U.S. Department of Energy Hydrogen and Fuel Cells Program:

2019 Annual Merit Review and Peer Evaluation Report

April 29–May 1, 2019
Arlington, Virginia

U.S. DEPARTMENT OF ENERGY

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U.S. Department of Energy Hydrogen and Fuel Cells Program

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and
Peer Evaluation Report

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NOTICE

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Prologue

Dear Colleague:

This document summarizes peer review comments and scores for the fiscal year (FY) 2019 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting (AMR), held April 29–May 1, 2019, in Arlington, Virginia. In response to direction from various stakeholders, including the National Academies, this review process provides project- and program-level evaluations of DOE-funded early-stage research, development, and analysis of hydrogen and fuel cell technologies.

This year's AMR included, for the second time, a dedicated two-day track on the DOE Office of Fossil Energy's Solid Oxide Fuel Cell Program, a one-day session on interagency- and state-level activities, and a fuel cell car ride-and-learn. The AMR kicked off with a research and development (R&D) discussion led by Dr. Alan Finkel, Australia's Chief Scientist, and Keith Schmid, the Chief Operating Officer of Plug Power. The plenary session also featured keynote remarks by Daniel Simmons, Assistant Secretary from the Office of Energy Efficiency and Renewable Energy (EERE); Michael Berube, Acting Deputy Assistant Secretary for Transportation, EERE; and program and subprogram overview presentations. The AMR was attended by close to 1,000 people, including close to 200 reviewers who reviewed 129 projects and more than 50 reviewers who were asked to provide feedback on the overall R&D program and subprograms.

DOE values the transparent public process of soliciting technical input on its projects and programs from relevant experts with depth and breadth of knowledge across a wide range of areas. The reviewers' recommendations are taken into consideration by DOE technology managers in generating future work plans. The summary table that follows lists the projects presented at the review and the overall evaluation score for each project, and Appendix A provides the scores and comments from the program reviewers. The individual reports present the reviewer comments to be considered during the upcoming fiscal year (October 1, 2019–September 30, 2020). The projects have been grouped according to subprogram and reviewed according to the appropriate evaluation criteria. To furnish principal investigators (PIs) with direct feedback, all of the evaluations and comments are provided to each presenter; however, the authors of the individual comments remain anonymous. DOE instructs the PIs to consider these summary evaluation comments fully, along with any other comments by DOE managers, in the PIs' FY 2020 plans. In addition, DOE managers contact each PI individually to discuss the comments and recommendations as future plans are developed.

Thank you to all 2019 AMR participants. I would like to express my sincere appreciation to the reviewers for your strong commitment, expertise, and dedication to advancing hydrogen and fuel cell technologies. You make this report possible, and we rely on your comments, along with other management processes, to help make project decisions for the new fiscal year. We look forward to your participation in the 2020 AMR, which is scheduled for May 19–21, 2020, in Arlington, Virginia.

Sincerely,

Sunita Satyapal
Director, Hydrogen and Fuel Cells Program
U.S. Department of Energy

Hydrogen Fuel R&D

Hydrogen Production R&D

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
P-102	Analysis of Advanced Hydrogen Production Pathways *Brian James, Strategic Analysis, Inc.*	3.4	X		
P-143	High-Temperature Alkaline Water Electrolysis *Hui Xu, Giner, Inc.*	3.2			X
P-177	Proton-Conducting Ceramic Electrolyzers for High-Temperature Water Splitting *Hossein Ghezel-Ayagh, Fuel Cell Energy*	3.5	X		
P-178	Industrially Scalable Waste Carbon Dioxide Reduction to Useful Chemicals and Fuels *Todd Deutsch, National Renewable Energy Laboratory*	3.3	X		

Hydrogen Production R&D: HydroGEN Seedling

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
P-148	HydroGEN Overview: A Consortium on Advanced Water-Splitting Materials *Huyen Dinh, National Renewable Energy Laboratory*	3.5	X		
P-152	Proton-Conducting Solid Oxide Electrolysis Cells for Large-Scale Hydrogen Production at Intermediate Temperatures *Prabhakar Singh, University of Connecticut*	3.3	X		
P-153	Degradation Characterization and Modeling of a New Solid Oxide Electrolysis Cell Utilizing Accelerated Life Testing *Scott Barnett, Northwestern University*	3.5	X		
P-154	Thin-Film, Metal-Supported High-Performance and Durable Proton–Solid Oxide Electrolyzer Cell *Tianli Zhu, United Technologies Research Center*	3.4	X		
P-155	High-Efficiency Polymer Electrolyte Membrane Water Electrolysis Enabled by Advanced Catalysts, Membranes, and Processes *Kathy Ayers, Proton OnSite*	3.5	X		

[*] HydroGEN seedling projects marked "Continue" are on track, but project continuation is contingent on passing a go/no-go decision.

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
P-156	Developing Novel Platinum-Group-Metal-Free Catalysts for Alkaline Hydrogen and Oxygen Evolution Reactions *Sanjeev Mukerjee, Northeastern University*	3.4	X		
P-157	Platinum-Group-Metal-Free Oxygen Evolution Reaction Catalysts for Polymer Electrolyte Membrane Electrolyzer *Di-Jia Liu, Argonne National Laboratory*	3.3	X		
P-158	High-Performance Ultralow-Cost Non-Precious-Metal Catalyst System for Anion Exchange Membrane Electrolyzer *Hoon Chung, Los Alamos National Laboratory*	3.3	X		
P-159	Scalable Elastomeric Membranes for Alkaline Water Electrolysis *Yu Seung Kim, Los Alamos National Laboratory*	3.3	X		
P-160	Best-in-Class Platinum-Group-Metal-Free Catalyst Integrated Tandem Junction Photoelectrochemical Water-Splitting Devices *Charles Dismukes, Rutgers University*	3.3	X		
P-161	Protective Catalyst Systems on III-V and Silicon-Based Semiconductors for Efficient, Durable Photoelectrochemical Water-Splitting Devices *Thomas Jaramillo, Stanford University*	3.5	X		
P-162	Novel Chalcopyrites for Advanced Photoelectrochemical Water Splitting *Nicolas Gaillard, University of Hawaii*	3.3	X		
P-163	Monolithically Integrated Thin-Film/Silicon Tandem Photoelectrodes for High-Efficiency and Stable Photoelectrochemical Water Splitting *Zetian Mi, University of Michigan*	3.4	X		
P-165	Accelerated Discovery of Solar Thermochemical Hydrogen Production Materials via High-Throughput Computational and Experimental Methods *Ryan O'Hayre, Colorado School of Mines*	3.5	X		
P-166	Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production *Charles Musgrave, University of Colorado Boulder*	3.5	X		
P-167	Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels *Chris Wolverton, Northwestern University*	3.1	X		

* HydroGEN seedling projects marked "Continue" are on track, but project continuation is contingent on passing a go/no-go decision.

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
P-168	Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for Solar Thermochemical Hydrogen *Ellen Stechel, Arizona State University*	3.4	X		
P-169	High-Temperature Reactor Catalyst Material Development for Low-Cost and Efficient Solar-Driven Sulfur-Based Processes *Claudio Corgnale, Greenway Energy*	3.3		X	
P-170	Benchmarking Advanced Water-Splitting Technologies: Best Practices in Materials Characterization *Kathy Ayers, Proton OnSite*	3.5	X		
P-175	Intermediate-Temperature Proton-Conducting Solid Oxide Electrolysis Cells with Improved Performance and Delivery *Xingbo Liu, West Virginia University*	3.4	X		
P-176	Development of Durable Materials for Cost-Effective Advanced Water Splitting Utilizing All-Ceramic Solid Oxide Electrolyzer Stack Technology *John Pietras, Saint-Gobain*	3.3	X		

Hydrogen Storage R&D

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
ST-001	System-Level Analysis of Hydrogen Storage Options *Rajesh Ahluwalia, Argonne National Laboratory*	3.6	X		
ST-100	Hydrogen Storage Cost Analysis *Brian James, Strategic Analysis, Inc.*	3.4	X		
ST-127	Hydrogen Materials—Advanced Research Consortium (HyMARC): A Consortium for Advancing Hydrogen Storage Materials *Mark Allendorf, Sandia National Laboratories, and Thomas Gennett, National Renewable Energy Laboratory*	3.4	X		
ST-128	Hydrogen Materials—Advanced Research Consortium (HyMARC): Sandia National Laboratories Technical Activities *Mark Allendorf, Sandia National Laboratories*	3.4	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
ST-129	Hydrogen Materials—Advanced Research Consortium (HyMARC): Lawrence Livermore National Laboratory Technical Activities *Brandon Wood, Lawrence Livermore National Laboratory*	3.6	X		
ST-130	Hydrogen Materials—Advanced Research Consortium (HyMARC): Lawrence Berkeley National Laboratory Technical Activities *David Prendergast and Jeffrey Long, Lawrence Berkeley National Laboratory*	3.4	X		
ST-131	Hydrogen Materials—Advanced Research Consortium (HyMARC): National Renewable Energy Laboratory Technical Activities *Thomas Gennett, National Renewable Energy Laboratory*	3.4	X		
ST-132	Hydrogen Materials—Advanced Research Consortium (HyMARC): Pacific Northwest National Laboratory Technical Activities *Tom Autrey, Pacific Northwest National Laboratory*	3.5	X		
ST-137	Hydrogen Materials–Advanced Research Consortium (HyMARC) Seedling: Electrolyte-Assisted Hydrogen Storage Reactions *Simon Jones, Liox Power*	3.2	X		
ST-143	Hydrogen Materials–Advanced Research Consortium (HyMARC) Seedling: Atomic Layer Deposition Synthesis of Novel Nanostructured Metal Borohydrides *Steven Christensen, National Renewable Energy Laboratory*	3.3	X		
ST-144	Hydrogen Materials—Advanced Research Consortium (HyMARC) Seedling: Optimized Hydrogen Adsorbents via Machine Learning and Crystal Engineering *Don Siegel, University of Michigan*	3.3	X		
ST-146	Precursor Processing Development for Low-Cost, High-Strength Carbon Fiber for Composite Overwrapped Pressure Vessel Applications *Matthew Weisenberger, University of Kentucky*	3.1	X		
ST-147	Developing a New Polyolefin Precursor for Low-Cost, High-Strength Carbon Fiber *Mike Chung, Pennsylvania State University*	3.1	X		
ST-148	Novel Plasticized Melt-Spinning Process of Polyacrylonitrile Fibers Based on Task-Specific Ionic Liquids *Sheng Dai, Oak Ridge National Laboratory*	3.1	X		

Fuel Cell R&D

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
FC-017	Fuel Cell System Modeling and Analysis *Rajesh Ahluwalia, Argonne National Laboratory*	3.3	X		
FC-135	FC-PAD: Fuel Cell Consortium for Performance and Durability *Rod Borup, Los Alamos National Laboratory*	3.5	X		
FC-140	Tailored High-Performance Low-Platinum-Group-Metal Alloy Cathode Catalysts *Vojislav Stamenkovic, Argonne National Laboratory*	3.4			X
FC-141	Platinum Monolayer Electrocatalysts *Jia Wang, Brookhaven National Laboratory*	2.6			X
FC-144	Highly Accessible Catalysts for Durable High-Power Performance *Anusorn Kongkanand, General Motors*	3.5	X		
FC-145	Corrosion-Resistant Non-Carbon Electrocatalyst Supports for Proton Exchange Fuel Cells *Vijay Ramani, Washington University*	3.1	X		
FC-146	Advanced Materials for Fully Integrated Membrane Electrode Assemblies in Anion Exchange Membrane Fuel Cells *Yu Seung Kim, Los Alamos National Laboratory*	3.4			X
FC-147	Advanced Ionomers and Membrane Electrode Assemblies for Alkaline Membrane Fuel Cells *Bryan Pivovar, National Renewable Energy Laboratory*	3.5			X
FC-155	Novel Ionomers and Electrode Structures for Improved Polymer Electrolyte Membrane Fuel Cell Electrode Performance at Low-Platinum-Group-Metal Loadings *Andrew Haug, 3M*	3.3	X		
FC-156	Durable High-Power Membrane Electrode Assemblies with Low Platinum Loading *Swami Kumaraguru, General Motors*	3.2	X		
FC-157	High-Performance Polymer Electrolyte Fuel Cell Electrode Structures *Mike Perry, United Technologies Research Center*	2.7		X	
FC-158	Fuel Cell Membrane Electrode Assemblies with Ultralow-Platinum Nanofiber Electrodes *Peter Pintauro, Vanderbilt University*	3.4	X		
FC-160	ElectroCat (Electrocatalysis Consortium) *Deborah Myers, Argonne National Laboratory, and Piotr Zelenay, Los Alamos National Laboratory*	3.3	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
FC-161	Advanced Electrocatalysts through Crystallographic Enhancement *Jacob Spendelow, Los Alamos National Laboratory*	3.4	X		
FC-162	Vapor Deposition Process for Engineering of Dispersed Polymer Electrolyte Membrane Fuel Cell Oxygen Reduction Reaction Pt/NbO_x/C Catalysts *Jim Waldecker, Ford Motor Company*	3.2	X		
FC-163	Fuel Cell Systems Analysis *Brian James, Strategic Analysis, Inc.*	3.4	X		
FC-170	ElectroCat: Durable Manganese-Based Platinum-Group-Metal-Free Catalysts for Polymer Electrolyte Membrane Fuel Cells *Hui Xu, Giner, Inc.*	3.0	X		
FC-171	ElectroCat: Advanced Platinum-Group-Metal-Free Cathode Engineering for High Power Density and Durability *Shawn Litster, Carnegie Mellon University*	3.4	X		
FC-172	ElectroCat: Highly Active and Durable Platinum-Group-Metal-Free Oxygen Reduction Reaction Electrocatalysts through the Synergy of Active Sites *Yuyan Shao, Pacific Northwest National Laboratory*	3.3	X		
FC-173	ElectroCat: Platinum-Group-Metal-Free Engineered Framework Nanostructure Catalysts *Prabhu Ganesan, Greenway Energy, LLC*	2.9		X	
FC-174	Highly Efficient and Durable Cathode Catalyst with Ultralow Platinum Loading through Synergetic Platinum-/Platinum-Group-Metal-Free Catalytic Interaction *Di-Jia Liu, Argonne National Laboratory*	3.4	X		
FC-178	Lab Call Fiscal Year 2018 (Membrane): Spirocyclic Anion Exchange Membranes for Improved Performance and Durability *Bryan Pivovar, National Renewable Energy Laboratory*	3.2	X		
FC-179	Lab Call Fiscal Year 2018 (Membrane): Stable Alkaline Membrane Based on Proazaphosphatranes Organic Superbase *Gao Liu, Lawrence Berkeley National Laboratory*	2.7			X
FC-180	Lab Call Fiscal Year 2018 (Membrane): High-Performing and Durable Pyrophosphate-Based Composite Membranes for Intermediate-Temperature Fuel Cells *Cortney Kreller, Los Alamos National Laboratory*	2.7		X	

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
FC-181	Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Microstructured Electrodes and Diffusion Layers for Enhanced Transport in Reversible Fuel Cells *Jacob Spendelow, Los Alamos National Laboratory*	3.4	X		
FC-182	Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Bipolar Membrane Development to Enable Regenerative Fuel Cells *Todd Deutsch, National Renewable Energy Laboratory*	2.9		X	
FC-183	Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Technology-Enabling Materials, Cell Design for Reversible Polymer Electrolyte Membrane Fuel Cells *Nem Danilovic, Lawrence Berkeley National Laboratory*	3.0	X		
FC-302	Developing Platinum-Group-Metal-Free Catalysts for Oxygen Reduction Reaction in Acid: Beyond the Single Metal Site *Qingying Jia, Northeastern University*	3.1	X		
FC-303	Mesoporous Carbon-Based Platinum-Group-Metal-Free Catalyst Cathodes *Jian Xie, Indiana University–Purdue University Indianapolis*	3.0	X		
FC-304	Fuel Cell Membrane Electrode Assemblies with Platinum-Group-Metal-Free Nanofiber Cathodes *Peter Pintauro, Vanderbilt University*	3.3	X		
FC-305	Active and Durable Platinum-Group-Metal-Free Cathodic Electrocatalysts for Fuel Cell Application *Alexey Serov, Pajarito Powder*	2.9		X	
FC-306	High-Performance Non-Platinum-Group-Metal Transition Metal Oxide Oxygen Reduction Reaction Catalysts of Polymer Electrolyte Membrane Fuel Cells *Timothy Davenport, United Technologies Research Center*	2.5		X	
FC-307	Cyclic Olefin Copolymer-Based Alkaline Exchange Polymers and Reinforced Membranes *Chulsung Bae, Rensselaer Polytechnic Institute*	3.3	X		
FC-308	Advanced Anion Exchange Membranes with Tunable Water Transport for Platinum-Group-Metal-Free Anion Exchange Membrane Fuel Cells *Michael Hickner, Pennsylvania State University*	3.4	X		
FC-309	Polymerized Ionic Liquid Block Copolymers and Ionic Liquids (PILBCP-IL) Composite Ionomers for High Current Density Performance *Joshua Snyder, Drexel University*	3.1	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
FC-310	Composite Polymer Electrolyte Membranes from Electrospun Crosslinkable Poly(Phenylene Sulfonic Acid)s *Ryszard Wycisk, Vanderbilt University*	3.5	X		
FC-311	Novel Non-Perfluorosulfonic Acid Proton Exchange Membrane for Fuel Cell Application *Taoli Gu, Xergy, Inc.*	3.2	X		
FC-312	Molten Hydroxide Dual-Phase Membranes for Intermediate-Temperature Anion Exchange Membrane Fuel Cells *Patrick Campbell, Lawrence Livermore National Laboratory*	3.2	X		
FC-313	Novel Bifunctional Electrocatalysts, Supports, and Membranes for High-Performing and Durable Unitized Regenerative Fuel Cells *Nem Danilovic, Lawrence Berkeley National Laboratory*	3.1	X		
FC-314	Efficient Reversible Operation and Stability of Novel Solid Oxide Cells *Scott Barnett, Northwestern University*	3.2	X		
FC-315	High-Efficiency Reversible Alkaline Membrane Fuel Cells *Hui Xu, Giner, Inc.*	3.3	X		
FC-316	Durable, High-Performance Unitized Reversible Fuel Cells Based on Proton Conductors *Meilin Liu, Georgia Institute of Technology*	3.0	X		
FC-317	Stationary Direct Methanol Fuel Cells Using Pure Methanol *Xianglin Li, University of Kansas Center for Research, Inc.*	3.0	X		
FC-318	Lab Call Fiscal Year 2019: Accessible Platinum-Group-Metal-Free Catalysts and Electrodes: ElectroCat *Jacob Spendelow, Los Alamos National Laboratory*	3.4	X		
FC-319	Lab Call Fiscal Year 2019: Low-Cost Gas Diffusion Layer Materials and Treatments for Durable High-Performance Polymer Electrolyte Membrane Fuel Cells *Rod Borup, Los Alamos National Laboratory*	3.2	X		
FC-320	Lab Call Fiscal Year 2019: Electrode Ionomers for High-Temperature Fuel Cells *Michael Hibbs, Sandia National Laboratories*	3.1	X		
FC-321	Lab Call Fiscal Year 2019: Solid Phase Processing for Reduced Cost and Improved Efficiency of Bipolar Plates *Ken Ross, Pacific Northwest National Laboratory*	3.0	X		
FC-322	Lab Call Fiscal Year 2019: Polymer Electrolyte Fuel Cell Electrode Structures with Encased Catalysts to Eliminate Ionomer Adsorption on Catalytic Sites *Deborah Myers, Argonne National Laboratory*	3.2	X		

Infrastructure and Systems R&D

Hydrogen Infrastructure R&D

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
IN-001	Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Steels *Chris San Marchi, Sandia National Laboratories*	3.7	X		
IN-004	Magnetocaloric Hydrogen Liquefaction *Jamie Holladay, Pacific Northwest National Laboratory*	3.1	X		
IN-005	Electrochemical Compression *Monjid Hamdan, Giner ELX, Inc.*	3.5	X		
IN-007	Metal Hydride Compression *Terry Johnson, Sandia National Laboratories*	3.4			X
IN-008	Dispenser Reliability *Michael Peters, National Renewable Energy Laboratory*	3.0	X		
IN-009	Advancing Hydrogen Dispenser Technology by Using Innovative Intelligent Networks *Darryl Pollica, Ivys Inc.*	3.4			X
IN-010	Hydrogen Dispensing Hose *Jennifer Lalli, NanoSonic*	3.3	X		
IN-011	Coatings for Compressor Seals *Shannan O'Shaughnessy, GVD Corporation*	2.8			X
IN-012	Low-Cost Magnetocaloric Materials Discovery *Robin Ihnfeldt, General Engineering & Research*	3.2	X		

Technology Acceleration

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
TA-001	Membrane Electrode Assembly Manufacturing Research and Development *Michael Ulsh, National Renewable Energy Laboratory*	3.4	X		
TA-005	In-Line Quality Control of Polymer Electrolyte Membrane Materials *Paul Yelvington, Mainstream*	3.3	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
TA-007	Roll-to-Roll Advanced Materials Manufacturing Lab Consortium *Claus Daniel, Oak Ridge National Laboratory*	3.1	X		
TA-008	Material–Process–Performance Relationships in Polymer Electrolyte Membrane Catalyst Inks and Coated Layers *Michael Ulsh, National Renewable Energy Laboratory*	3.2	X		
TA-009	Maritime Fuel Cell Generator Project *Lennie Klebanoff, Sandia National Laboratories*	3.4	X		
TA-011	FedEx Express Hydrogen Fuel Cell Extended-Range Battery Electric Vehicles *Phillip Galbach, FedEx Express*	3.4	X		
TA-012	Northeast Demonstration and Deployment of FCRx200 *Abas Goodarzi, US Hybrid*	3.2		X	
TA-013	Fuel Cell Bus Evaluations *Leslie Eudy, National Renewable Energy Laboratory*	3.7	X		
TA-014	Hydrogen Station Data Collection and Analysis *Sam Sprik, National Renewable Energy Laboratory*	3.4	X		
TA-015	Dynamic Modeling and Validation of Electrolyzers in Real-Time Grid Simulation *Rob Hovsapian, Idaho National Laboratory*	3.5	X		
TA-016	Fuel Cell Hybrid Electric Delivery Van *Jason Hanlin, Center for Transportation and the Environment*	3.1	X		
TA-017	Innovative Advanced Hydrogen Mobile Fueler *Sara Odom, Electricore*	3.4	X		
TA-018	High-Temperature Electrolysis Test Stand *James O'Brien, Idaho National Laboratory*	3.2	X		
TA-019	Modular Solid Oxide Electrolyzer Cell System for Efficient Hydrogen Production at High Current Density *Hossein Ghezel-Ayagh, FuelCell Energy*	3.4	X		
TA-020	Optimal Stationary Fuel Cell Integration and Control (Energy Dispatch Controller) *Genevieve Saur, National Renewable Energy Laboratory*	3.2	X		
TA-021	Integrated Systems Modeling of the Interactions between Stationary Hydrogen, Vehicle, and Grid Resources *Samveg Saxena, Lawrence Berkeley National Laboratory*	3.4	X		
TA-022	H2@Scale: Experimental Characterization of Durability of Advanced Electrolyzer Concepts in Dynamic Loading *Shaun Alia, National Renewable Energy Laboratory*	2.9	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
TA-023	Hydrogen Stations for Urban Sites *Brian Ehrhart, National Renewable Energy Laboratory/ Sandia National Laboratories*	3.5			X
TA-024	Analysis of Fuel Cells for Trucks *Ram Vijayagopal, Argonne National Laboratory*	3.0	X		

Systems Analysis

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
SA-044	Cost–Benefit Analysis of Technology Improvement in Medium- and Heavy-Duty Fuel Cell Vehicles *Aymeric Rousseau, Argonne National Laboratory*	3.0	X		
SA-169	Market Segmentation Analysis of Medium- and Heavy-Duty Trucks with a Fuel Cell Emphasis *Chad Hunter, National Renewable Energy Laboratory*	3.6	X		
SA-170	Analysis of Cost Impacts of Integrating Advanced Onboard Storage Systems with Hydrogen Delivery *Amgad Elgowainy, Argonne National Laboratory*	3.2	X		
SA-171	H2@Scale Analysis *Mark Ruth, National Renewable Energy Laboratory*	3.6	X		
SA-172	Hydrogen Demand Analysis for H2@Scale *Amgad Elgowainy, Argonne National Laboratory*	3.5	X		

Safety, Codes and Standards

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
SCS-001	National Codes and Standards Deployment and Outreach *Carl Rivkin, National Renewable Energy Laboratory*	3.3	X		

Project Number	Project Title *Principal Investigator Name & Organization*	Final Score	Continue	Discontinue/ Further Review	Completed
SCS-005	Research and Development for Safety, Codes and Standards: Materials and Component Compatibility *Chris San Marchi, Sandia National Laboratories*	3.5	X		
SCS-007	Fuel Quality Assurance Research and Development and Impurity Testing in Support of Codes and Standards *Tommy Rockward, Los Alamos National Laboratory*	3.5	X		
SCS-010	Research and Development for Safety, Codes and Standards: Hydrogen Behavior *Ethan Hecht, Sandia National Laboratories*	3.5	X		
SCS-011	Hydrogen Quantitative Risk Assessment *Alice Muna, Sandia National Laboratories*	3.5	X		
SCS-019	Hydrogen Safety Panel, Safety Knowledge Tools, and First Responder Training Resources *Nick Barilo, Pacific Northwest National Laboratory*	3.7	X		
SCS-021	National Renewable Energy Laboratory Hydrogen Sensor Testing Laboratory *William Buttner, National Renewable Energy Laboratory*	3.5	X		
SCS-022	Fuel Cell and Hydrogen Energy Association Codes and Standards Support *Karen Quackenbush, Fuel Cell & Hydrogen Energy Association*	2.9	X		
SCS-026	Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Polymers *Kevin Simmons, Pacific Northwest National Laboratory*	3.5	X		

Table of Contents

Introduction

The fiscal year (FY) 2019 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (the Program) Annual Merit Review and Peer Evaluation Meeting (AMR) was held April 29–May 1, 2019, in Arlington, Virginia. This report is a summary of comments by AMR peer reviewers about the hydrogen and fuel cell projects funded by DOE's Office of Energy Efficiency and Renewable Energy (EERE). Projects supported by other state agencies and DOE offices (including the Office of Fossil Energy Solid Oxide Fuel Cell Program [FE-SOFC)], Office of Science [Basic Energy Sciences], Office of Nuclear Energy [NE], Advanced Research Projects Agency–Energy [ARPA-E], and EERE Bioenergy Technologies Office) in areas relevant to hydrogen and fuel cells were also presented at the FY 2019 AMR. DOE uses the results of this merit review and peer evaluation, along with additional review processes, to make funding decisions for upcoming fiscal years and help guide ongoing performance improvements to existing projects.

The objectives of this meeting included the following:

- Review and evaluate FY 2019 accomplishments and FY 2020 plans for DOE laboratory programs; industry/university cooperative agreements; and related research, development, and demonstration (RD&D) efforts.
- Provide an opportunity for stakeholders and participants (fuel cell and hydrogen system manufacturers, component developers, and others) to provide input to help shape the DOE-sponsored RD&D program in order to address the highest-priority technical barriers and facilitate technology transfer.
- Foster interactions among the national laboratories, industry, and universities conducting RD&D.

The peer review process followed the guidelines in the *Peer Review Guide* developed by EERE. The peer review panel members, listed in Table 1, provided comments about the projects presented. Panel members included experts from a variety of backgrounds related to hydrogen and fuel cells, and they represented national laboratories; universities; various government and non-government organizations; and developers and manufacturers of hydrogen production, storage, delivery, and fuel cell technologies. Each reviewer was screened for conflicts of interest as prescribed by the *Peer Review Guide*. A subset of these reviewers was also asked to provide overall Program and subprogram review feedback. The results of this Program Review feedback are included in Appendix A. A complete list of the meeting participants is presented in Appendix B.

Table 1: Peer Review Panel Members

No.	Name	Organization
1	Kareem Afzal	PDC Machines, Inc.
2	Rajesh Ahluwalia	Argonne National Laboratory
3	Paul Albertus	University of Maryland
4	Ilse Alcantara	NASA
5	Shaun Alia	National Renewable Energy Laboratory
6	Laurent Antoni	CEA (French Atomic Energy and Alternative Energies Commission)
7	Mirela Atanasiu	Fuel Cells and Hydrogen Joint Undertaking (FCH JU)
8	Katherine Ayers	Proton OnSite
9	Chulsung Bae	Rensselaer Polytechnic Institute
10	Bamdad Bahar	Xergy Inc
11	Nick Barilo	Pacific Northwest National Laboratory
12	Jean Baronas	California Energy Commission
13	Olga Baturina	U.S. Navy, Naval Research Laboratory
14	Matthew Beckner	General Motors
15	Guido Bender	National Renewable Energy Laboratory
16	William Bergeson	Federal Highway Administration
17	Naveen Berry	South Coast Air Quality Management District
18	Bart Biebuyck	Fuel Cells and Hydrogen Joint Undertaking (FCH JU)
19	Bryan Blackburn	Redox Power Systems
20	Rodney Borup	Los Alamos National Laboratory

No.	Name	Organization
21	Nico Bouwkamp	California Fuel Cell Partnership
22	Antonio Bouza	U.S. Department of Energy
23	Ken Boyce	UL
24	Kyle Brinkman	Clemson University
25	Albert Burgunder	Praxair, Inc.
26	Susan Burke	U.S. Environmental Protection Agency
27	Jimmy Burns	University of Virginia
28	Scott Calabrese Barton	Michigan State University
29	Pietro Caloprisco	Fuel Cells and Hydrogen Joint Undertaking (FCH JU)
30	Patrick Campbell	Lawrence Livermore National Laboratory
31	Marcelo Carmo	Forschungszentrum Jülich
32	Kevin Centeck	U.S. Army, Tank Automotive Research, Development and Engineering Center (TARDEC)
33	Franklin Chang Díaz	Ad Astra Rocket Company, Costa Rica
34	Bryan Chapman	Exxon Mobil Corporation
35	Santanu Chaudhuri	Argonne National Laboratory
36	Praveen Cheekatamarla	Atrex Energy, Inc.
37	Dejun Chen	Georgetown University
38	Biswajit Choudhury	DuPont
39	Yachun Chow	California Air Resources Board
40	William Collins	Consultant
41	Hector Colon-Mercado	Savannah River National Laboratory
42	Amedeo Conti	Nuvera Fuel Cells, Inc.
43	Chris Cornelius	University of Nebraska
44	Stephen Creager	Clemson University
45	David Cullen	Oak Ridge National Laboratory
46	Ismaila Dabo	Pennsylvania State University
47	Nilesh Dale	Nissan Technical Center North America, Inc.
48	Nemanja Danilovic	Lawrence Berkeley National Laboratory
49	Timothy Davenport	United Technologies Research Center
50	Emory De Castro	Advent Technologies, Inc.
51	Daniel DeSantis	Strategic Analysis, Inc.
52	Todd Deutsch	National Renewable Energy Laboratory
53	Eric Dirschka	NASA
54	Tabbetha Dobbins	Rowan University
55	Francesco Dolci	European Commission Joint Research Centre, Energy, Transport and Climate
56	Andreas Dorda	Austrian Federal Ministry for Transport, Innovation and Technology
57	Martin Dornheim	Helmholtz-Zentrum Geesthacht
58	Mihai Dorobantu	Eaton Vehicle Group
59	David Edwards	Air Liquide
60	Glenn Eisman	Rensselaer Polytechnic Institute
61	Lior Elbaz	Israel Fuel Cells Consortium, Institute of Nanotechnology and Advanced Materials, Israel National Research Center for Electrochemical Propulsion, and Bar-Ilan University
62	William Elrick	California Fuel Cell Partnership
63	Elif Ertekin	University of Illinois
64	Sylvie Escribano	CEA (French Atomic Energy and Alternative Energies Commission)
65	Leslie Eudy	National Renewable Energy Laboratory
66	Matt Fairlie	Next Hydrogen
67	David Farese	Air Products and Chemicals, Inc.

No.	Name	Organization
68	Gary Flood	GSF Consulting
69	Nicole Forester	Commonwealth Scientific and Industrial Research Organisation, Australia (CSIRO)
70	Katrina Fritz	KM Fritz, LLC
71	Bernard Frois	CEA (French Atomic Energy and Alternative Energies Commission)
72	Livio Gambone	Nikola Motor Company
73	Prabhu Ganesan	Savannah River Consulting, LLC
74	Jürgen Garche	Ulm University
75	Mario Garcia-Sanz	ARPA-E
76	Monterey Gardiner	BMW Group
77	Thomas Gennett	National Renewable Energy Laboratory
78	Dominic Francis Gervasio	University of Arizona
79	Hossein Ghezel-Ayagh	FuelCell Energy
80	William Gibbons	University of Maryland
81	François Girard	National Research Council Canada, Energy, Mining and Environment
82	Leslie Goodbody	California Air Resources Board
83	Colin Gore	Redox Power Systems, LLC
84	Leo Grassilli	Consultant
85	Matt Gregori	Sempra Utilities
86	Ulf Groos	Fraunhofer Institute for Solar Energy Systems ISE, Fuel Cell Systems, Hydrogen Technologies
87	Tom Gross	Energy Planning and Solutions
88	Stephen Grot	Ion Power
89	Katrina Groth	University of Maryland
90	Ram Gupta	Virginia Commonwealth University
91	Jennifer Hamilton	California Fuel Cell Partnership
92	Dan Hancu	U.S. Department of Energy
93	Aaron Harris	Air Liquide
94	Alex Harris	Brookhaven National Laboratory
95	Kevin Harrison	National Renewable Energy Laboratory
96	William Harrison	Nanosonic, Inc.
97	Jason Hattrick-Simpers	National Institute of Standards and Technology
98	Andrew Haug	3M Company
99	Ethan Hecht	Sandia National Laboratory
100	Thorsten Herbert	NOW GmbH (National Organisation Hydrogen and Fuel Cell Technology)
101	Michael Hibbs	Sandia National Laboratories
102	Darren Hickey	Cummins
103	Michael Hickner	Pennsylvania State University
104	James Hinkley	Commonwealth Scientific and Industrial Research Organisation, Australia (CSIRO)
105	Jamie Holladay	Pacific Northwest National Laboratory
106	Chang Huajian	State Power Investment Corporation Research Institute
107	Kevin Huang	University of South Carolina
108	Yu Huang	University of California, Los Angeles
109	Chad Hunter	National Renewable Energy Laboratory
110	Nick Irvin	Southern Company
111	Levi Irwin	U.S. Department of Energy
112	Ian Jakupca	NASA
113	Brian James	Strategic Analysis, Inc.

No.	Name	Organization
114	Will James	Savannah River National Laboratory
115	Hongfei Jia	Toyota North America
116	Qingying Jia	Northeastern University
117	Scott Jorgensen	SBC Global
118	James Kast	Toyota Motor Corporation
119	Douglass Kauffman	National Energy Technology Laboratory
120	Jay Keller	Consultant
121	Ron Kent	Southern California Gas Company
122	John Khalil	United Technologies Research Center
123	Yu Seung Kim	Los Alamos National Laboratory
124	Sarah Kleinbaum	U.S. Department of Energy
125	Shanna Knights	Ballard Power Systems
126	Tomonari Komiyama	JX Nippon Oil
127	Anusorn Kongkanand	General Motors
128	John Kopasz	Argonne National Laboratory
129	Theodore Krause	Argonne National Laboratory
130	Ahmet Kusoglu	Lawrence Berkeley National Laboratory
131	Xianglin Li	Kansas University
132	Ludwig Lipp	T2M Global
133	Shawn Litster	Carnegie Mellon University
134	Di-Jia Liu	Argonne National Laboratory
135	Gao Liu	Lawrence Berkeley National Laboratory
136	Meilin Liu	Georgia Institute of Technology
137	Miguel Maes	NASA
138	Jim Manusco	Westport Power, Inc.
139	Radenka Maric	University of Connecticut
140	Olga Marina	Pacific Northwest National Laboratory
141	Andrew Martinez	California Air Resources Board
142	Sara Marxen	CSA Group
143	David Masten	General Motors
144	Luca Mastropasqua	University of California, Irvine
145	Paul Matter	PH Matter
146	Scott Mauger	National Renewable Energy Laboratory
147	Anthony McDaniel	Sandia National Laboratories
148	Stephen McDougle	NASA
149	Noah Meeks	Southern Company
150	Nalini Menon	Sandia National Laboratories
151	Nguyen Minh	University of California, San Diego
152	Cortney Mittelsteadt	Giner, Inc.
153	Miguel Modestino	New York University
154	Mohsen Mosleh	Howard University
155	Christopher Muhich	Arizona State University
156	Rangachary Mukundan	Los Alamos National Laboratory
157	Christopher Munnings	Electrochemical Energy Systems
158	Vivek Murthi	Nikola Motor Company
159	William Mustain	University of South Carolina
160	Kenneth Neyerlin	National Renewable Energy Laboratory
161	Tien Nguyen	Independent
162	Madeleine Odgaard	IRD Fuel Cells
163	Bob Oesterreich	Air Liquide
164	Tadashi Ogitsu	Lawrence Livermore National Laboratory

No.	Name	Organization
165	Gregory Olson	Consultant
166	Kevin Ott	Los Alamos National Laboratory, retired
167	Benjamin Paczkowski	U.S. Army, Tank Automotive Research, Development and Engineering Center (TARDEC)
168	Andrew Park	Chemours
169	George Parks	FuelScience, LLC
170	Pinakin Patel	Fuel Cell Energy, Inc.
171	Tapan Patel	U.S. Army
172	Mike Perry	United Technologies Research Center
173	Michael Peters	National Renewable Energy Laboratory
174	Guillaume Petitpas	Lawrence Livermore National Laboratory
175	Aaron Petri	U.S. Army
176	John Pietras	Saint-Gobain
177	Peter Pintauro	Vanderbilt University
178	Bryan Pivovar	National Renewable Energy Laboratory
179	Olga Polevaya	Nuvera Fuel Cells, Inc.
180	Karen Quackenbush	Fuel Cell & Hydrogen Energy Association
181	Glenn Rambach	SiGNa Chemistry Inc.
182	Jeffrey Reed	University of California, Irvine
183	Brian Rice	University of Dayton Research Institute
184	Denzel Robertson	Air Liquide
185	Aashish Rohatgi	Pacific Northwest National Laboratory
186	Subir Roychoudhury	Precision Combustion, Inc.
187	Tecle Rufael	Chevron Energy Technology Company
188	Antonio Ruiz	Nikola Motor Company
189	Christian Sattler	German Aerospace Center (DLR)
190	Birgit Schwenzer	National Science Foundation
191	Alexey Serov	Pajarito Powder, LLC
192	Godwin Severa	University of Hawaii
193	Stephen Sikirica	U.S. Department of Energy
194	Kevin Simmons	Pacific Northwest National Laboratory
195	Prabhakar Singh	University of Connecticut
196	Joshua Snyder	Drexel University
197	Grigorii Soloveichik	U.S. Department of Energy
198	Xueyan Song	West Virginia University
199	Herie Soto	Shell Oil Company
200	Jacob Spendelow	Los Alamos National Laboratory
201	Vojislav Stamenkovic	Argonne National Laboratory
202	Andy Steinbach	3M Company
203	Nadia Steiner	Université de Franche-Comté
204	Gary Stottler	General Motors, retired
205	Ian Sutherland	General Motors
206	Scott Swartz	NexTech Materials LTD
207	Karen Swider-Lyons	U.S. Navy, Naval Research Laboratory
208	Andrei Tchouvelev	A.V. Tchouvelev & Associates Inc.
209	Pascal Tessier	Air Liquide
210	David Tew	ARPA-E
211	Michael Toney	SLAC National Accelerator Laboratory
212	Jianhua Tong	Clemson University
213	John Trocciola	CSRA
214	Hiroyuki Usuda	New Energy and Industrial Technology Development Organization

No.	Name	Organization
		(NEDO)
215	Mike Veenstra	Ford Motor Company
216	David Viano	Commonwealth Scientific and Industrial Research Organisation, Australia (CSIRO)
217	James Waldecker	Ford Motor Company
218	Jia Wang	Brookhaven National Laboratory
219	Adam Weber	Lawrence Berkeley National Laboratory
220	Marcel Weeda	TNO innovation for life
221	Douglas Wheeler	DJW Technology, LLC
222	Mark Williams	AECOM
223	Brandon Wood	Lawrence Livermore National Laboratory
224	Stephen Woods	NASA
225	Ryszard Wycisk	Vanderbilt University
226	Jian Xie	Indiana University–Purdue University Indianapolis
227	Hui Xu	Giner, Inc.
228	Michael Yandrasits	3M Company
229	Fuming Yang	State Power Investment Corporation Research Institute, China
230	Eleni Zafeiratou	Fuel Cells and Hydrogen Joint Undertaking (FCH JU)
231	Piotr Zelenay	Los Alamos National Laboratory
232	Xiao-Dong Zhou	University of Louisiana at Lafayette
233	Jonathan Zimmerman	Sandia National Laboratories
234	Barr Zulevi	Pajarito Powder, LLC

Summary of Peer Review Panel's Crosscutting Comments and Recommendations

AMR panel members provided comments and recommendations regarding selected DOE hydrogen and fuel cell projects, overall management of the Hydrogen and Fuel Cells Program, and the AMR peer evaluation process. The project comments, recommendations, and scores are provided in the following sections of this report, grouped by subprogram. Comments about Program and subprogram management are provided in Appendix A.

Analysis Methodology

A total of **129** Fuel Cell Technologies Office (FCTO) projects were reviewed at the meeting. As shown in the table above, **234** review panel members participated in the AMR process, providing a total of **677** project evaluations. These reviewers were asked to provide numeric scores (on a scale of 1–4, including half-point intervals, with 4 being the highest) for five aspects of the work presented. Sample evaluation forms are provided in Appendix C. Scores and comments were submitted using laptops (provided on site) to a private online database, allowing for real-time tracking of the review process. A list of projects that were presented at the AMR but not reviewed is provided in Appendix D.

For the Hydrogen Fuel R&D; Fuel Cell R&D; Infrastructure and Systems R&D; and Safety, Codes and Standards subprograms, scores were based on the five criteria and weights provided below. The Hydrogen Fuel R&D subprogram includes two project categories—Hydrogen Production R&D and Hydrogen Storage R&D—that were similarly evaluated. The Infrastructure and Systems R&D subprogram includes three project categories: Hydrogen Infrastructure R&D, Technology Acceleration, and Systems Analysis; these were similarly evaluated.

Score 1: Approach to performing the work (20%)
Score 2: Accomplishments and progress toward overall project and DOE goals (45%)
Score 3: Collaboration and coordination with other institutions (10%)
Score 4: Relevance/potential impact on DOE Program goals and RD&D objectives (15%)
Score 5: Proposed future work (10%)

For each project, individual reviewer scores for each of the five criteria were weighted using the formula in the box below to create a final score for each reviewer for that project. The average score for each project was then calculated by averaging the final scores for individual reviewers. The individual reviewer scores for each question were also averaged to provide information on the project's question-by-question scoring. In this manner, a project's final overall score can be meaningfully compared to that of another project.

Final Overall Score = [Score 1 x 0.20] + [Score 2 x 0.45] + [Score 3 x 0.10] + [Score 4 x 0.15] + [Score 5 x 0.10]

A perfect overall score of "4" indicates that a project satisfied the five criteria to the fullest possible extent; the lowest possible overall score of "1" indicates that a project did not satisfactorily meet any of the requirements of the five criteria.

The Hydrogen Fuel R&D category also includes a subcategory for Hydrogen Production R&D: HydroGEN Seedling projects. The evaluation form for these projects (included in Appendix C) was modified to address their unique features; the scores for these projects were based on the following five criteria and weights:

Score 1: Approach to performing the work (20%)
Score 2: Relevance/potential impact on DOE Program goals and RD&D objectives and the HydroGEN Consortium mission (15%)
Score 3: Accomplishments and progress toward overall project and DOE goals and the HydroGEN Consortium mission (30%)
Score 4: Collaboration effectiveness with HydroGEN and, as appropriate, other institutions (25%)
Score 5: Proposed future work (10%)

The 2019 AMR also included some recently awarded projects that were placed in a separate scoring panel with modified scoring criteria and weights. The evaluation form for these projects is included in Appendix C. The scores for new projects were based on the following five criteria and weights:

Score 1: Approach to performing the work (40%)
Score 2: Accomplishments and progress toward overall project and DOE goals (10%)
Score 3: Collaboration and coordination with other institutions (15%)
Score 4: Relevance/potential impact on Hydrogen and Fuel Cells Program goals (15%)
Score 5: Proposed future work (20%)

For this new projects panel, reviewers were given the option not to evaluate Score 2: Accomplishments. (In such instances, the other criteria were re-weighted to total 100%.) Scores for new projects were then included in their respective panels—Fuel Cell R&D or Hydrogen Infrastructure R&D—after the weighted averages for each panel were computed using normal weighting. The minimum, average, and mean scores were then computed for the entire panel (new projects included).

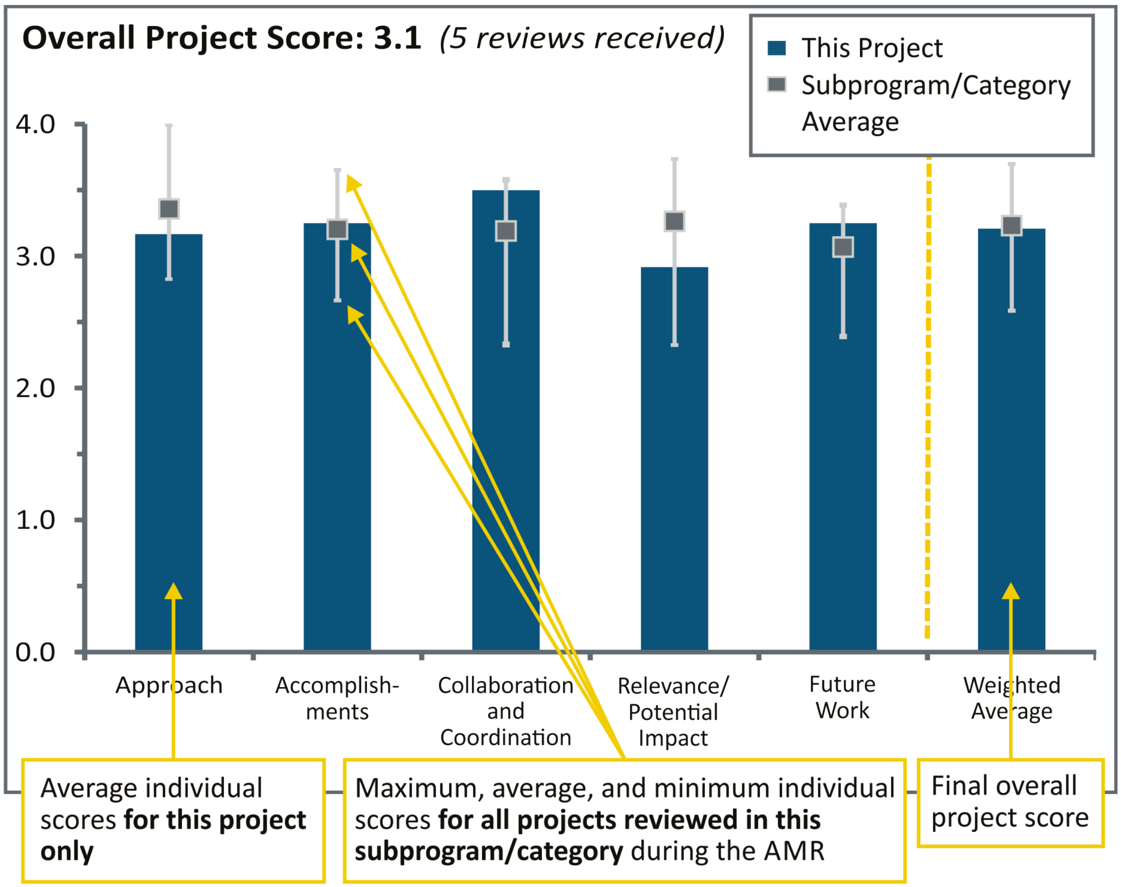
For all projects, reviewers were also asked to provide qualitative comments regarding the five criteria, specific strengths and weaknesses of the project, and any recommendations relating to the work scope. These comments were also entered into the private online database for easy retrieval and analysis.

Organization of the Report

The project comments and scores are grouped by subprogram (Hydrogen Fuel R&D; Fuel Cell R&D; Infrastructure and Systems R&D; and Safety, Codes and Standards). In the case of Hydrogen Fuel R&D, project comments and scores are grouped by category (Hydrogen Production R&D, Hydrogen Production R&D: HydroGEN Seedling, and Hydrogen Storage R&D). Infrastructure and Systems R&D projects are also grouped by category (Hydrogen Infrastructure R&D, Technology Acceleration, and Systems Analysis). Each of these sections begins with a brief description of the general type of research and development or other activity being conducted. Next are the results of the reviews of each project presented at the 2019 AMR, including the qualitative comments for each project.

Each individual project report also includes a graph showing the overall project score and a comparison of how each project aligns with all of the other projects in its subprogram or category. Projects are compared based on the consistent set of criteria described above. Each project report includes a chart with bars representing that project's average scores for each of the five designated criteria. The gray vertical hash marks that overlay the blue bars represent the corresponding maximum, average, and minimum scores for all of the projects in the same subprogram or category. A sample graph is provided.

Sample Project Score Graph with Explanation



For clarification, consider a hypothetical review in which only five projects were presented and reviewed in a subprogram. Table 2 displays the average scores for each project according to the five rated criteria.

Table 2: Sample Project Scores

	Approach (20%)	Accomplishments (45%)	Collaboration and Coordination (10%)	Relevance/ Potential Impact (15%)	Future Work (10%)
Project A	3.4	3.3	3.3	3.2	3.1
Project B	3.1	2.8	2.7	2.7	2.9
Project C	3.0	2.6	2.7	2.8	2.9
Project D	3.4	3.5	3.4	3.2	3.3
Project E	3.6	3.7	3.5	3.4	3.4
Maximum	3.6	3.7	3.5	3.4	3.4
Average	3.3	3.2	3.1	3.0	3.1
Minimum	3.0	2.6	2.7	2.7	2.9

Using these data, the chart for Project A would contain five bars representing the values listed for that project in Table 2. A gray hash mark indicating the related maximum, average, and minimum values for all of the projects in Project A's subprogram or category (the last three lines in Table 2) would overlay each corresponding bar to facilitate comparison. In addition, each project's criteria scores would be weighted and combined to produce a final, overall project score that would permit meaningful comparisons to other projects. Below is a sample calculation for the Project A weighted score.

Final Score for Project A = [3.4 x 0.20] + [3.3 x 0.45] + [3.3 x 0.10] + [3.2 x 0.15] + [3.1 x 0.10] = 3.3

2019 – Hydrogen Fuel R&D
Summary of Annual Merit Review of the Hydrogen Fuel R&D Subprogram

The Hydrogen Fuel R&D subprogram focuses on early-stage research and development (R&D) to reduce the cost and improve the reliability of technologies used to produce and store hydrogen from diverse domestic energy resources. The subprogram is divided into two categories: (1) Hydrogen Production R&D and (2) Hydrogen Storage R&D. Efforts in each area leverage expertise and capabilities at the national laboratories and encourage collaboration witth industry through the Hydrogen Materials–Advanced Research Consortium (HyMARC) and the HydroGEN consortium. Both consortia are part of the U.S. Department of Energy's (DOE's) Energy Materials Network (EMN). The subprogram also covers early-stage R&D in materials for hydrogen production and storage; this work is specifically targeted to support the H2@Scale initiative.

In fiscal year (FY) 2019, production projects focused primarily on early-stage R&D for advanced water-splitting materials and systems funded through HydroGEN. Production pathways under investigation included advanced high- and low-temperature electrochemical water splitting and direct solar thermochemical (STCH) and photoelectrochemical (PEC) water splitting. Hydrogen storage projects in FY 2019 focused on materials-based hydrogen storage R&D through HyMARC, including the discovery, design, synthesis, and validation of metal–organic frameworks (MOFs), metal hydrides, and other innovative concepts with the potential to reach high energy densities as well as favorable kinetics and thermodynamics. A new effort on hydrogen carriers (also under HyMARC) started in FY 2019 to address challenges associated with transporting and storing large quantities of hydrogen and to enable progress toward achieving the H2@Scale vision. The subprogram continued early-stage R&D for onboard high-pressure storage through the development of precursor fibers for low-cost, high-strength carbon fiber. All projects under the Hydrogen Fuel R&D subprogram continued to be evaluated with respect to their potential to meet DOE's cost and performance targets for the near and long terms.

Summary of Hydrogen Fuel R&D Subprogram and Reviewer Comments

Reviewers of the Hydrogen Production R&D category commented that the projects were focused on achieving DOE cost and performance targets across the various technology pathways. The reviewers responded favorably to the approach of these early-stage R&D efforts, mentioning that they were logical and show high probability of impact. Projects were also commended for their combination of experimental and computational methods in their approach to advancing fundamental understanding of underlying concepts, as well as meeting project targets. The advanced water-splitting projects were praised for their strong interaction with the national laboratories and successful leveraging of capabilities through the HydroGEN consortium. Projects were also commended for their contributions of resources to the HydroGEN Data Hub. Reviewers commented that they would like to see increased attention to accurate cost models as these projects move into the next phase.

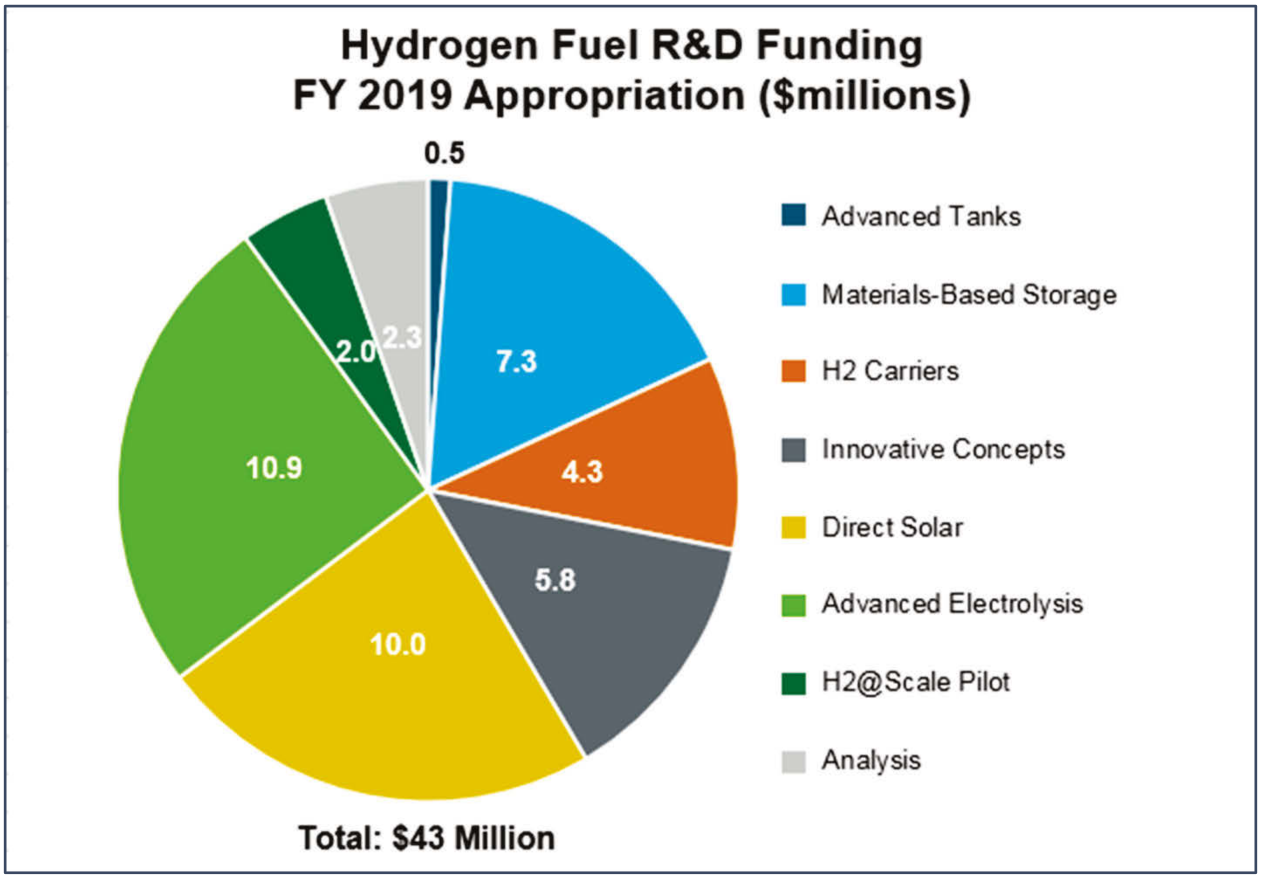
Within the Hydrogen Storage R&D category portfolio, reviewers highlighted the continued synergy of resources, priorities, and technical goals. The reviewers are encouraged that closer integration of early-stage production and storage R&D efforts will lead to successful overlap with infrastructure activities to maximize R&D impact and increase the likelihood of success for the overall Hydrogen and Fuel Cells Program (the Program). Reviewers praised the subprogram category's world-class team members, productive collaborations, project management, and open communication with stakeholders. The reviewers commended the Program's consistent engagement and flexibility to meet industry needs. HyMARC continued to be highly regarded as the nucleus to influence foundational scientific understanding and world-class resources and facilities across multiple institutions. The consolidation of the HyMARC and Hydrogen Storage Characterization Optimization Research Effort (HySCORE) teams has broadened the scope and provided a more streamlined way to address R&D with limited overlap and duplication among the seedling projects. While the material-based hydrogen storage work was generally commended, reviewers did note a desire for additional work and portfolio balance with more traditional high-pressure storage tanks.

Twenty-five hydrogen production projects were reviewed, with overall favorable scores ranging from 2.9 to 3.7, with 3.4 as the average score. The Hydrogen Storage R&D portfolio was represented by fourteen oral presentations and eight posters (including one Small Business Innovation Research project) in FY 2019. Out of the fourteen projects reviewed, nine focused on materials development, two on analysis, and one on engineering. In general, the reviewers' scores for the projects were good, with scores of 3.6, 3.1, and 3.3 for the highest, lowest, and average scores, respectively.

Each of the individual project reports in this section contains a project summary, the project's overall score and average scores for each question, and the project-level reviewer comments.

Hydrogen Fuel R&D Funding

The FY 2019 appropriation for the Hydrogen Fuel R&D subprogram totaled $39 million, with an additional $4 million from the Hydrogen Infrastructure R&D appropriations to support the hydrogen carrier development activities. Of these appropriations, $30 million was allocated for hydrogen production research and $13 million for hydrogen storage research, as shown in the figure below. Projects funded in the Hydrogen Production R&D portfolio are expected to accelerate materials development for advanced water-splitting technologies toward meeting DOE targets, and this emphasis is expected to continue into FY 2020.



* Note: FY 2019 funding includes $4 million from Hydrogen Infrastructure R&D to support hydrogen carrier R&D

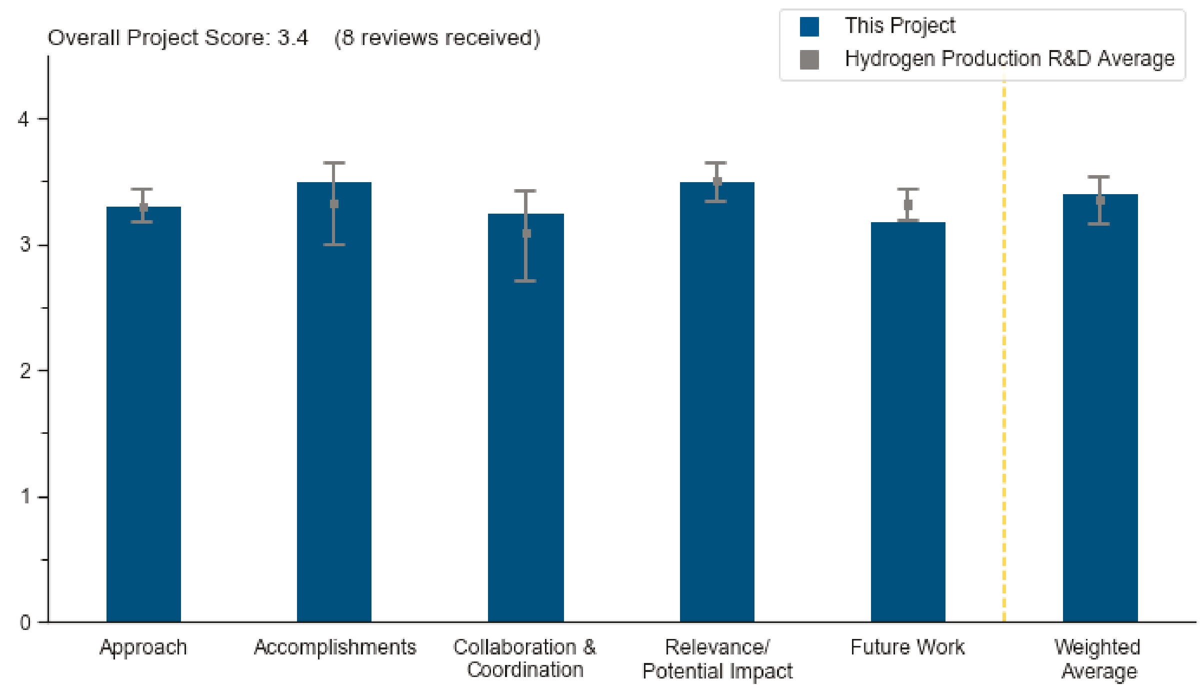
Project #P-102: Analysis of Advanced Hydrogen Production Pathways

Brian James, Strategic Analysis, Inc.

Brief Summary of Project

This project investigates high-priority hydrogen production and delivery pathways selected or suggested by the U.S. Department of Energy (DOE), and subsequently analyzes them with respect to economic and technical drivers. The project provides complete hydrogen production and delivery pathway definition, performance, and economic analysis not elsewhere available. The current effort is updating the Hydrogen Analysis (H2A) model cases for polymer electrolyte membrane (PEM) and solid oxide electrolysis with updated performance and cost data. The project addresses several DOE-identified barriers related to transmission methods for energy carriers and hydrogen generation by water electrolysis. The prime (Strategic Analysis, Inc. [SA]) is collaborating with project partners National Renewable Energy Laboratory (NREL), Argonne National Laboratory (ANL), electrolyzer companies, and other technology experts to model state-of-the-art (SOA) and future systems (e.g., photoelectrochemical [PEC] hydrogen production and solar thermochemical hydrogen [STCH] production).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approaches used for the hydrogen production and the energy transmission analyses are sound. The attempt to obtain performance and cost data from six electrolyzer companies and research groups is excellent. Similarly, the approach to the analysis of energy transmission methods is sound and informative. In particular, comparison of total cost of transmission using multiple metrics (i.e., dollars per mile, dollars per megawatt-mile, and dollars per megawatt-hour) provides level comparisons and meaningful insight.
- The approach is based on industry surveys followed by in-depth technoeconomic analysis (TEA). The methods used for PEM electrolysis and energy transmission are appropriate. Particularly noteworthy is the modification of the energy transmission cost parameter from cost per mile to cost per megawatt-hour per

mile. This metric shows a significant difference in the performance of the energy transport technologies. The solid oxide electrolysis work is in its infancy but is likely to succeed if it follows the protocols outlined for PEM.

- The bottom-up cost-modeling approach taken by SA provides the community with critical insights into technology pinch points and scale-up challenges to tackle.
- The project is very diverse, ranging from an in-depth summary of electrolysis accounting and cost to a comparison of energy transfer and infrastructure costs for gas and liquid pipelines versus high-voltage transmission lines. The project uses a quantitative approach wherein all assumptions are explicitly spelled out. Any cost study will be a continuously moving target as compared to a more physics-based approach founded on materials, energy consumption, and book-end efficiencies.
- The analysis of several of the barriers associated with hydrogen generation via electrolysis is interesting and insightful, as is the comparison of hydrogen as an energy-carrying medium with other fuel options. The investigators' presentation choices for hydrogen generation analysis results are sometimes difficult to understand. For example, the team distributes capital cost information for mechanical balance of plant (BOP) over the amount of hydrogen produced per day; however, information is not provided indicating the period of time for which this cost rate is anticipated (i.e., the period of time over which these costs are spread before replacement costs will be incurred). Similarly, lifetimes of electrical BOP components are not mentioned. The investigators also mention that their analyses should address system efficiency and manufacturing; however, their analysis for PEM electrolysis does not appear to contain explicit metrics associated with these barriers. The degree to which these barriers affect the investigators' work is unclear. The presentation method for the analysis of energy transmission was more coherent and well thought out. However, the small number of references on which the team bases the analysis is concerning. Only a few pipeline cost models are cited. On the other hand, the small number of references may only underscore the need for more rigorous analysis and model validation and development within the community.
- The project does not take spikes, off time, lower capacity factors, or scaling for peak and non-peak types and multiple stacks into account. The results of other studies such as Lawrence Berkeley National Laboratory's report, *A Total Cost of Ownership Model for Solid Oxide Fuel Cells in Combined Heat and Power and Power-Only Applications*, should be considered, as it is possible that their results may translate to electrolysis. Transmission work should inform other parts of the DOE Hydrogen and Fuel Cells Program (the Program). Furthermore, transmission work should consider carriers and non-pipeline transmission of hydrogen including trucking in both high-pressure and liquid states.
- As with any analysis conducted at any level of fidelity, the inputs and assumptions in this analysis have a significant and indelible imprint on the result. SA's work flow and analytical results carry caveats warning of sparse information throughout their approach. Nonetheless, the investigators decided to conduct the analysis. The investigators should communicate the effect sparse information has on the result to inspire more confidence in the result.
- Some assumptions were clearly "cherry-picked," to the detriment of competing technologies. For example, it seems disingenuous to assume combustion for a natural gas re-electrification pathway achieves 33% efficiency and assume a fuel cell achieves 50% efficiency in the hydrogen case.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- These unbiased updates to the electrolysis cases are extremely valuable to the hydrogen community. SA's efforts to thoughtfully improve the modeling approach to increase the robustness of the results should be applauded. Modeling dollars per square centimeter versus dollars per kilowatt for electrolyzers is an example of one such improvement. The electrolyzer updates, especially the long-distance energy transmission cost analysis, should be published in a DOE record as soon as possible. The energy transmission work should also be published in the peer-reviewed open literature as soon as possible. The publication of this work will have a large influence on discussions around investing in electricity versus hydrogen infrastructure, which are taking place globally.
- Approach and assumptions aside, the progress made by the investigators has been excellent. Their results on hydrogen production cost using PEM electrolysis provide insight into the primary cost drivers and the

degree to which these drivers may override cost reduction potential in future systems. It should be noted that several offsets are present that limit, and indeed eliminate, the possibility of cost reduction in future systems. Rather than directly commenting on this elimination, these results may indicate how aspects of the investigators' methodology have limiting assumptions, for example, the degree to which the investigators do or do not assess future technology to be less costly than current technology. Although not presented directly here, the analysis may show where breakthrough innovations must happen in order for hydrogen production cost to meet, if not exceed, DOE targets. Likewise, progress on energy transmission analysis and the conclusions drawn so far offer fascinating insight into the costliness of electricity transmission and the potential for hydrogen and other fuels to dramatically lower this portion of overall cost.

- SA was able to generate a great deal of work, given the limited budget. The effort involved in gathering information and forging an analytical result from it is appreciable.
- The investigators have made good progress toward project goals. Many milestones were achieved several months in advance. The April 2019 milestone is not shown to be completed, but this is likely a result of the Program Annual Merit Review occurring one month after presentations are submitted.
- Significant progress has been made, particularly in terms of PEM and transmission analysis. The analysis reports its findings in ways that are highly quantitative and seemingly transferable. One area that could be improved is the rate of industrial survey response, though this improvement is likely difficult to achieve.
- It is unclear why the investigators believe dollars per square centimeter to be a better cost metric. On slide 7, a desire "to decouple cost from performance" is expressed. Clarification on the benefits of decoupling cost from performance may suffice to answer this question. The Current Central case requires four ~25 MW systems, and the Future Central case relies on two 50 MW systems—perhaps these assumptions are based on the survey. Only Giner ELX has mentioned a (very) large 5 MW stack, so a 25 MW stack seems impressive.
- The results from the electrolysis (i.e., the hydrogen production via water splitting) portion of the study appear modest and incremental. Although the team successfully reached out to six electrolyzer manufacturers for data collection, the data quality and response rate are unclear. For that matter, it is unclear how many manufacturers are in favor of PEM versus solid oxide electrolyzers. The project team reports "general agreement" on current density and voltage data. However, it would be beneficial to quantify the sample representativeness of the blinded respondents' responses, perhaps in the form of standard deviation or uncertainty ranges. Similarly, the project team indicated they obtained limited data on cost. It would be helpful to specify a measure of reliability of the cost-related data. Slide 10 indicates that the study results for future stack costs appear to be more reliable than the current case. These results may signal that the uncertainty assumptions should be revisited.
- It is unclear whether the electrolysis accounts for capacity factors. Furthermore, it is unclear whether costs are consistent with the current SOA, especially when combined with delivery that is much higher than that projected.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project team forged good connections with NREL and ANL. It is great to see that industrial collaborators, though unnamed, are contributing information to the analysis and participating in the review process. It would be interesting to discuss the industry view of the methods and results. It would also be helpful to understand whether the industry finds this level of information useful or would be likely to develop a business case from these results.
- The team has shown good integration with partners, particularly NREL, for project modeling and validation.
- The collaboration and data collection from the electrolyzer manufacturers and outside research groups appear to be valuable. Although the blinding of manufacturer names is understandable, it is unclear why the research groups were not named.
- As the technologies being investigated by SA mature, it is naturally becoming more difficult to obtain survey responses high in quality and quantity. DOE may have a role to play in facilitating the acquisition of what may be considered confidential information in a way that ensures complete anonymity and precludes

damage to the provider. In other words, SA requires DOE's assistance in order to achieve very high collaboration ratings.
- The project received good input from DOE and from other national laboratories. Unfortunately, the missing electrolysis input and the literature-focused comparison of infrastructure and pipeline costs indicate that industry was not extremely integrated in the project. Given the breadth of the technology review, the preference to focus on literature comparisons is understandable.
- The project team collaborated well but may not have obtained enough industrial feedback. The role of the national laboratories is unclear, and it seems there may be overlap, as many laboratories have strong TEA, life-cycle analysis (LCA), and total cost of ownership (TCO) scientists.
- The investigators acknowledge their collaborators and are somewhat clear on the contributions these individuals make to the overall effort. The presentation slides use somewhat ambiguous language regarding collaborator contributions (e.g., "assisted with model runs," "vetted process work"). Clarifying these contributions in future reviews is recommended.
- The team is strong. However, the PEM electrolyzer questionnaire sent in December of 2018 seems far too detailed. With over 40 questionnaire parameters ranging from catalyst loading to operation and maintenance (O&M) costs, more than half of which are labeled "critical," it is not surprising that the project team received such a limited number of responses.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This impact of this project lies in its reevaluation of H2A models. This reevaluation is necessary to ensure that the model used for evaluating systems is valid and current.
- SA TEAs such as the ones presented here are a gold standard used by industry to understand key hydrogen technologies.
- The relevance of the hydrogen production cost update portion of the study is straightforward and needed, especially considering the ongoing reduction of renewable electricity price and increased shipments in PEM units. However, the relevance and potential impact of the energy transmission analysis portion of the project is very strong. The results are significant and novel in that they challenge the commonly accepted notion that electrical grid is the preferred means of renewable energy transmission to consumers.
- The periodic cost updates for electrolysis, along with information on fossil fuel energy transmission, are very relevant to keeping DOE research programs on track. The cost analysis helped demonstrate changes in raw materials and capital costs between the 2019 and 2013 studies. Since simple scaling was used, it is not clear that the project will have a large impact on how existing projects are managed or evaluated.
- This project offers important contributions to stakeholders and may also be important for designing targets.
- The investigators provide information useful to the Fuel Cell Technologies Office (FCTO) and the entire hydrogen fuel cell community. The impact of this project is somewhat limited by its lack of certain types of information and by the presence of several unstated assumptions. It would be useful to provide these details in the reports produced and delivered to DOE and later share these details with the larger community. The impact of the analyses performed could be made even stronger by tying the results to conclusions about ways in which technology needs to change (in performance or cost) to reach DOE targets. This is perhaps outside of the scope of the project but would add tremendous value and reduce the need for such analysis by others at a later date.
- It would be more helpful to show today's actual capital costs converted to dollars per kilogram. Large (by today's standards) projects in the 5–10 MW range for energy storage are in development; therefore, it would be nice to have this data more readily available. It will be many years before "Current Cases" for hydrogen production are anywhere near $5/kg (as stated on slide 14), and this production value is very near the value assumed for "Future Cases." A "current" case should be achievable within roughly a year.
- The notion that electricity cost makes the largest contribution to the ultimate hydrogen cost for PEM electrolysis is not news, and revisiting this case study is not useful. It would perhaps be more useful to dedicate resources elsewhere. The energy transmission study is very intriguing, and the result is counter-intuitive for a lay person. Order-of-magnitude differences in cost for carrying energy via electricity

transmission versus other fuel types are notable and have the potential to influence a range of issues that concern policy makers and industrialists.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The future work builds on the progress made so far. It is specific, relevant, and well planned. This project is on track to update the H2A for relevant hydrogen technologies and serve as a good comparison for energy transmission costs, which are important when considering a nationwide energy grid.
- The future sensitivity analysis on the PEM electrolysis and the future exploration of industry feedback will be very interesting and helpful, considering the scale and increased number of projects in North America and around the world. Solid oxide electrolyzers still appear to be an out-year technology in the long term, similar to PEC objectives. The primary value is breaking down silos across FCTO subareas and ensuring that different areas are using a similar basis for reports and technology prioritizations (i.e., delivery, analysis, and target-setting coordination).
- Solid oxide electrolysis is a very good target for an updated analysis.
- The stated future work for the PEM and solid oxide analysis looks good, especially the error and sensitivity analyses. It is suggested that the team carry out a simple data quality or representativeness analysis on the collected industry data. On the other hand, there is no meaningful operational or demonstration data for PEC- or STCH-based hydrogen production technologies to justify similarly detailed cost analyses at this time. Instead, it is strongly recommended that the project team publish the energy transmission results in a peer-reviewed journal. The results are significant and impactful enough to necessitate a wide distribution beyond the internal DOE report. Furthermore, the project team should consider future work that includes the cost of a combination of various energy production and transmission pathways.
- Many of the future activities for analysis of hydrogen generation technologies mentioned in this project (e.g., sensitivity and error analyses, non-electrolysis methods) are important, and the plan for their inclusion is appreciated. Perhaps a similar suite of activities should be developed for the transmission analyses. Additionally, the project may benefit from exploring ways in which the information can best be used by the energy community.
- Transmission should be expanded to other possibilities. For solid oxide and PEM fuel cells, there has already been Design for Manufacture and Assembly work done. Therefore, it is necessary to determine key differences for electrolysis and leverage those differences.
- More work on PEM H2A analysis seems redundant. Also, both PEC and STCH water-splitting technologies are at very low technology readiness levels. One might suggest postponing these studies until sufficient data emerges to provide a robust outcome to the analysis. Otherwise, predictions for these technology pathways to attain commercial viability, or even meet DOE cost targets, are not believable.
- The “cherry-picking” should be reduced, and actual current cases ($15/kg H_2) should be shown. This would be more helpful for audience members who work with utilities to develop large-scale energy storage projects.

Project strengths:

- Availability of empirical or manufacturer data provides a strong foundation for the electolyzer portion of the project. However, the energy transmission study is undoubtedly the highlight of the project. It offers a unique and an interesting approach with potentially impactful results based on an energy-normalized cost of transmission.
- The project uses both survey data and internal analysis to develop cost models. Internal assumptions are checked and validated by the surveys, and the responses are validated by analysis. This dual validation system seems a positive way to “keep them honest” in both respects and therefore is good for building H2A schemes. Particularly interesting and important is the change in metrics for energy transport from cost per mile to cost per mile per energy unit.
- Much of the work performed brings a deep level of understanding of the costs associated with these technologies and uses. The work on energy transmission in particular is excellent, and both analyses have

the potential to provide insight into technological transformations needed to reduce the cost of hydrogen as an energy carrier and storage medium.

- Methods are sound and consistent with obtaining low-fidelity results, given limited budget resources. Investigators demonstrate good interactions with collaborators. Results of the energy transmission case study are intriguing and may warrant a much deeper dive using more data and more rigorous methods.
- The project demonstrates a very diverse effort with a deep technical dive. The derivations of project assumptions are well documented. The majority of the effort was directed toward the electrolysis work, but many assumptions were somewhat simplified with respect to scaling factors and cost savings between distributed and central scales. The project offers a good across-the-board comparison of energy transmission options.
- Investigators demonstrate strong methodology, knowledge of staff, and familiarity with DOE objectives and a breadth of technologies in the hydrogen space.
- The project is well organized and has a strong team. The questionnaire was a good start but needs to be simplified to improve responses.
- The analysis informs targets and explores new metrics for transmission.

Project weaknesses:

- Some assumptions appeared to be too high-level. The comparison of infrastructure pipelines may not have much use without context of the value of the final energy (e.g., comparison on a megawatt-hour basis without taking into account the efficiency losses of conversion). A simple introduction that explains why the comparison is being done and how the results will be used to steer project or Program end goals would be helpful.
- The weakness is the reliance on slow survey data from the industry. It is critical to have data, and it will be difficult to increase response rates, but more data would nonetheless help speed the project.
- The only weaknesses are the lack of quantity and reliability in the stack cost data on PEM/solid oxide and the subsequent lack of clarity on related uncertainties.
- More detail is needed on some of the assumptions used in the electrolysis analysis, particularly with regard to the lifetime of systems and the depreciation and durability limitations of the capital equipment used.
- The cost estimation methodology is so detailed that it is difficult to get a clear understanding of the critical performance metrics for a technology.
- Budgets seem high for this incremental and continued support to SA.
- The case is closed on PEM electrolysis. It seems that no matter how hard the commercial enterprise drives reductions in performance-enhancing hardware development costs, operating costs, or manufacturing costs, electricity costs nonetheless dominate. Unless and until this landscape changes, DOE should not be devoting resources to PEM electrolysis technology development, or the analysis thereof.

Recommendations for additions/deletions to project scope:

- The project team should consider ways in which the results from these studies could affect and drive further research and development in the science and engineering communities.
- Publication of the energy transmission results in a peer-reviewed journal is strongly recommended. The study team should subsequently carry out an expanded follow-up study to include both given energy production and transmission costs. The team should drop or defocus future PEC or STCH cost analysis efforts, since input data for meaningful study does not exist.
- More effort should be focused on analysis of biomass pathways. Regarding solar pathways, a definitive comparison of photovoltaics+PEM electrolysis and a comparison to PEC would be more impactful than updating STCH. The project team should consider how to put the results of each analysis into a learning rate model context, which is often the preferred context for discussing future costs of new technology.
- The project team should continue with future work to ensure as much industry input and review as reasonable within the scope of budget and resources available.
- Relative differences between PEM and alkaline in terms of capital, installation, and O&M should be shown.
- The project team should evaluate more scalable systems for water splitting, such as particle-based systems and possibly PEC. Furthermore, the team should work with laboratory experts to account for externalities and LCA and TCO.

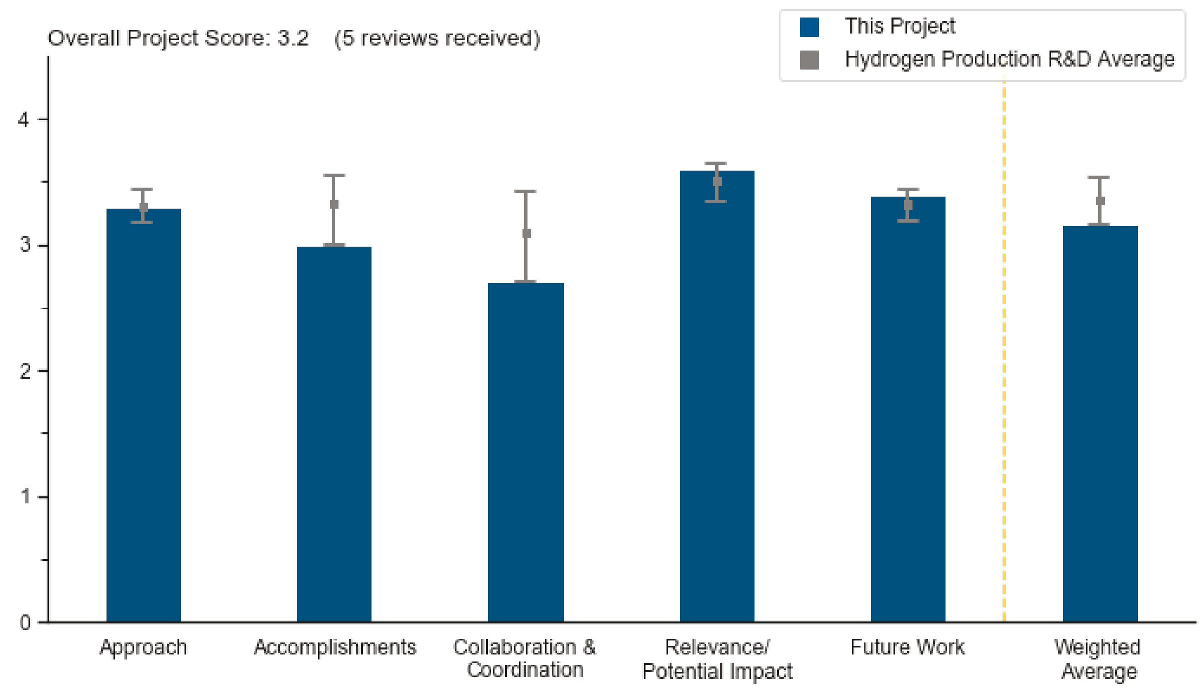
Project #P-143: High-Temperature Alkaline Water Electrolysis

Hui Xu, Giner, Inc.

Brief Summary of Project

This project aims to develop high-temperature molten alkaline electrolyzers with improved electrical efficiency and reduced cost. The electrolyzer will operate in the temperature range of 300°C–550°C. Specific project tasks include (1) development of porous ceramic oxide matrices, (2) incorporation of molten hydroxide electrolytes into the porous matrices, (3) selection of anode and cathode catalysts, (4) assembly and testing of single cells, (5) construction and testing of a 1.8 kW electrolyzer stack, and (6) system and economic analysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach to addressing the identified technical barriers is reasonable and logical.
- The project is well designed, feasible, and identifies and addresses critical barriers. The degree of integration with other relevant efforts is unclear. Short-stack efforts seem to be on the sideline. The reason for this is not apparent since single-cell progress is meeting targets.
- The approach of using molten salt electrolytes to increase electrolysis efficiency at elevated temperatures is good. This approach allows for obtainment of higher ionic conductivity and a potential for non-noble metal electrodes. Three major technical challenges to this approach are electrode materials, sealing materials, and corrosion. It is difficult to assess how effectively these challenges are being addressed. For example, the cell performance data used to meet the go/no-go milestone were obtained at 550°C; however, elsewhere in the presentation, it was stated that lower temperatures were needed to reduce corrosion issues. The lower-temperature data that were presented indicated substantially lower performance (confirming that electrodes were less active). Furthermore, button-cell testing (and presumably low steam utilization) was used to

collect performance data. Though button-cell testing is fine for assessing intrinsic performance, sealing issues are masked by using this method.
- Alkaline electrolysis promises lower cost due to lower cost of stack construction materials. However, there is usually a performance penalty compared to acid-based membrane systems. The higher temperature is expected to improve performance of the alkaline system. Matrix microstructure is correctly identified as a key parameter.
- The presentation suggests a good approach; however, the slides do not clearly lay out the approach. The milestones chart provides some information about the approach, but the previous slide is practically useless for understanding what the project team is doing to accomplish the targets.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Significant progress has been made toward the project objectives.
- Achieving good durability in this temperature range is quite challenging. Lowering temperature improves durability but also lowers performance to unacceptable levels. Performance improvements at lower temperatures appear to be going in the right direction. Resistance measurements should be reviewed and explained.
- Progress toward overall goals is sufficient. The team may need to increase spend rate and to return to short-stack efforts, as single-cell progress is meeting targets.
- Technical challenges have been identified, and progress has been made to address them. However, the investigators are already two years into a three-year project, and it seems that there is a long way to go to achieve the project's stated objectives. The original goal of demonstrating >90% lower heating value (LHV) efficiency in a stack appears to have been abandoned.
- Based on the milestone chart, the team has completed or is nearing completion of their goals. The slides do not do a good job of showing these accomplishments. Slide 20 suggests improvement at 450°C and suggests that the comparison to be made is on another slide. Given how much room is on the slide and the fact that this is a primary accomplishment, the comparison should be on one slide.

Question 3: Collaboration and coordination

This project was rated **2.7** for its engagement with and coordination of project partners and interaction with other entities.

- Interactions with the University of Connecticut have been very helpful. Their excellent images are very useful in understanding the materials.
- The collaboration with the University of Connecticut brings needed skills to the team. However, collaboration with a subsidiary company is not true collaboration. If Zircoa was simply providing off-the-shelf materials, then this does not seem like a collaboration either.
- Although the level of collaboration is sufficient, the investigators' communication of collaborative efforts requires expansion.
- Collaboration with an organization or company that may be interested in using the technology for hydrogen production is recommended.
- There is only one other collaborator outside of Giner, Inc., and its subsidiaries. Vendors are not collaborators. It would be helpful to provide details about the collaborators' data or information contributions in the Accomplishments slides.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- If both capital and operating costs can be lowered as predicted, it will lead to a significant reduction in production cost of hydrogen.
- The molten salt electrolyte concept is sound and has significant potential, if successfully developed.
- Impressive progress is made toward performance targets.
- The work is directly relevant to the goals of DOE regarding water splitting.
- This project aligns with the DOE Hydrogen and Fuel Cells Program.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The project offers a logical plan to further investigate lower operating temperatures and perform durability tests at 450°C. Transitioning the technology to a stack is important.
- The project's proposed future work is reasonable. More focus on corrosion issues and cell performance degradation is recommended.
- The future work seems appropriate.
- Based on the project's current stance, future work aimed at evaluating the newly discovered matrix material and optimizing performance at lower temperatures makes more sense than proceeding with stack development. Additional work performed to demonstrate sealing materials and approaches would be beneficial. A primary focus of additional testing work should be long-term durability of cell and seal materials (for durations much longer than 120 hours).
- Short-stack efforts require more comprehensive discussion and presentation.

Project strengths:

- The work up to this point shows substantial accomplishment. The project is fairly comprehensive, ranging from material stability to cost estimation.
- The project concept for increasing electrolysis efficiency is good. The electrochemical testing and discovery of new matrix materials are project strengths.
- Progress toward the performance target is excellent. Collaboration appears to be going well.
- The main project strength is its approach to addressing identified technical barriers.
- The team and the team's approach are good.

Project weaknesses:

- The presenter was very unclear about the results and when answering questions. Some slides displayed too many small, unreadable graphs, and other slides displayed incomplete datasets from which conclusions could not be drawn. This led to confusing statements and answers during the question-and-answer session. Specifically, it was unclear that the performance improvement at 450°C on slide 20 was being compared to data on another slide. The presenter was seemingly suggesting the performance was better at 450°C than 550°C.
- The project's main weakness is the investigators' choice to back away from the short-stack effort. Both processes should be approached in parallel (single-cell/short-stack development), particularly considering the remaining time and budget.
- The project requires an increased focus on technical "death threats." The project demonstrates limited technical progress toward achieving a viable materials set.
- The main project weakness is its lack of identification of or coordination with an organization or company that may be interested in developing the technology further after the project ends.
- The technique for resistance measurement needs improvement.

Recommendations for additions/deletions to project scope:

- Durability testing should be increased from a few hundred hours to 1000 hours.
- Focus on long-term durability and corrosion mitigation should be increased. Electrode performance should be assessed using impedance spectroscopy testing. Seal performance demonstration is necessary.

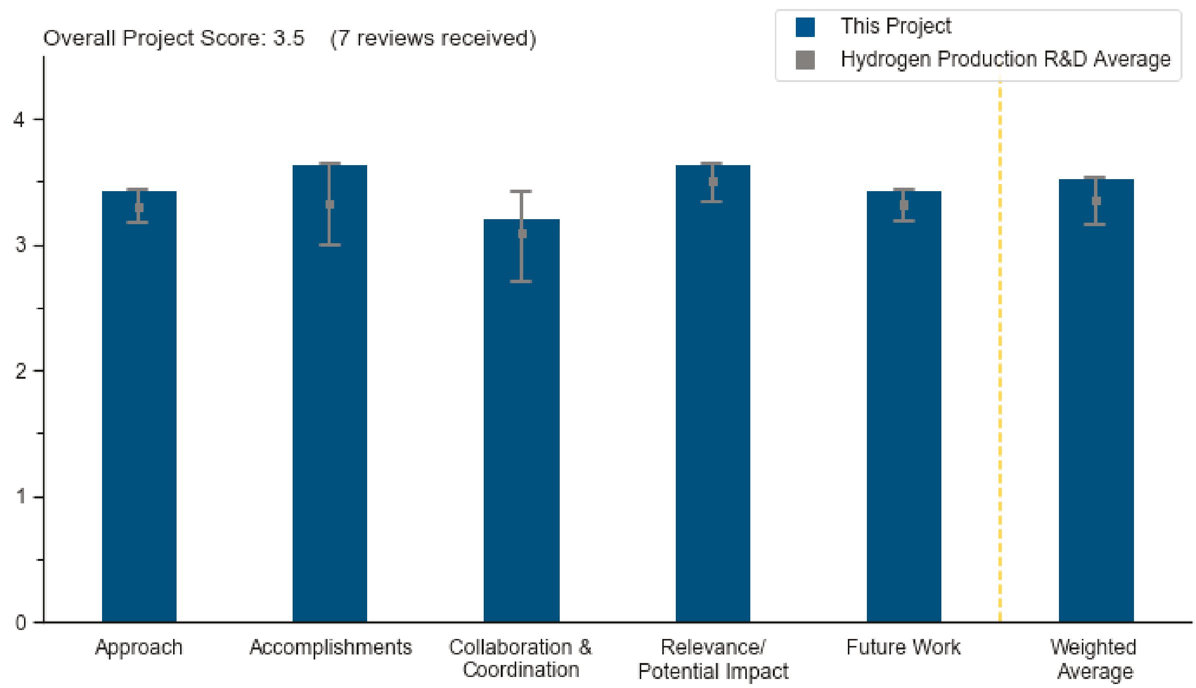
Project #P-177: Proton-Conducting Ceramic Electrolyzers for High-Temperature Water Splitting

Hossein Ghezel-Ayagh, Fuel Cell Energy

Brief Summary of Project

The project objective is to develop an advanced high-temperature water-splitting system for the production of hydrogen with a cost less than \$2/kg H_2 using a proton-conducting ceramic (P-SOEC) electrolyzer. The project targets improved cell and stack electrical efficiency (≥95% lower heating value [LHV] H_2) at current density >1 A/cm^2 at an operating temperature ≥500ºC. The project also seeks to reduce degradation to <1%/1,000 hours, showing a pathway to ultimately reach a stack lifetime of at least seven years. The cell area will be scaled up to 100 cm^2, and a stack with a capacity for producing more than 1 kg H_2/day will be demonstrated. A cell and stack manufacturing process will be developed that incorporates high-yield ceramic processing technologies.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- There are some compelling reasons to consider proton-conducting ceramic electrolytes for electrochemical water splitting to produce hydrogen. Temperatures are high enough that precious metal electrodes are not required in the electrodes, yet not so high that thermal integration is challenging. The ionic conductivity of proton-conducting ceramic electrolytes at 600°C can be similar to oxygen-ion-conducting ceramic electrolytes at 800°C. The electrode-supported electrolyte membrane architecture targeted in this project is a good way to minimize resistance (and power consumption) during electrolysis. A challenge is that the best proton-conducting ceramics (based on barium zirconate) require very high sintering temperatures for densification, which makes it difficult to achieve the targeted porous-electrode-supported, dense-thin-film electrolyte architectures. Another challenge is that the design of electrochemically active and stable electrode materials for operation at 600°C is not easy.

- The project demonstrates a comprehensive and balanced approach, and good progress has been made thus far.
- The approaches to addressing technical barriers and meeting milestones are reasonable and logical.
- The technical approach to achieving project objectives is well thought out and effective.
- The overall approach is very complete and promising.
- This work takes a logical developmental approach. Manufacturing medium to large proton-conducting membrane cells is difficult. Converting the cells to a stack is even harder. It is unclear where the innovation is or if the approach will be successful. The investigators' proposal is similar to other unsuccessful projects done in the literature.
- The area for the tall stack with a capacity of 1 kg H_2 per day should be roughly estimated based on the targeted current density and stack efficiency. A stack lifetime longer than seven years is one of the project objectives; therefore, an appropriated estimation approach is needed.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The researchers achieved outstanding achievements within the short term of this project thanks to their strong research background in this field. The achievement so far guarantees the success of the overall project objective and DOE goal.
- Excellent progress has been achieved, and several milestones have been completed ahead of schedule.
- Significant progress has been made toward project objectives.
- The project is off to an excellent start.
- Excellent progress has been made toward fabrication of the co-sintered membrane architectures. It will be interesting to observe whether similar microstructures can be obtained on larger area and stack intent cells. The degradation of the steam electrode may be problematic. This degradation will need to be addressed for the project to survive its first go/no-go milestone.
- The project goals are on track. The project should evaluate the degradation during thermal cycling.
- This project is just starting; therefore, investigators reported mostly plans and data from previous work. The initial data looks interesting.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- Close collaboration with other institutions and partners is demonstrated. This collaboration has produced results that are important to achieving the objectives of the project.
- The project demonstrates reasonable and balanced contributions from collaborators.
- This project is a good example of collaboration between university and industry. The inclusion of national laboratories would improve this collaboration even further.
- Interactions between collaborators are reasonable.
- This project has three team members, although it could be argued that a wholly owned subsidiary of Fuel Cell Energy (FCE) should be considered as a separate team member. There does not appear to be interaction with other organizations, although at this stage such interactions may not be necessary.
- Investigators are collaborating with Colorado School of Mines (CSM). CSM provides some good materials but has been unable to scale up. FCE is skilled at scaling up, so this collaboration makes sense. It is not clear why investigators list Versa Power Systems (VPS) as a collaborator since VPS is owned by FCE.
- The way in which the fabrication effort is coordinated with VPS is unclear.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Solid oxide electrolysis is a key component of DOE's emerging portfolio of hydrogen production technologies. FCE has demonstrated solid oxide fuel cell (SOFC) stacks and systems at very large scales, and if this project is successful, FCE will be positioned to complete system development and ultimately produce large-scale solid oxide electrolyzer systems. Thus, this project has high relevance and a significant potential impact.
- High-temperature electrolysis is very important to H2@Scale. It does not require the expensive materials (Pt and Nafion) used by low-temperature electrolysis, and it requires less electricity. If the investigators can get the proton-conducting membranes into reasonable (>100 cm^2) cells and stacks, the achievement may have a large impact. The lower operating temperature of proton-conducting membranes enables the use of lower-cost metals for the interconnects and should have lower degradation.
- The proposed current density, operating temperature, long-term durability, hydrogen production scale, and efficiency can potentially help to move toward DOE's target of $2/kg.
- This is a very important, very high-impact project.
- The project is relevant to high-temperature water electrolysis.
- The project aligns well with the Hydrogen and Fuel Cells Program (the Program) and DOE research, development, and demonstration objectives.
- The project aligns well with the Program.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- Much remains to be done, but progress thus far is impressive. The future work outlined is possible, given time and budget.
- Plans clearly build on past progress and are sharply focused on critical barriers to project goals.
- The proposed future work is excellent. It would be helpful for the team to include the methodology they used to predict a stack lifetime longer than seven years.
- The proposed future work is a logical continuation of the presented effort. Thermal cycling should be included in future testing.
- The three focus areas of future work are acceptable. Stabilization of the steam electrode is critical. It appears to be a fundamental materials problem, and new materials sets may need to be explored.
- The investigators must demonstrate that they can build cells and stacks with good performance.
- The approaches to be used to improve cell Faradaic efficiency and reduce cell performance degradation are unclear.

Project strengths:

- This project demonstrates a balanced and systematic approach to each facet of the protonic ceramic fuel cell/electrolytic cell and stack manufacture. The project draws on vast experience and institutional knowledge from collaborators. The team appears very solid. Manufacturing defects are low, and cell strength is high.
- The main strength of the project is the complementary expertise of the team members: FCE, CSM, and VPS.
- The team has experts in proton-conducting membranes. If the team is able to manufacture the cells and stacks, it will be very impactful.
- The project has been effectively planned and well executed, with good progress achieved.
- In general, the project achieved excellent progress in the short term, which is very promising.
- The project benefits from its use of FCE's proven and scaled-up SOFC stack platform.
- The project is well structured and holistic.

Project weaknesses:

- There are no obvious weaknesses.
- A more explicit discussion and characterization of cell and stack leak rates is needed and would offer a substantial addition to the project. Since performance and progress are impressive and cell strength is high, sealing should not be an issue.
- Cell degradation in the fuel cell mode seems to be a challenge. Some effective approach may be needed to achieve the project milestones set for degradation rate.
- The degradation of the steam electrode must be addressed.
- Investigators' anticipated future testing lacks thermal cycling.
- It is hard to see what the innovation is in cell and stack manufacturing that will allow larger cells and the assembly of the cells into a stack.

Recommendations for additions/deletions to project scope:

- A greater focus on cell leaks, stack leaks, and source tracking is recommended.
- The steam electrode degradation needs to be addressed. Project focus on this issue should be increased before expending resources on other project activities.
- The investigators should distinguish between current progress and literature data.
- Greater effort should be directed toward materials stability and durability under operating conditions.
- There are no recommendations for additions/deletions to project scope.
- No additions or deletions are recommended.

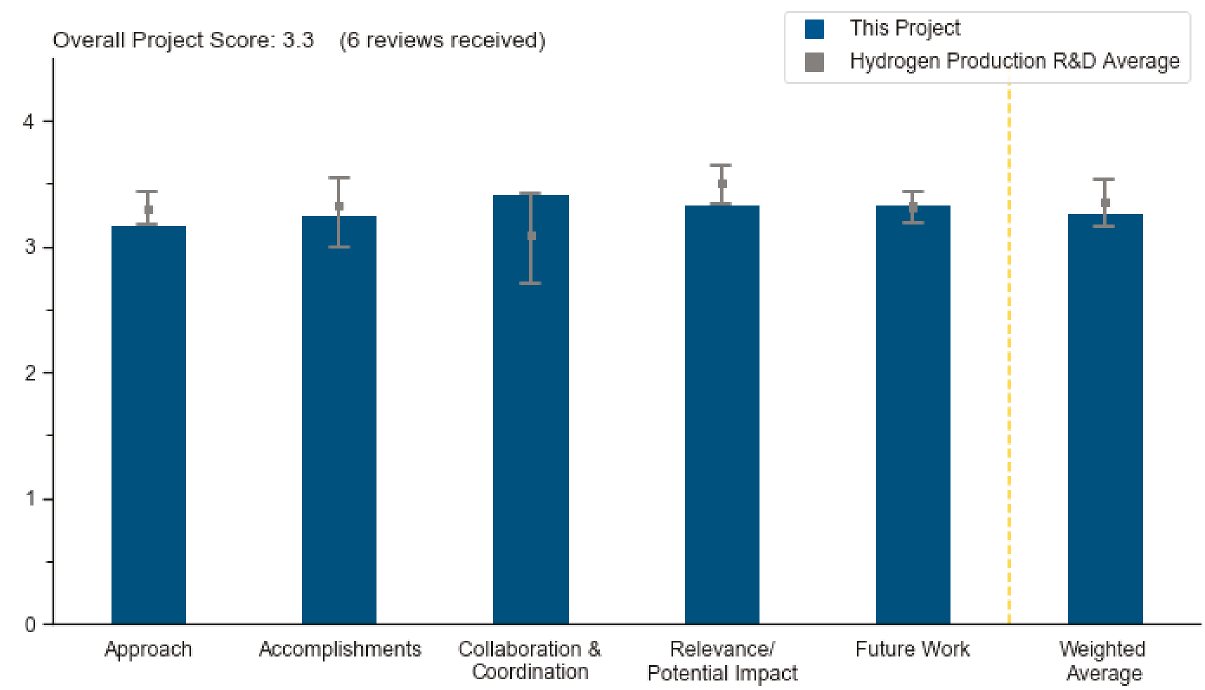
Project #P-178: Industrially Scalable Waste Carbon Dioxide Reduction to Useful Chemicals and Fuels

Todd Deutsch, National Renewable Energy Laboratory

Brief Summary of Project

The goal for this project is to develop an electrochemical reactor that accelerates the rate of the limiting reaction steps for converting CO_2 into liquid fuels and valuable chemicals so that the device operates at power densities commensurate with the rate of point-source CO_2 emissions. This new reactor utilizes a CO_2–water electrolyzer that stores inexpensive renewable electricity as hydrogen and carbon bonds in these products. This device has the potential for improved energy efficiency, chemical selectivity, and throughput compared to conventional thermochemical processes. The project addresses technical barriers through (1) CO_2 mass transport limitations for reduction current density; (2) advanced membranes and membrane architectures (e.g., bipolar membranes); (3) Ni-P catalyst development; and (4) in situ electrochemical component integration.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production R&D projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project and its approach are ambitious in simultaneously tackling four significant problems. The approach is described succinctly and logically. Coupling experimentation with modeling is a good practice, and the use of modeling from the very beginning is wise. The approach does not rely on material breakthrough but rather on rational combination of materials, structures, and logical approaches.
- This project focuses on electrolyzer design, a critical component for realizing large-scale CO_2 conversion technologies. Components such as membrane, flow field configuration, and catalyst loading all impact the overall cell performance and Faradaic efficiency. A thorough effort is needed to understand how all these parameters work together. Furthermore, optimization is needed. The National Renewable Energy Laboratory (NREL) is leveraging its extensive expertise and capability in water electrolyzer design to

create a benchmark technology for CO_2 electrolysis. NREL is also pursuing 2D modeling (e.g., COMSOL and Fluent) to clarify the roles of mass transport of products and reactants, liquid water flow, electrochemical reaction kinetics, and charge and heat transfer on device performance. NREL is also leveraging other X-ray characterization capabilities at Argonne National Laboratory (ANL) for nanoscale synchrotron X-ray computed tomography (nano-CT) to analyze catalyst and electrode structure. Finally, Rutgers University will develop nickel phosphide (NiP) catalysts for the cathodic CO_2 reduction reaction. Rutgers University has reported that this NiP catalyst can produce C1–C4 liquid products at very low over-potentials, but it appears to produce significant H_2 at larger applied potentials. This could be problematic to achieving high current density and desirable product selection. The initial six months show good progress with the construction of a contained CO_2 electrolysis test station. Further work will incorporate product detection using mass spectrometry. However, quantification of gaseous products is typically done with gas chromatography (GC), so future efforts will require incorporating in-line GC for real-time analysis and quantification of product formation rates, selectivity, and Faradaic efficiency.

- The project approach is good. Most important barriers are identified (slide 4) and addressed by some effort. The approach can be strengthened by performing a rough assessment of the largest rate-limiting steps such that efforts may be directed in proportion to relative size of limitation. The assessment would also be useful to inform systematic study. As an example, it is difficult for the reviewer to determine the relative magnitude of CO_2 solubility limitation as compared to the impact of water management. It is likely that the range of possible current densities is small enough to render a passive water management scheme sufficient under most or all applications. The team reports that a model has been developed and is to be published (slide 8), but it would be reasonable to report some preliminary results to reviewers to allow for recommendations regarding the overall approach going forward.
- The conversion of waste CO_2 to useful products is a clearly identified objective. The barriers related to mass transport, membrane, catalysts, and component integration are well identified.
- The stated research and development (R&D) approach, especially regarding the improvement of mass transport via the use of gaseous diffusion electrodes and membrane electrode assembly (MEA), sounds reasonable. Also, starting with known CO_2 reduction catalysts makes sense. It appears that the team's approach is to carry out two distinct electrochemical processes, CO_2 reduction and H_2O oxidation, in a single cell. This approach may not be the most effective approach, given the early stage of knowledge of these systems. Instead, the team might initially consider a two-step approach in which hydrogen (from the well-understood water electrolysis system) is fed to a separate CO_2 electrolyzer to systematically isolate parameters and gain mechanistic understanding of the various steps.
- The approach is not defined. It seems that investigators will build a test stand, but investigators did not specify what products they will be making. The catalysts were not identified. Furthermore, there was no experimental plan. It is good that the investigators plan on modeling, but without specific products and conditions, it is unclear what they will be modeling. The innovations described relate to improving the CO_2 transport and using a non-platinum-group-metal catalyst. However, it was anticipated that the CO_2 transport would use hydrophilic and hydrophobic channels, which is a variation of what is already being done in polymer electrolyte membrane fuel cells. It is not evident that investigators can achieve significant advancement in the state of the art with their approach. The approach incorporated no technoeconomic analysis. Investigators failed to identify and address the key challenge to CO_2 reduction. In their model on slide 8, they identify synthesis gas and methane as products. However, thermochemical conversion of CO_2 to synthesis gas and methane is already well established in the literature. It is very unlikely that a low-temperature electrochemical approach will be more efficient and less expensive than current state-of-the-art thermochemical production. When asked about their choice to produce synthesis gas and methane, investigators stated that they did not plan to produce synthesis gas and methane but, in fact, plan to produce other products. If this is the case, it would be beneficial for the investigators to list the products they actually plan to produce and eliminate time spent developing models that make products the investigators do not intend to make experimentally.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team's achievements are substantial, given that the project is still in its early stages. The project has already demonstrated improved polarization from catalyzed electrospun electrodes. The multiphysics model is useful for conceptualization and prediction of operational metrics. The development of a custom electrolysis test stand shows ingenuity and creativity.
- The team has made good progress in the first six months of the project timeline. The project has constructed an electrolyzer test station with controlled humidity and fluid and gas delivery systems. The test station will harness the capability of an in-line mass spectrometer to detect products formed at the cathode. Team members have met the Quarter 1 (Q1) and Q2 milestones. The Q3 milestone is on track, and the go/no-go decision points in Q4 seem reasonable.
- The team has made good progress in dealing with materials that are difficult to electrospin. Substantial effort was required to achieve MEA production using the low-throughput electrospinning approach.
- The team's progress toward the milestones appears satisfactory. The system is operational, with needed safety and automation.
- The project is too new to produce meaningful accomplishments, but it is off to a good start. It will be interesting to see how the project develops between this year and the next.
- It took the team five months to build the test stand, begin developing models, and produce samples. Given the time and budget, this is a reasonable amount of progress. The team should have identified the first products and reaction conditions to be evaluated and modeled.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- This project demonstrates good collaboration with other national laboratories and with Rutgers University. NREL has taken the lead with its development of the electrolyzer hardware and test station. This development includes building the CO_2 electrolyzer and verifying its performance, an endeavor that suits the laboratory's expertise in water electrolysis device construction and operation. NREL is constructing the ionomer and bipolar membrane, as well as fabricating the gas diffusion electrode (GDE) and MEA. NREL will conduct modeling to determine how each component of the electrode affects system performance. Los Alamos National Laboratory (LANL) will contribute to the project by developing advanced cathode structures. LANL will also conduct nano-CT characterization of the electrode–catalyst structure. Rutgers University is responsible for developing the NiP catalyst to incorporate into cathodes.
- The project has a very strong team of collaborators that include experienced individuals and organizations. Team members are funded at substantial levels commensurate with their contributions.
- The team appears motivated and collaborates well.
- LANL, ANL and Rutgers University are strong partners that bring much value to the team. Based on the presentation, it appears the project innovation is coming from the team members. The poster should distinguish between NREL's partners and the groups with which NREL is coordinating. For example, the poster lists LANL as a partner but also lists other parts of NREL as partners; however, it is assumed that these other parts of NREL are merely groups with which NREL is coordinating.
- Collaboration among the national laboratories and Rutgers University looks good. That said, the team should also seek industry input to strengthen the project.
- Investigators demonstrate adequate collaboration and coordination. However, since there is no collaboration with industrial partners, the team may be missing out on the industrial perspective.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The field needs a standardized testing station technology for catalyst benchmarking and confirmation of performance. Currently, most laboratories have their own electrolyzer devices that may or may not use standardized components. This makes comparison between different groups and reports extremely difficult. This project will address this challenge by developing a standardized testing architecture for evaluating catalysts and verifying system performance.
- The project has the potential to enable an entire class of reactors applicable to many synthesis pathways. The project is directly aligned with DOE goals to reuse waste CO_2 as a pathway to lowering overall CO_2 release into the atmosphere.
- The project demonstrates a high-impact, reasonable approach.
- The project is relevant to CO_2 utilization efforts. The principal investigator should ensure that results can be translated into industrial processes by including fundamental scientific details.
- The project is aiming to develop an electrochemical process that "…could greatly improve the energy efficiency and selectivity compared to thermochemical processes starting from water and CO_2." However, this benchmark may not be very meaningful since there are no such commercial thermochemical processes for comparison. Instead, benchmarks should include known processes with renewable energy input, either as direct electricity use or hydrogen via electrolysis. In other words, this project (and other upcoming e-fuel concepts) need to demonstrate the most efficient and sensible use of renewable energy, i.e., an existing process such as direct use, battery storage, or hydrogen or new processes such as converting $CO_2 + H_2O$ back to hydrocarbon fuels or chemicals.
- CO_2 reduction has historically been achieved by DOE Basic Energy Sciences and Fossil Energy programs. It is unclear how this project distinguishes itself from those other programs. Since investigators did not identify what products they will make or what catalysts they plan to develop, it is difficult to provide feedback on the potential impact. While the reuse of CO_2 may be impactful, it is difficult to determine the extent of the impact without a technoeconomic analysis. The analysis should compare the cost of producing the target products electrochemically versus thermochemically. Investigators should include the market size along with other relevant factors in their consideration.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The project demonstrates a thorough assessment of future work. It may be useful to determine the impact or cost of separation of the large product distribution on the overall process. That is, operation at low current density with a very narrow product distribution may offer substantial advantages over higher current densities and broader product distribution. Impact could initially be determined using a separate model. It is recommended that investigators attempt to increase overall pressure of operation to allow for CO_2 concentration control while maintaining pressure balance across membranes.
- The team plans to complete an electrolyzer testing station with incorporation of mass spectrometry. The team also plans to demonstrate technology with NiP electrocatalysts on a GDE cathode. The progress on milestones and go/no-go decision points in Q4 will determine whether the project continues. From there, the team will be able to begin benchmarking catalysts and confirming the performance of novel catalyst materials. Challenges will likely occur when translating the performance of aqueous cell catalysts into an operating electrolyzer MEA architecture. These challenges will become apparent only once full testing has begun, and electrode/catalyst characterization will likely identify mitigation strategies to overcome these challenges and improve system performance.
- The proposed future work sounds reasonable based on the limited data so far. Understandably, at this point, the project is too new to propose data-driven actions.
- The proposed future work is satisfactory.
- Considering that most of the project lies ahead, the team's proposed future work is quite broad.

- The proposed future work is vague; more specificity is required. Though the investigators propose to "build more CO_2 test stations" and "test catalysts in MEAs," it is unclear which catalysts and membranes they intend to use and what the innovation will be. Investigators should identify the number one challenge limiting electrochemical CO_2 reduction and determine how to meet this challenge. Their current plan does not do so. Investigators need to identify what their target molecules are and why. They should also include a technoeconomic analysis to justify their work.

Project strengths:

- The project demonstrates impressive achievement, considering that the team has been under contract for less than six months. The project plan is well constructed and ambitious. The team is very strong in the relevant technical areas.
- This project will establish a standardized testing platform to benchmark and evaluate catalyst performance. This is certainly needed in the field. The project leverages the excellent capabilities of NREL, ANL, LANL, and Rutgers University.
- The project appears to be well positioned and focused to tackle the key technical aspects of improved catalyst and membrane developments.
- The project offers a multidimensional approach.
- The project is supported by a large budget and good partners.
- The project is high-impact.

Project weaknesses:

- The project's only real weakness may be the choice of catalyst. For example, the chosen catalyst has been demonstrated to produce a variety of liquid products at very low over-potentials, but H_2 evolution will become an issue at larger applied potentials. The team may need to consider a catalyst with a less complex product distribution for initial electrolyzer testing, evaluation, and electrode optimization.
- The list of factors that affect operation must be refined. The experimental space is vast, so it is necessary to pare down the variables to be studied. Several of the R&D challenges listed on slide 4 may be eliminated without affecting the outcome of the project. These may be revisited after the technology develops further.
- The project lacks industrial collaboration. In the absence of an industrial viewpoint, the team may develop technology that may not translate into industrial practice.
- The project's weaknesses are related to lack of system-level considerations, such as the lack of an appropriate reference system for benchmarking, insufficient overall cell or system mass and energy balance discussions, and gas separation or recycling challenges due to likely non-ideal CO_2 conversion efficiency.
- Investigators do not address the key limitation to room-temperature CO_2 reduction. Their experimental plan is extremely vague. Investigators do not justify the work they are doing with technoeconomic analysis. They do not identify materials, catalysts, or products to be made. However, the characterization the team plans to do looks to be very good.
- There is insufficient discussion of performance projections and metrics for success. A target or expected product compound is not clearly stated.

Recommendations for additions/deletions to project scope:

- The project forms an excellent basis to assess the performance and functionality of the basic concept. If positive results are shown, the scope of the project should be expanded to other catalysts.
- The team should use the model and verify its results experimentally to remove factors that make little impact. The team should also consider scaling up the electrospinning setup.
- The term "waste CO_2" should not be used, as it can be misleading. The term gives the impression that CO_2 is free, or even available at negative prices. The clear majority of CO_2 byproduct that enters the atmosphere comes in the form of very dilute concentrations that require additional processing and significant capital investment to achieve the pure form used as feedstock in such electrochemical systems. In fact, the high cost of concentrating and capturing CO2 can potentially be a showstopper in the economics of most commodity-type utilization and conversion processes. CO2 may be undesirable, but it is almost certainly not cheap.

- Investigators need to identify what products they are targeting and provide a technoeconomic analysis showing that those products can be reasonably synthesized. NREL has excellent technoeconomic analysis capabilities, so it was surprising that they were not included in the project. The project needs to develop an experimental plan in addition to the test station construction plan. Additionally, the team needs to improve the model approach. There has been extensive reaction and reactor modeling of CO_2 reduction, and it is not clear that this literature is being used.

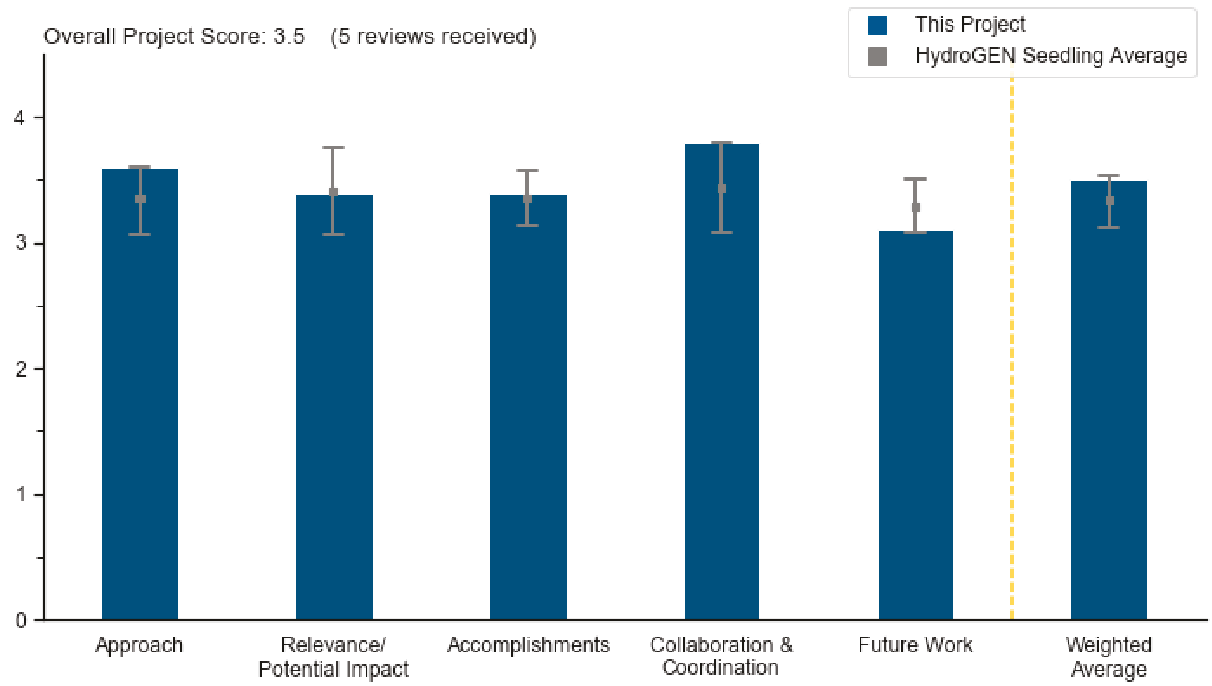
Project #P-148: HydroGEN Overview: A Consortium on Advanced Water-Splitting Materials

Huyen Dinh, National Renewable Energy Laboratory

Brief Summary of Project

The HydroGEN Consortium's objective is to facilitate collaborations between federal laboratories, academia, and industry to evaluate and accelerate the research and development (R&D) of innovative, advanced materials that are critical and necessary to advanced water-splitting technologies for clean, sustainable, and low-cost hydrogen production. Water-splitting technology pathways supported by HydroGEN include (1) photoelectrochemical (PEC), (2) solar thermochemical (STCH), (3) low-temperature electrolysis (LTE), and (4) high-temperature electrolysis (HTE).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach is strong and targets key areas in PEC, STCH, and LTE and HTE to achieve the U.S. Department of Energy (DOE) target of $2/kg. The consortium's offered capabilities in synthesis, characterization, and theory and computation are clearly an invaluable asset to consortium participants. There are multiple layers of engagement with participants and collaborators across capability nodes, the Energy Materials Network, and the Data Hub and ample opportunities for collaboration, with many accomplishments already. As the consortium matures, it may be helpful to establish formal internal mechanisms for self-assessment, deciding future directions, identifying existing barriers, and selecting concrete steps to take to overcome these to maximize the impact of the nodes and ensure adaptability. It was unclear whether such mechanisms exist (perhaps through the steering committee) to set strategy to ensure a continued effective approach.

- The consortium is aiming to reach $2/kg of hydrogen, and various technologies are going to be used to reach this target: from PEC to STCH and LTE and HTE. This project's approach is surely going to open a wide range of possibilities to reach that goal. This shall also be facilitated by using cross-cutting innovation and theunique capabilities found in the 80 nodes within HydroGEN. The task to coordinate and organize information in a multinode platform shall guide the scientists to reach their specific targets and to properly compare the achievements.
- The project appears to be well managed, with excellent collaboration among the six national laboratory partners. Through its nodes and the Data Hub, HydroGEN makes available a wide range of unique national laboratory capabilities, expertise, and data that support the development of the four advanced water-splitting technologies being pursued. The initiation of the supernodes, which help to support R&D efforts within the partner laboratories in their areas of technical expertise, should provide significant additional "value" to HydroGEN toward meeting the DOE hydrogen production goal of $2/kg.
- This effort appears well structured to leverage DOE dollars by combining expertise residing in different national laboratories and aggregating the knowledge from different groups to solve materials challenges.
- HydroGEN is more of a program than a project. The structure is very well defined, and the partners are very well connected. It is of very high value that a wide range of different technologies are combined, which helps with understanding other technologies and identifying synergies between them. The project management seems to be very efficient. The communication structure is close and seems to work very well. However, the size of HydroGEN makes it difficult for all partners to be aware of all developments.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- To meet the DOE hydrogen production price goal of $2/kg, HydroGEN and its focus on developing advanced water-splitting technologies for producing cost-competitive hydrogen are critical to DOE and the Fuel Cell Technologies Office (FCTO), given that many of the companies involved in some aspect of these nascent technologies do not have the resources available to pursue the level of fundamental R&D necessary to make these technologies commercially viable. Through its "node" approach, HydroGEN leverages and makes available the collective unique capabilities and expertise of its partner national laboratories to the broader scientific community, which should help accelerate the development of these technologies.
- Advancing electrolysis systems for energy conversion and storage can be achieved only by substantial innovation in materials synthesis. Only by demonstrating novel materials will the goal of $2/kg be achieved. Therefore, with select expertise and unique capability aligned with strong collaborative work, a substantial impact and relevance in the field of hydrogen production is expected.
- According to the website, a majority of the nodes are being used, which shows engagement with the community toward helping DOE reach its targets. The consortium can point to several technical accomplishments, as well as a dedicated effort toward benchmarking, all of which are very valuable. Activities are distributed broadly across a variety of R&D areas, and many of the individual projects already cite several notable technical achievements toward the hydrogen targets. One challenge in assessing impact is that it is a little difficult to assess the specific, concrete contributions of the nodes toward helping the projects meet these targets (that is, whether node involvement is generally critical, important, or tangential to project success). While making this assessment is rather challenging, it may be useful to identify clear examples or evidences of how the nodes have affected the progress of the individual R&D efforts.
- By managing the materials characterization within the national laboratory complex, HydroGEN helps industrial–academic teams focus on making progress toward their performance and durability targets.
- HydroGEN is strategically focused on materials development to achieve faster breakthroughs in this key area. The project is very strong in this respect. However, cost reductions will not be determined by reactive materials, in the end, but by land use, receiver and reactor efficiencies, and the market. These parts are nearly not covered in HydroGEN. Taken the timeline for implementing renewable hydrogen production, it seems to be difficult for HydroGEN to provide the necessary fast input for the already growing market. If there are no machines that produce hydrogen, even with less efficient materials, better materials will never make it into application.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The consortium's suite of accomplishments is quite impressive, and the members are clearly enabling a diverse set of activities around advanced water-splitting technologies. Specifically, the consortium is to be commended for the level of involvement of the core laboratories in HydroGEN activities via the nodes and now the supernodes, which was evident throughout the presentations. The visibility and accessibility via the website are high. The establishment of the standard technology transfer agreements between consortium partners will be a very useful approach to streamline access and overcome a common barrier. The establishment of the supernodes to merge capabilities is also a valuable asset. Finally, the benchmarking effort for materials characterization supported by the consortium will be very useful moving forward, especially for assessing progress toward targets. The establishment of the HydroGEN Data Hub and its degree of utilization within the consortium are solid, and clearly a good deal of effort has gone into making the Data Hub accessible and user-friendly through the development of interfaces, visualization tools, etc. As the Data Hub grows further, additional metrics beyond the number of files uploaded may be useful in assessing the impact and value added of the Data Hub itself. These could be, for example, the extent to which data are being shared among different consortium members or cited in forthcoming publications.
- The project is still in its initial phase. However, substantial progress can be observed by the number of contributions to the Data Hub and the volume of data already available. It is also very interesting to see the number of high-quality seedling projects applied for and approved within the consortium. Progress over the initial phase is also showing. Within a few seedling projects, a few milestones have been already achieved, showing that the consortium is on excellent track toward achieving and reaching the proposed goals.
- HydroGEN's overarching mission aligns well with FCTO's mission to develop renewable hydrogen production technologies capable of producing hydrogen at \$2/kg. The accomplishments presented for each of the four water-splitting technologies appear to demonstrate good to excellent progress, although it is very difficult to put into perspective how much these accomplishments are moving the needle toward meeting the DOE production goal of \$2/kg of hydrogen for the individual technologies. One of the major challenges for HydroGEN is that while its \$22 million in funding is substantial, it is a challenge to determine how to best allocate its funding across four distinctly different water-splitting technologies. Based on five funding opportunity announcement awards for each of the four technology areas, it appears that FCTO is showing no "favoritism" toward one technology or another, which is understandable at this early stage. However, as HydroGEN moves toward its renewal, FCTO, along with HydroGEN, should do a "deep dive" to evaluate the state of each technology toward meeting the DOE target, as well as the technology's market readiness, to decide how to best allocate its limited funding.
- As the project is so big, there must be differences between the seedling projects. Not everything can be outstanding. However, the progress reported is excellent. None of the technologies seems to be on a dead-end road, and all showed how their developments can potentially contribute to the goal of \$2/kg hydrogen very well.
- From this presentation, it is challenging to assess progress measured against performance indicators. The go/no-go decision points and criteria are not mentioned in the slides.

Question 4: Collaboration effectiveness

This project was rated **3.8** for its collaboration and coordination with HydroGEN and other research entities.

- The structure of HydroGEN is really impressive. The projects are very well connected. A benchmarking process is established. The Data Hub is the perfect vehicle to allow the whole consortium to interact with each other and get value from the achieved results. The reported communication between the partners in the projects, and also between the projects, is outstanding. It is fantastic to observe how HydroGEN supports the different communities growing together.
- The HydroGEN Consortium is clearly valuable to the research community, particularly to academic partners who are obviously benefiting from the capabilities of the core laboratories in synthesis, characterization, and theory and computation. There is substantial visibility through the website, which

makes capabilities clear and has clearly resulted in good utilization of laboratory capabilities among HydroGEN participants. Efforts at facilitating collaboration via the Data Hub, the benchmarking efforts, and the streamlined technology transfer agreements show targeted efforts to engage the community.
- Based on the testimonials, there appears to be significant benefit to the broader scientific community's ability to access the expertise and capabilities of HydroGEN's partner laboratories through the nodes. One of the project's key activities is the development of benchmarking protocols that will provide the basis for evaluating and comparing the performance of the new materials toward meeting the FCTO technical targets, using well-defined experimental approaches and metrics that allow for a fair and unequivocal comparison. There has been a significant increase in the cumulative data added to the Data Hub, as well as in the number of HydroGEN members participating over the past year, although it does appear that the vast majority of data added was around the time leading up to and including last year's Annual Merit Review. While the type of experimental data added was presented, it would be interesting to know to which technology the data added aligns. It would also be interesting to know if members of the broader scientific community who are not members of HydroGEN find the data, as presented and available in the Data Hub, useful and of value. Given that platinum-group-metal (PGM)-free oxygen evolution reaction and hydrogen evolution reaction catalysts for LTE is one of HydroGEN's major focus areas, it would be interesting to know the extent to which HydroGEN is collaborating with and able to leverage the R&D being conducted in ElectroCat, whose mission is to develop PGM-free catalysts for polymer electrolyte membrane systems.
- Within the results presented, the strong collaboration between the project partners and other R&D peers across the community is clear to see. However, it is recommended that a list of achieved publications be presented, so that the multi-laboratory collaboration within HydroGEN and with other institutions can be easily identified.
- The National Renewable Energy Laboratory appears to effectively facilitate interaction between teams and HydroGEN nodes. Working groups help to foster exchange among similar projects.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project's proposed future effort continues to coordinate the many parallel efforts and integrate the research. Benchmarking to quantify the progress of each competing technology will be very important.
- The proposed future work is logical and will be the right way to efficiently achieve the goals. However, as HydroGEN is so big, it is difficult to follow everything in every project.
- On the whole, the proposed future activities are a logical and reasonable continuation of ongoing efforts. HydroGEN shows solid efforts to continue and expand their ongoing activities. Some proposed activities shown, such as "integrate the whole system," are a little vague, and it is not clear what concrete steps are to be taken for this integration or how they have been determined. Similarly, for the proposed activity "Continue to develop a user-friendly, secure, and dynamic HydroGEN Data Hub," it is not clear what aspects of the Data Hub will be targeted in the short, middle, and long terms.
- Much of the proposed future work lacks focus and distinct metrics or goals. It is not clear what "integrate the whole system" means toward accelerating the R&D of HydroGEN. Likewise, the "collaborate and perform integrated research in the five supernodes" lacks focus and goals or objectives. The establishment of benchmarking standard protocols is a critical aspect of this project. Given that HydroGEN is nearing the end of its initial funding period and is probably up for renewal within the next year or so, it was expected that one future work action would have been to begin to develop the framework for the next phase of HydroGEN.
- The project's proposed future work is excellent, but it is not clear how the proposed tasks are going to be implemented.

Project strengths:

- HydroGEN has a logical and very well-established structure. It clearly helps strengthen communication between different scientific communities. Therefore, it is the perfect tool to bring together researchers with different backgrounds and create synergies. This will help overcome problems faster. The exchange of data is outstanding. It gives all participants the possibility to act faster and to put results in this large framework. The benchmarking is very important and will help with following the actions and results efficiently.

- The project appears to be well managed, with excellent collaboration among the six national laboratory partners. Through its nodes and the Data Hub, HydroGEN makes available a wide range of unique national laboratory capabilities and expertise, as well as data that supports the development of the four advanced water-splitting technologies being pursued. To date, there appears to be good utilization of the nodes. The initiation of the supernodes, which help to support R&D efforts within the partner laboratories in their areas of technical expertise, should add significant additional value to HydroGEN in meeting the DOE hydrogen production goal of $2/kg.
- The project's strengths include its ambitious target, the expertise among the different players within the consortium, the team's unique capability to perform the proposed tasks, the awareness to create a user-friendly and super-necessary R&D information platform (Data Hub), the ability to perform cross-cutting R&D among laboratories, the awareness of the necessity of a solid benchmark, and the ability to achieve fast results.
- The project's strengths include its effective and dynamic collaborations that engage laboratories in R&D activities toward DOE hydrogen targets. The project's further strengths include the community-building efforts through the Data Hub, the benchmarking efforts, and the expertise and capabilities of the laboratories.
- The project manages a complex effort of coordinating many researchers and different technologies for hydrogen production at varying technology readiness levels (TRLs).

Project weaknesses:

- It is difficult to put in perspective to what extent the accomplishments presented have moved each of the four technologies toward meeting the $2/kg goal. Furthermore, it is difficult to put in perspective where each of the four technologies stands relative to meeting the $2/kg goal. While it is not necessarily a weakness, it would be beneficial to understand how the funding is allocated among the four water-splitting technologies, with which of the four technologies the nodes being utilized align, from which technology data is being accessed, etc. This understand would provide a better understanding of how the capabilities, expertise, and R&D for each technology is being utilized.
- HydroGEN's strength is also a weakness. The communication within HydroGEN is extremely positive, but having so many partners involved takes a good deal of time and resources that could be used for achieving the project's goals. However, the question is whether communication is not the better way to accelerate the process.
- It is not clear how to directly assess the impact of the consortium as a whole on progress toward DOE targets. This is admittedly a challenging problem. While the individual projects themselves have clearly defined go/no-go decision points and can point to performance metrics and demonstrations, assessment of the consortium and its contributions in tandem is much more challenging. It may be beneficial to consider ways of showing evidence of the impacts of the nodes themselves on the success of HydroGEN activities.
- The project's weaknesses include that it is covering a broad range of R&D areas and fields, which presents a communication challenge and brings into question whether scientists can speak the same "language." Other weaknesses include how the project team will break down the main goal of $2/kg of hydrogen into subtargets for different R&D tasks for materials development, as well as internal competition.
- An overview of measurable progress in each technology was not provided. Go/no-go milestones appear to be missing from the presentation.

Recommendations for additions/deletions to project scope:

- The project scope is just right, given that HydroGEN's goals are focused on materials. If the market introduction of clean hydrogen were the goal, much more effort on engineering topics and product development would be necessary.
- As HydroGEN moves toward its renewal, a "deep-dive" technical evaluation of each of the four water-splitting technologies being pursued should be considered. The evaluation would help in understanding where each of the four technologies stands toward meeting the DOE target relative to the other three technologies, what the major challenges are that need to be addressed, and what the likelihood is of

addressing those challenges, with the purpose of best deciding how to allocate funding and resources. While it is understood that DOE does not pick winners, and picking a winner is not necessarily being advocated, how to best allocate limited funding is a critical issue.

- The project team should find a way to quantify progress of all parallel efforts and associate timeline and TRL with it.

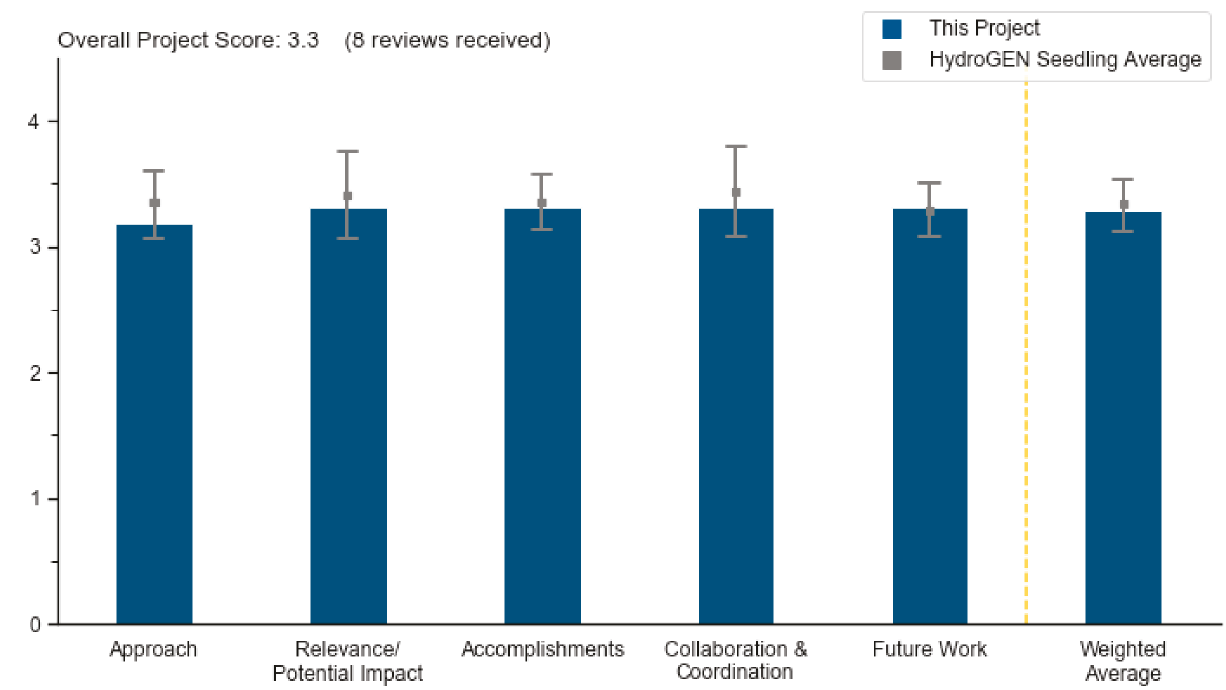
Project #P-152: Proton-Conducting Solid Oxide Electrolysis Cells for Large-Scale Hydrogen Production at Intermediate Temperatures

Prabhakar Singh, University of Connecticut

Brief Summary of Project

The primary objective of this project is to identify novel materials and processing techniques to develop cost-effective and efficient proton-conducting solid oxide electrolysis cells (H-SOECs) for large-scale hydrogen production at intermediate temperatures (600°C–800°C). New proton-conducting electrolytes, tailored hydrogen and oxygen electrodes, and optimized cell designs for lowering the electrode polarization and resistive losses will be developed. Following synthesis and characterization of new electrolyte and electrode materials, they will be used for the fabrication of solid oxide electrolysis cells (SOECs) and tested for performance and durability. The project will examine degradation mechanisms and optimize materials chemistry and component structures to mitigate any degradation.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- This is primarily a materials development effort aimed at the "BZCY-Yb" proton-conducting ceramic electrolyte material, which has some interesting attributes for high-temperature electrolysis systems. The team is pursuing a sol–gel approach for BZCY-Yb powder preparation, which has shown promise in reducing sintering temperature. Reducing the sintering temperature is essential for designing a practical cell fabrication process. Without details on the sol–gel process being used, it is difficult to assess the cost-effectiveness.

- In general, the project's research approaches are excellent. It would be good if there were clearer motivation for lowering sintering temperature below 1400°C and using the sol–gel method to prepare powder.
- The approach focuses on non-noble, non-Pt, low-cost materials and scalable processing. Emphasis is placed on low-temperature processing (i.e., targeting low-temperature kilns that use cheaper Kanthal elements, ~1300°C and below), while preserving the bulk, interfacial, and surface properties required for electrolyzer operation. The interaction between fluorite and perovskite materials was also probed.
- The approaches to address the identified technical barriers are logical and reasonable.
- This project has a comprehensive approach.
- This is a sound approach; however, the uniqueness of the project is not completely clear.
- The project team is advised to review the instructions of creating Hydrogen and Fuel Cells Program (the Program) Annual Merit Review slides carefully. The instructions advise listing the technical barriers being addressed, as described in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (MYRDDP). The authors have not identified these barriers in accordance with the MYRDDP. The approach to improving the material performance and fabrication seems sound, but it is unclear how some of the work will affect the barriers in question. It would be beneficial to understand which barriers were being addressed by various tasks.
- The oral presentation and presentation materials do not give a good sense that the project is grounded in solving one or two key problems. There seem to be multiple moving parts to this project, and it is not apparent how they mesh.

Question 2: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The focus of this project is on industrially relevant parameters rather than on record-setting (but short-term and unstable) performance. The processing focus should prove useful for assessing the feasibility of manufacturing SOEC stacks using conventional, scalable technology in optimal ways. The emphasis on lowering the processing temperature is one of the project's unglamorous but very useful efforts, since typical SOEC materials like Zr are highly refractory but also contain volatile elements, such as Ba, that evaporate and have deleterious effects on the defect chemistry of the vital components. It also should be cheaper to process at lower temperatures, if the dwell times are also reasonable.
- Solid oxide electrolysis is a key component of the DOE's emerging portfolio of hydrogen production technologies. If this project is successful, a new materials set will be available for designing solid oxide electrolyzer systems. Thus, this project has relevance and a significant potential impact. The challenge will be to take the materials technology developed on this project to the full-scale stack level and, ultimately, to large-scale system levels.
- In general, the project has significant potential to meet DOE goals. The synthesis and fabrication processes based on the sol–gel method and infiltration should be justified for large-scale production, and the cost estimation should be reasonably included in the future technoeconomic analysis (TEA).
- The impact of this project is quite clear and beneficial to H-SOEC systems. It would be beneficial to see the impact of the new materials, not just under electrical testing but under a hydrogen production test as well.
- The project is relevant to high-temperature water electrolysis.
- The impact and relevance are clearly seen. There are no issues to raise.
- The project aligns well with the Program.
- It is not apparent that the project is addressing a critical path issue for steam electrolysis. Lowering the sintering temperature sounds useful, but it is not clear that this is one of the top hurdles for the success of the technology. However, the project does seem to be engaged and contributing to the HydroGEN network.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project is pursuing solutions to one of the major challenges that has limited the potential of high-temperature proton-conducting ceramics, specifically the need for excessively high temperatures for densification. The team has made good progress on this. They also have demonstrated high proton conductivities in their low-temperature sintered materials.
- The project achieved significant progress within one year by showing promising current density and lower sintering temperature. In general, the project's accomplishments are outstanding.
- The project is proceeding as proposed. Excellent progress has been made with respect to current density and electrolyte thickness.
- The project has made excellent progress toward its overall goals.
- The project goals are on track; however, it seems like little progress was shown in the presentation as compared to the review from the previous year. Other aspects should be evaluated, such as the effects of Cr poisoning on durability. The 3% H_2O during testing seems rather low.
- The project has met Phase 1 milestones. It would be helpful if the principal investigator (PI) would clarify that the cells being tested were prepared using the lower-temperature sintering approach.
- The project team has achieved budget period (BP) 1 milestones. The use of ZnO as a sintering aid has been covered by Liu's group before (see citation below) and others in the past, and there is a great deal of work that can be found in literature on sintering aids and less refractory dopants for BZY. The combinatorial sintering aid study in BP 2 needs to work harder to advance sintering aid knowledge, beyond what is already known. (Wenping Sun, Zhen Shi, Mingfei Liu, Lei Bi, and Wei Liu. "An Easily Sintered, Chemically Stable, Barium Zirconate-Based Proton Conductor for High-Performance Proton-Conducting Solid Oxide Fuel Cells." *Advanced Functional Materials* 24, no. 36 (2014): 5695-5702. doi:10.1002/adfm.201401478.)
- The accomplishments of this project do not seem overly significant, considering the primary objective of the project is to create H-SOEC electrolyte materials at low temperatures and to provide lower-cost hydrogen production capability. First, the temperature reduction from 1450°C to 1350°C is small. Most industrial equipment that operates at 1350°C can also operate at 1450°C, suggesting that there would be little material cost savings in production equipment. The operating costs to go from 1350°C to 1450°C would be insignificant to industrial equipment that can operate at temperatures greater than 1000°C. If there are cost savings to be found, they should be addressed directly. Secondly, while the authors are commended for performing a durability test, 50 hours is extremely short. It would beneficial to show the test data and let it run to failure. Finally, the authors should consider showing the performance of the current state of the art on many of their metrics. It would be beneficial to show the audience how large the improvements being made to the state of the art are or how close the new technology has come to providing a function similar to the state of the art.

Question 4: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- These two organizations (the University of Connecticut [UConn] and Pacific Northwest National Laboratory [PNNL]) have been at the forefront of solid oxide fuel cell technology for many years. It is good to see these two powerhouses collaborating on a project such as this one. DOE is also commended for setting up the H2@Scale program to facilitate collaborations between project teams and national laboratory nodes funded under the HydroGEN program. This enables many resources to be brought to bear on addressing challenging technical issues.
- This appears to be a well-integrated effort, with UConn, Idaho National Laboratory (INL), National Renewable Energy Laboratory (NREL), and PNNL all contributing. However, the PI could do a better job of articulating the roles and responsibilities of the different organizations. For example, it is not entirely clear what the UConn researchers have contributed.

- In general, the collaboration between the team, institution, and Energy Materials Network (EMN) nodes is excellent. If the connection between the NREL's screening and the validation of the material can be further improved, it would be better.
- There are several collaborators involved in this project. The EMN is being leveraged, NREL will do combinatorial work on sintering aids, and INL is performing the cell testing. However, no direct references were made to how the project is leveraging or contributing to the HydroGEN Data Hub.
- The project's collaboration and coordination are adequate and as proposed.
- The interactions between collaborators are appropriate.
- No issues were identified with the project's collaboration.
- It is unclear how the modeling effort at Sandia National Laboratories is being used to support the project's experimental work.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- A very useful focus included in the future work will be to analyze and present the contributions for each conducting species in order to assess whether a useful transference number is attainable, especially with the lower firing compositions where sintering aids could create unwanted electronic defects.
- The proposed future work is a logical continuation of the presented effort. Thermal cycling should be part of future testing.
- This project appears to be on track, and future work is aimed at addressing the project's remaining milestones.
- The project team should just keep up the momentum. They are doing good work.
- The proposed future work is excellent. It would be better if the team could show a stronger connection between the theoretical and experimental work.
- The PI did not have time to convey plans for future work during the presentation, so the following comments are based off of the presentation materials. Generally, the Phase II plan seems sound. It is questionable that the team will be able to "demonstrate...cost of H_2 production <$2/gge" by quarter 12, as listed under (e) on the "Proposed Future Work" slide.
- More details should be given on the proposed approaches for future work.

Project strengths:

- The project has integrated multiple efforts into one and has achieved an outstanding current density. The proposed roll-to-roll fabrication of cells and stacks is very interesting. It would be good if the team could include the new innovative synthesis and fabrication in TEA.
- The project's strengths include the technical prowess of the team, the powder synthesis technology that is being applied to reduce the sintering temperature of the electrolyte material, and the fabrication process that is being used to fabricate cells.
- The project's strengths include the quality of the team. This is a good technology area on which to work (e.g., steam electrolysis, proton-conducting electrolyte).
- The project's strengths include the large network it has to work within. The electrical results seem encouraging, the new synthesis operations seem to be producing good cells, and the project is meeting technical targets.
- The project has a reliance on and is using the strengths of its collaborators. Excellent progress has been made with respect to optimizing electrochemical performance.
- The project's main strength is in the approaches that have been taken to address the critical technical issues to date.
- The emphasis is on industrially relevant parameters. The project team has achieved the BP 1 milestones.
- The project is incrementally improving SOEC performance.

Project weaknesses:

- The actual hydrogen generation rates need to be measured. This will be done as part of the transference number calculations in BP 2, but it is vital to the meaningful interpretation of the I–V curves for the tested cells that have been presented. There remains room for innovation in the approaches to decreasing the processing temperature and maintaining performance of the cells. Judging by the apparent cell shrinkage during firing, the fabrication of cells with 25 cm^2 of active area will be extremely challenging.
- The presentation needs improvement. The presenter used up most of his time before reaching slide 6. This limits the time available to view and understand the technical data. Despite being a major project goal, no information was reported on cost reduction—or even notional cost reduction for future cases. It is also unclear from the presentation how some technical barriers are being addressed.
- The project's weaknesses include the clarity of the presentation and the project's time management. The project team needs to articulate why specific project objectives are on the critical path for steam electrolysis, as well as what the size of the prize is.
- The targets for performance and stability may have been set too conservatively. The milestones have been met with ease. It may be possible to be more aggressive going forward.
- The endpoint of the project is the testing of a three-cell stack; there will be a long way to go after the project is completed.
- The team needs to better demonstrate the uniqueness of the project.

Recommendations for additions/deletions to project scope:

- The project team should be sure to probe the transference numbers and ensure that the materials are in equilibrium when doing so. This is not trivial but vital to getting useful data about the materials. There are some conflicting data in the field at the moment.
- Materials modeling is recommended to help guide and explain experimental results, which would better enable future research and development to build off the results of this effort.
- A small effort is recommended to determine the mechanical properties (e.g., fracture toughness) of the electrolyte.
- If time allows, the project team should increase stability test duration.
- Test conditions and characterization parameters are missing on most figures. No changes to the project scope are suggested.

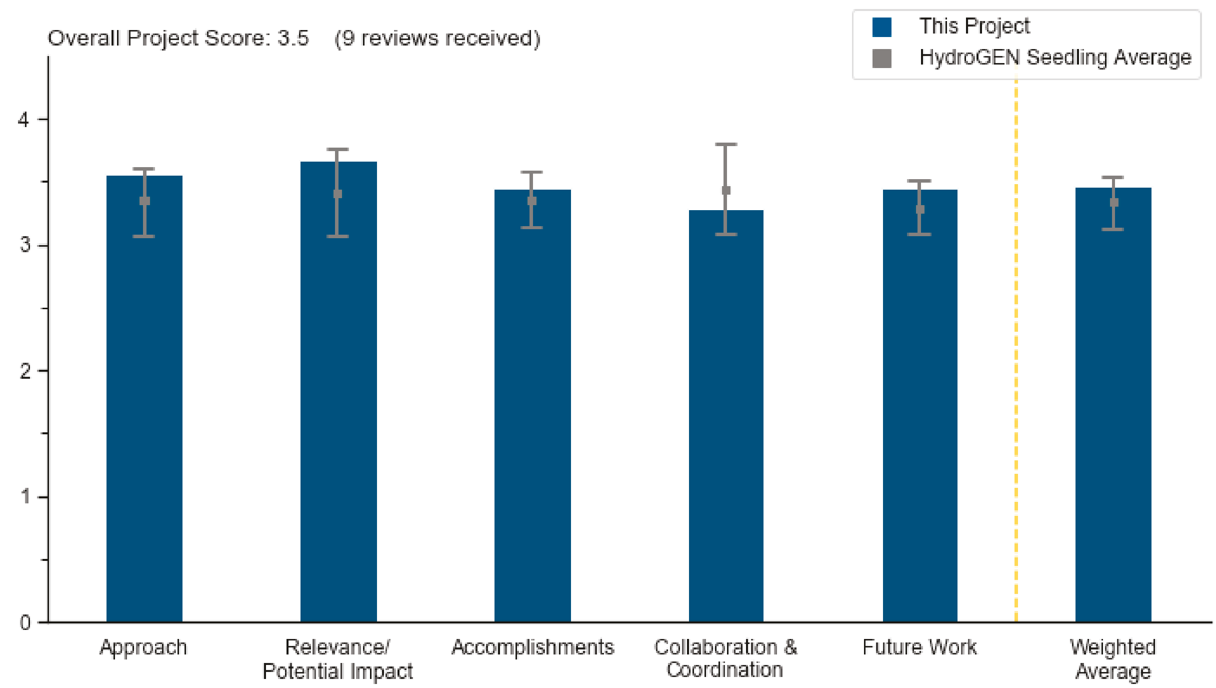
Project #P-153: Degradation Characterization and Modeling of a New Solid Oxide Electrolysis Cell Utilizing Accelerated Life Testing

Scott Barnett, Northwestern University

Brief Summary of Project

Solid oxide electrolysis cells (SOECs) have the potential for high electricity-to-hydrogen conversion efficiency, but these cells lack long-term stability, particularly at high current density, and the degradation mechanisms in SOECs are poorly understood. The project aims to develop mechanistic degradation models that realistically predict long-term SOEC durability, using input data from accelerated electrochemical life testing combined with quantitative microstructural and microchemical evaluation. Also, a promising SOEC cell type with high performance will be further developed. The understanding achieved by combining experimental results and theory will be used to guide improvements in long-term SOEC durability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach of this project brings much-needed fundamental analysis to SOECs to help explain a common electromechanical failure mode of the cells. Testing and theory are coupled in this work, allowing for far-reaching results that could enable insights into other material sets as well.
- This project is aimed at understanding and addressing degradation in SOEC electrodes, which will be essential for the successful development and deployment of high-temperature electrolyzers. The project approach includes an appropriate balance of theory, new materials development, and long-term durability testing.
- The project has a clearly defined research objective, which is the quantitative prediction of SOEC durability, and a plan to combine experiments and modeling to get there.

- The approach is outstanding, which is enough to perform the proposed work and fulfill the milestones and the U.S. Department of Energy's goals.
- There is excellent incorporation of theory and modeling from the Energy Materials Network resources.
- The approach seemed reasonable. The use of experimental data to validate the models is important.
- The approaches are reasonable and logical.
- The approach to this work seems sound. The modeling efforts support the hypothesis that overpotential is related to failure. A comprehensive set of materials is being tested. However, the current densities selected for study are seemingly out of place. To begin with, the approach slide suggests that the state-of-the-art current density is at 0.5 A/cm^2, yet solid oxide tests are often run at 1 A/cm^2. Some companies have reported that they could run above this current density, but they do not find it to be advantageous to do so. Failure studies were conducted at only 0.8 A/cm^2 and 1.6 A/cm^2. Studies should be presented at some midpoint current density as well.
- The approach is clear; however, it seems to be lacking other degradation mechanisms that could affect the model.

Question 2: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- Solid oxide electrolysis is a key component of DOE's emerging portfolio of hydrogen production technologies. Understanding cell degradation modes under the unique conditions intrinsic to solid oxide electrolysis (e.g., high steam contents on fuel electrodes and high overpotentials on air electrodes) will be critical for the successful development and deployment of large-scale solid oxide electrolysis systems. Thus, this project has high relevance and significant potential impact.
- The work is highly relevant to SOEC development because it combines experimental work with fundamental defect chemistry and the mechanics of the materials. The critical findings can educate other material sets used for SOECs—and likely for other devices as well. Calculating a critical overpotential for degradation that is informed by oxygen pressure and material strength should have far-reaching impacts, as it is relevant to more than just this set of materials.
- Solid oxide electrolyzer degradation is a key challenge to SOECs. It is important to understand the degradation mechanism in order to develop new materials and cell designs that can mitigate the degradation. The degradation models being developed here can be integrated into the cell, stack, and system models for better projection of stack performance.
- The highest-efficiency electrolysis approach is very relevant. The project is demonstrating substantial progress toward SOECs with long lifetimes.
- The project is highly needed for the prediction of long-term stability, which directly answers long-term stability goals.
- The project is relevant to high-temperature water electrolysis, addressing one of the failure mechanisms in SOECs.
- The project is focused on a critical path issue for steam electrolysis: durability.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program.
- The work is directly relevant to improving solid oxide electrolysis projects; however, it seems that the expected operating conditions for such projects are not in line with the tested conditions presented here.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project's accomplishments include the correlation of testing conditions (e.g., current density) with degradation rates and cell failure, stable cell operation at 1 A/cm^2 with the novel $Sr(Ti_{0.3}Fe_{0.7-x}Co_x)O_{3-\delta}$ (STFC) air electrode for 1,000 hours, and agreement between the model predictions and observed failures at the air–electrode/electrolyte interface.

- The elucidation of oxygen potential and fracture conditions is very important. It would be good to see the team include outside data in the analysis and make connections to groups that could provide more robust values for key physical properties, such as the fracture toughness of novel materials involved in the SOEC formulations.
- The project team has successfully completed the budget period 1 milestones. The project has demonstrated theoretical work that matches observed experimental failures and conveniently correlates with the available strength data for materials.
- The project has achieved outstanding progress and is on the perfect track to meet its milestones.
- The work is progressing as proposed and exceeding expectations year to year (the proposal was ambitious).
- The project goals are on track, with good progress made during the last year.
- The authors are making excellent strides toward achieving their goals. The go/no-go decision seems somewhat unclear. It is not clear whether they are aiming to predict cell degradation to within 30% accuracy or to improve degradation rates by a similar factor.
- The integration of a reference electrode was well done. This will be key in understanding the failure mechanisms. The identification that failure occurs when the overpotential is above 200 mV is important. It is unclear whether failure for this material set starting at overpotentials above 200 mV can be extrapolated to other material sets and other temperatures. Slide 11 says the voltage degradation is flattening out; however, the data do not support this assertion. It clearly looks like the voltage is continuing to degrade. The researchers should have continued the test. The modeling work examining the effect of operating conditions assumes a uniform current density across the cell. However, the current density will vary depending on the position in the cell. The model needs to account for the varying current density. It is well known that high current densities and high steam contribute to the degradation. This work is starting to quantify the levels at which cracking and damage occurs.
- It is not clear once the degradation is identified what the path forward is to prevent it; it could be material selection, careful selection of operating conditions, etc. It would also be beneficial to know how the cost of hydrogen will be affected, following the model's suggestions. Other aspects such as Cr poisoning effects on durability, processing parameters, and thermal cycling should be considered.
- The information presented does not convincingly demonstrate that overpotential or current density is the only root cause for cracks experimentally observed in the electrolyte that is formed experimentally by sintering. For example, other considerations may include defects in the electrolyte; defects in the sintered electrolyte could cause cracking under high current flow.

Question 4: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- The metal-supported SOEC testing at Lawrence Berkeley National Laboratory (LBNL) is an interesting start in the use of that cell structure. It will be insightful to see where the limitations and improvements of that approach will be. Cell testing at Idaho National Laboratory (INL) provides experimental data to educate the modeling work, in addition to the testing at Northwestern University (NU). This provides a third-party dataset that should help strengthen the signal of useful correlations and dampen noise of the contributions of confounding variables that are operator- or facility-related. The team specifically mentions utilizing and providing information for the Data Hub.
- This is a good start to engaging with the HydroGEN nodes and is set to grow. The project team is strongly encouraged to make plans to share and obtain datasets via the Data Hub. The team should be actively seeking datasets to further test and validate modeling.
- While the HydroGEN team seems well utilized, the authors may wish to reach out to industry experts to confirm their capabilities and operating conditions.
- The collaboration with the national laboratories is outstanding. It would be better if collaboration with other universities could be included.
- The interactions between collaborators are reasonable.
- No issues are observed; collaboration is proceeding as expected.
- The team members are fairly well coordinated.
- Communication with the benchmarking project is very important. The research team needs to get additional degradation data to compare the project theory with work done by others. INL has extensive data, so it was

surprising not to see this mentioned in the data used in the project. Considerable degradation modeling has been done by the Solid State Energy Conversion Alliance (SECA) for solid oxide fuel cells (SOFCs). While some conditions are different, there is some knowledge that could be gained from discussions with SECA participants at the National Energy Technology Laboratory (NETL), Pacific Northwest National Laboratory (PNNL), and West Virginia University, who have been doing modeling of SOFCs. NU is encouraged to reach out to them and see if there is possible collaboration or work that can be leveraged.
- It is not clear that there is much coordination between the work being done at NU and the work being performed by LBNL and INL.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work for fulfilling the milestones is outstanding. If the starting work for a new protonic ceramic electrolyzer system is initialized, it would be fantastic.
- The proposed future work is a logical continuation of the presented effort. Thermal cycling should be part of future testing and considered in the model.
- Continuing to study the correlation of critical overpotentials with lifetimes will be useful, especially for the different cell types.
- The researchers are looking to continue validating their models and expanding the materials set tested, which is excellent.
- The proposed future work seems well thought out and will provide excellent progress for this project.
- This is a very good use of DOE funds.
- The future work is commensurate with the stated objectives of the project.
- Reasonable future work is proposed.
- The proposed future work is logical, but more details should be given, especially regarding the approaches.

Project strengths:

- This project effectively combines theory and experimental results in an impressive fashion. The strength of the correlation between interface overpotential and mechanical failure has intuitive appeal from a fundamentals point of view, and it appears to be born out of a meaningful quantity of experimental data.
- The project provides a unique and effective methodology for predicting long-term stability based on the optimization of operating conditions and materials selection, etc. The success of this project will help the commercialization of high-temperature electrolysis significantly.
- The project is focusing on a critical issue for steam electrolysis. The team has a clear hypothesis and plans to test it, and team members are utilizing both modeling and experiments.
- The project's strengths include its focus on degradation and its novel electrode materials, which are showing promise.
- The project team is using a good combination of experiment, characterization, and theory to develop the degradation models. The researchers have a solid background in this area.
- There is good focus on a critical subject. This is a strong team, with good research expertise and seemingly strong modeling and predictive capabilities.
- The main strength of the project is the complementary expertise of the team (including NU, INL, and LBNL).
- The project is identifying operating conditions in which cell failure can occur.
- The model is providing reasonable predictions, even without fitting parameters.

Project weaknesses:

- There are no obvious project weaknesses yet.
- The project team needs to ascertain whether the very simplified Butler–Volmer approach is appropriate for all the situations that have been considered. The team needs to determine what is causing the steam variability during long-term testing. The cycling can be deleterious to the cells and could be a confounding variable that is not adequately controlled.

- The researchers are using a limited set of materials. They should reach out to INL and SECA, who have additional data that may be useful. The models have some assumptions that need to be adjusted. For example, they are assuming constant current density across the cell. This is a poor assumption. There are additional SOEC models that can describe how current changes, which could be used to give better results. PNNL and NETL have models that can do this for SOECs.
- The project team needs to confirm operating conditions for current density. It is suggested that the project do a wider range of failure tests at different current densities and reach out to industry for review and input.
- The project team is not getting as much out of HydroGEN as it probably could.
- The model seems to target only one degradation mechanism.

Recommendations for additions/deletions to project scope:

- If the initial study on proton-conducting SOECs were added, the scope would be fantastic.
- The project team should consider including additional elements in the model, e.g., fuel effects and current density gradient. The project should verify that, as the model gets more detailed, it does not turn out that the early promising results were just fortuitous.
- The project team should relate these degradation processes to their effect on limiting the efficiency of SOEC operation under different conditions (e.g., temperature and reactant flows).
- Test conditions and characterization parameters are missing on most figures.

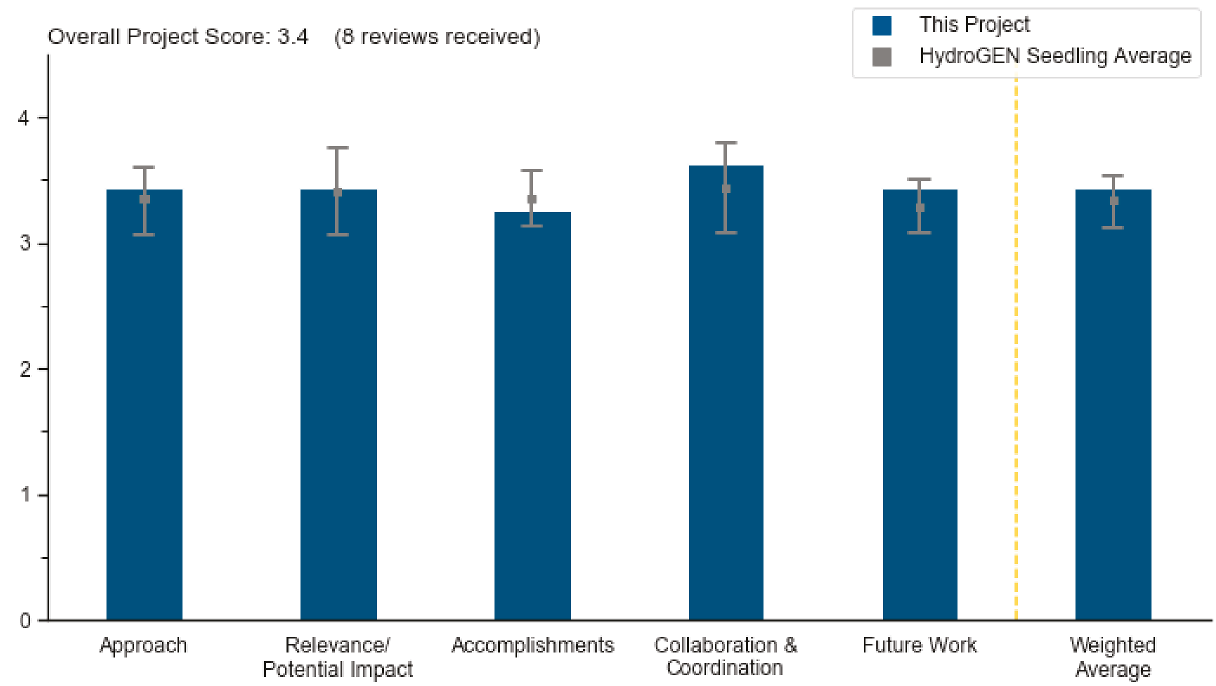
Project #P-154: Thin-Film, Metal-Supported High-Performance and Durable Proton–Solid Oxide Electrolyzer Cell

Tianli Zhu, United Technologies Research Center

Brief Summary of Project

This project is developing a thin-film, durable, metal-supported solid oxide electrolysis cell (SOEC) using a proton-conducting electrolyte at targeted operating temperatures of 550°C–650°C. This advanced SOEC will provide a highly efficient, cost-competitive high-temperature electrolysis process for hydrogen production. Initial efforts focus on demonstrating the feasibility of the proposed concept by further advancing metal-supported single cells based on work completed previously for solid oxide fuel cell (SOFC) applications. Cell fabrication, especially electrolyte deposition via suspension plasma spray (SPS) processes, is a focus.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The project has a reasonably comprehensive strategy to develop a lower-cost fabrication approach to proton-conducting SOECs (P-SOECs), building off of previous SOFC experience. The approach is integrating fabrication, characterization, testing, and modeling.
- The project has a viable approach, low-cost production and assembly, and an opportunity for a high-durability system.
- The project's approaches to addressing the identified technical barriers are logical and appropriate.
- Plasma spray for proton-conducting membranes may solve several of the manufacturing challenges that are associated with this technology. By operating at temperatures less than 700°C, the team may be able to use lower-cost materials and have lower degradation.
- In general, the proposed approaches are excellent. If the project adds an approach to further improve SPS fabrication of the dense electrolyte and the porous electrode, it will be better.

- There are some compelling reasons to consider proton-conducting ceramic electrolytes for electrochemical water splitting to produce hydrogen. The temperatures are high enough that precious metals are not required in the electrodes, yet not so high that thermal integration is challenging. The ionic conductivity of proton-conducting ceramic electrolytes at 600°C can be similar to that of oxygen-ion-conducting ceramic electrolytes at 800°C. The metal-supported, thin-film electrolyte SOEC architecture that is targeted in this project makes a lot of sense for minimizing resistance (and power consumption) during electrolysis. A significant challenge is that barium-zirconate-based proton-conducting ceramics require very high sintering temperatures for densification, which makes it difficult to achieve high-density electrolyte architectures. The approach being pursued in this project is even more challenging because the barium-zirconate electrolyte coatings need to be sintered under conditions that are compatible with the porous metal support. There is a concern that it will be extremely difficult to achieve sufficiently high electrolyte density while simultaneously achieving proper morphologies of the metal support and fuel electrodes. Another challenge is that it is not easy to design electrochemically active and stable electrode materials for operation at 600°C.
- The overall approach is very complete and promising; however, the plasma spray might be a risky technique to control all parameters.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- Solid oxide electrolysis is a key component of DOE's emerging portfolio of hydrogen production technologies. If this project is successful, a promising metal-supported cell technology will be available for subsequent development of stack technology and ultimately large-scale solid oxide electrolyzer systems. Therefore, this project has relevance and a significant potential impact.
- Materials development for water splitting is relevant to DOE work. The state of the art for SOEC performance seems low compared to what is in other presentations. There are several groups achieving >1 A/cm^2 at <1.4 V and 800°C. The target of 4 mV/1000 hours seems reasonable. If cells can be manufactured at the projected cost in low volume, this will accelerate SOEC commercialization.
- The achievement of the project objectives can align well with the DOE target for long-term, low-cost, and efficient high-temperature electrolysis. The metal-supported P-SOEC represents one of the most promising research efforts among SOECs.
- This project relates very well to the goals of improving solid oxide performance as it pertains to DOE targets. The authors have also included a suggested cost analysis for hydrogen produced from the proposed system. The low costs do seem highly dependent on the electrical cost being $0.04/kWh, which is very low for electrical costs.
- The project is relevant to high-temperature water electrolysis that uses an alternative to traditional fabrication processes.
- The performance, durability, and stated costs indicate the potential for a viable electrolysis system.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program.
- It is not clear that manufacturing cost is one of the top barriers to SOECs. It would be beneficial to see a stronger connection to durability. However, the team is clearly leveraging and contributing to the HydroGEN Consortium.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- There are substantial and meaningful results across the different research thrusts. The project has not been all smooth sailing, which usually means the team is working on the important parts.
- The project has made excellent progress.
- The project goals are on track, with good progress made during the last year. It is not clear how far the present system is from the assumed conditions for hydrogen cost. The team needs to consider what needs to

be achieved to reach a $1.35/kg cost target for hydrogen. The project takes a holistic approach in addressing different aspects for cell fabrication. Thermal cycling should be a part of the stability testing.

- Thus far, the results are promising and meet the Phase I targets. However, it is noted that the steam concentration required to achieve some of these targets is very low, less than 20% H_2O. Ideally, this concentration would be higher for large-scale operating.
- This project has made progress, but it looks like the issues to be addressed are quite challenging.
- The project fulfilled its go/no-go milestone. The electrolyte property can be further improved.
- The 3% steam content for some of the tests seems very low and does not represent what a real system would experience. It would be helpful if the presentation included the flow rate and steam utilization. If the project is using a high flow rate and low utilization, the steam content may not be a problem. However, a high flow rate and low utilization may skew the performance, making it look better than it actually is. The data indicate that as the steam content was decreased, the performance increased. This was surprising since the reverse is true in most of the literature. The researchers should explore this result, as it could have significant impact on the operation of the stack. The use of a metal support limits how high the sintering temperature can be. Therefore, it is not surprising that defects in the electrolyte are apparent, since a low sintering temperature is being used.
- Although the Phase I go/no-go milestone and performance target was met, the density of the SPS-processed electrolyte is not sufficient and contains unreacted $BaCO_3$. Also, the performance target was met with a fuel-electrode-supported cell rather than a metal-supported cell.

Question 4: Collaboration effectiveness

This project was rated **3.6** for its collaboration and coordination with HydroGEN and other research entities.

- This project has a strong team involving an extremely qualified consultant, the University of Connecticut, as a subcontractor and several HydroGEN national laboratory nodes. The ultimate SOEC technology that is being developed will require contributions from all of these team members.
- This project is one of the best examples of a team engaging multiple HydroGEN nodes to make key contributions to the project.
- The collaboration appears vibrant and effective. No issues are apparent.
- The project team seems well suited, and work seems to be progressing fluidly.
- There are good interactions occurring with the nodes.
- The team has outstanding collaborations. If the electrochemical modeling information can be used as guidance for other processes, it will be better.
- The coordination between the team members has been effective, but closer coordination may be needed between the fabrication and material development team members.
- The collaboration seems to be well organized. The project is using the HydroGEN nodes well. Pacific Northwest National Laboratory and Boston University are listed as collaborators, but they are not on the project. The team should clarify how those institutions are contributing.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The future work seems to cover all the steps necessary to improve this technology.
- The proposed future work is consistent with the project objectives. The major focus should be on increasing electrolyte density and achieving the performance target on a metal-supported cell.
- The focus is on production optimization and durability testing. This is where effort should be spent. More cost information is desired; this is in large part as a result of the very enticing cost numbers that were reported. To be candid, the SPS process seems almost too inexpensive. Future work should indicate the assumptions related to the process scale used to estimate cell and stack production costs.
- In general, the proposed future work is excellent. If the team can improve the clarity for targeting the remaining challenges, it will be better.

- The proposed future work is a logical continuation of the presented effort. Thermal cycling should be a part of future testing.
- The proposed future work is appropriate; however, some details on the proposed approaches are needed.
- It is hard to judge the proposed future work based on the brief outline in the presentation materials. It would be helpful to see a milestones chart for the current phase.
- The use of a metal support limits the sintering temperature, resulting in defects in the electrodes. The researchers do not give a strategy for how they will develop a dense electrode layer without the high-temperature sintering required. The future work focuses on the issues of electrode densification and durability. It would be good to see the details of the cost analysis.

Project strengths:

- The project's strengths include its collaborations and its leveraging of the HydroGEN nodes. The team has a strong research plan and is working on valuable objectives (e.g., steam electrolysis, P-SOECs).
- The project has a very strong, collaborative team, and the approach of metal-supported, thin-film P-SOECs is unique. SPS fabrication is promising and may be cost-effective.
- The project's strengths include the development of a unique fabrication technique that can lower fabrication costs.
- The project is well organized, with excellent results to start. The team included a cost analysis with promising results.
- This is a strong team. Plasma deposition is an interesting approach. The project is using the HydroGEN nodes well.
- The project's main strength is in the approaches being conducted to address the technical barriers.
- The project has the potential for a viable system that meets DOE targets.
- This is a strong team. There is a potential for lowered costs.

Project weaknesses:

- The project has no major project weaknesses, although it appears that the issues are quite challenging, considering the level of effort.
- The team may need to consider further processing steps or different fabrication techniques if sufficient densification is not achieved.
- The team should consider the cost of electricity for analysis. The team needs to explain or increase the steam concentration for the feed.
- The researchers need to test their cells with more realistic steam levels and steam utilization. They are using a metal support with materials that require high-temperature sintering. This will be very difficult to solve.
- There is a focus on fabrication versus durability.
- The cost estimations appear too optimistic. Greater detail should be reported.
- There is extreme technical difficulty associated with achieving project success.

Recommendations for additions/deletions to project scope:

- The team needs to focus on achieving high electrolyte density in the final metal-supported platform.
- There should be an increased level of detail regarding cost estimation.
- No additions or deletions are suggested.

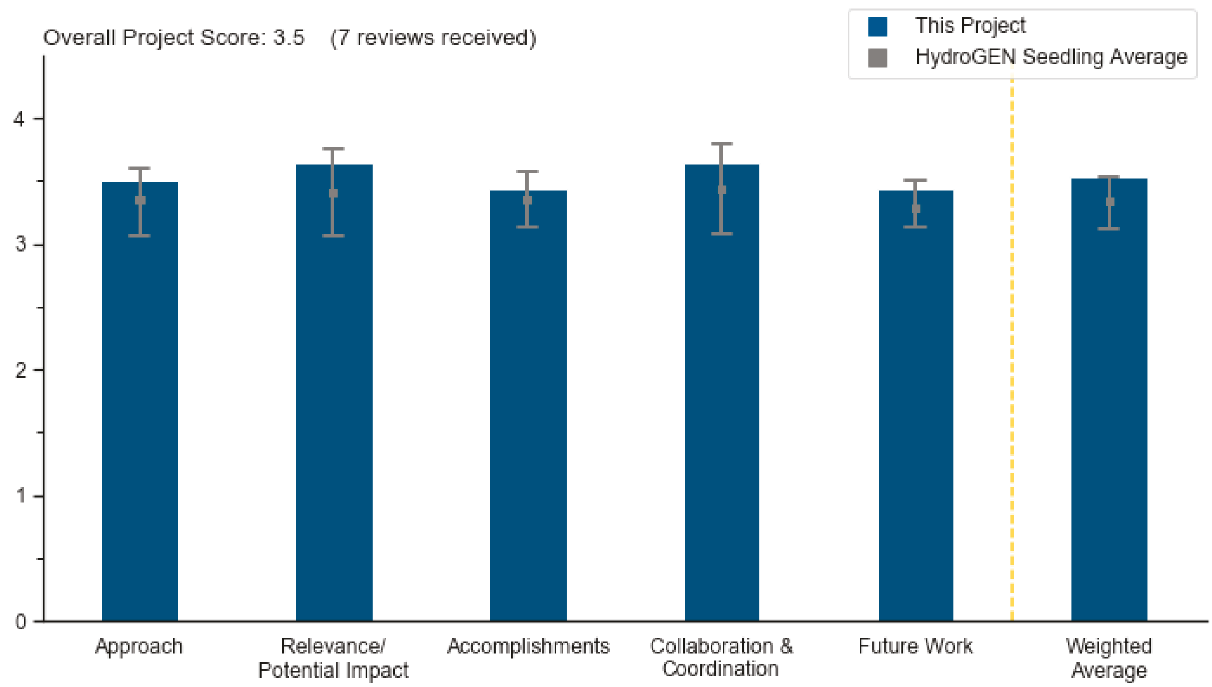
Project #P-155: High-Efficiency Polymer Electrolyte Membrane Water Electrolysis Enabled by Advanced Catalysts, Membranes, and Processes

Kathy Ayers, Proton OnSite

Brief Summary of Project

This project will develop an advanced, highly efficient polymer electrolyte membrane water electrolysis (PEMWE) membrane electrode assembly (MEA) by addressing membrane, catalyst, catalyst layers, and their interfaces. Four areas affecting cost and efficiency will be developed: (1) thinner membranes, (2) lower catalyst loadings, (3) optimized gas diffusion layer and porous transport layer materials and structures, and (4) increased operating temperature. Successful demonstration and integration of these four areas require a deeper understanding of the scientific and technical aspects of PEMWE MEAs. Proton Onsite will partner with University of California, Irvine, and Oak Ridge National Laboratory (ORNL)—with support from the National Renewable Energy Laboratory (NREL) and Lawrence Berkeley National Laboratory (LBNL)—to integrate advanced cell designs and materials and fundamentally characterize performance.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The general approach of this project is to improve catalyst materials, reduce membrane thickness, and increase operational temperature. This is very reasonable for achieving better electrolyzer efficiency and lowering the cost of hydrogen production. Based on results obtained previously, the team is continuing studies on durability, membrane material hydration and down-selection, the electrode preparation process, and advanced characterizations. These are all appropriate for reaching the project's final goals.
- Thinner membranes and alternative catalysts have shown promise for the stable operation of polymer electrolyte membrane (PEM) electrolyzers with improved efficiency. This project advances material performance and integrates components, while leveraging fundamental characterization to understand and

push design limits. The project is taking a multifaceted approach to understand the effect of catalyst, electrode, and membrane performance on overall cell performance. The issues that need to be addressed are identifying active and durable membranes with thicknesses below 50 microns, reducing the catalyst loading by a factor of 10 while avoiding catalyst dissolution at low loading, synthesizing and integrating higher-activity oxygen evolution reaction (OER) catalysts into the anode, understanding how the electrode and substrate porosity affects performance, refining the cell architecture, and completing the imaging and characterization of the electrode after operation. The goal is to reduce catalyst loading by a factor of approximately 10 and achieve hydrogen production at or below $2/kg.

- PEM electrolyzers are still based on rudimentary catalyst-coated membrane concepts, with thick membranes, high catalyst loadings, and platinum-group-metal (PGM) coatings on almost all components. To reduce cost and increase efficiency, membrane thickness is the easy aspect to tackle. By combining that with tuning the catalyst composition and loading, Proton OnSite and the project partners are pursuing the best and quickest approach to achieve $2/kg.
- This project (and the U.S. Department of Energy) is solving a huge problem for the hydrogen fuel cell industry: the capital expense around electrolysis systems. Ayers and the team are taking a "holistic" approach and leveraging fuel cell research, mainly decreasing membrane thickness and catalyst loading. This is very ambitious, considering that funding levels are fairly low. This is also supporting others' research. It is not clear why the membrane hydration versus temperature is being studied. It seems that the size and cost of the heat rejection system would also have to be included for fair assessment. Some more clarification would be helpful. The team has done a nice job with the physical characterization and modeling attempt.
- The overall approaches include optimizing the catalyst component, reducing membrane thickness, and improving the structure of the porous transport layer. These approaches address two critical barriers: (1) long-term durability of the electrolysis system and (2) higher defect sensitivity with advanced materials and operation. The approaches to addressing the barriers are effective and closely correlated with each other. The interface characterization that is being done with electrode cross-section imaging reveals the interface between the catalyst layer and the porous transport electrode. The obtained data provides the information needed for MEA system modeling. The simulation model indicates that the relatively thinner membrane can reduce overvoltage of the cell, which supports and is evidenced by the MEA test results. Meanwhile, the thinner membrane's impact on stress and creep is also understudied. The weakness of the catalyst design approach is the reliance on precious group metals, which limits further reduction of the capital cost of the water electrolyzer. It would be better if the team would clearly state the way the current approach could lead to the ultimate deliverable (an advanced electrolysis stack producing hydrogen at 43 kWh/kg and $2/kg H_2).
- The selected approach to evaluate the performance mechanisms for water electrolysis emphasizes a methodical and logical structure. The membrane, coatings, and modeling work done during the second year progressed logically from the catalyst and modeling work done during the first year. It would be preferred to see some discussion of sustained performance. Short-term performance during an innovation activity may not extend into a deployed system. For many electrochemical systems, a 500-hour test barely qualifies as a fabrication check-out test. While such testing may not be in the project scope, it would be beneficial to have some discussion on how the performance gains from this research activity can be transferred to a fielded system.
- Thinner membranes and higher operating temperature are a good opportunity, as long as the durability does not suffer.

Question 2: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- When considering the market maturity of PEM electrolyzers, it seems that, of all electrolyzer types within HydroGEN, PEM might be the only one able to reach $2/kg in such a short period of time. When considering the proposed approach and current results, it seems that this project shall be the only one with proper impact, and therefore it has the largest potential among the projects within HydroGEN.

- This project has the potential to address outstanding cost and performance issues with electrocatalytic hydrogen evolution by evaluating how each component affects overall system performance. For example, results have shown that membranes composed of short-chain polyfluorosulfonic acids with 50–90 micron thickness demonstrated change in hydration at varying temperatures, compared with other compositions. This result implies improved stability and mechanical strength, as well as superior current density from electrolyzer cells constructed with 50- and 90-micron-thick membranes. Additional studies with catalyst dispersion have identified the optimum ionomer dispersants needed, which will prevent catalyst agglomeration and boost overall performance. In addition, both the distribution on the catalyst and electrode porosity need optimization. These studies will identify how to improve overall efficiency and allow for cost-effective hydrogen production through electrolysis.
- This project aligns well with the objective of the DOE hydrogen production target ($2/kg of hydrogen, 43 kWh/kg of hydrogen). As noted in the presentation, the final deliverable is an advanced electrolysis stack producing hydrogen at 43 kWh/kg and at costs of $2/kg. If successful, the project would have a huge impact since the DOE ultimate target would be reached.
- The potential impact is significant, as PEM electrolyzers are well understood and the target decrease in specific energy consumption can have an immediate benefit, which is relatively straightforward to translate to larger systems with higher technology readiness levels.
- The research has high impact on several levels; it is drawing attention to the issues around decreasing the cost of electrolysis systems. The project is also being open and not secretive with the results, which is also very helpful and broadly strengthens the research community and technology.
- This activity both generates new studies and verifies historical characterization studies of the water electrolysis process. The resulting data enables understanding of the process in sufficient detail to adjust the design and fabrication trade space to craft the required performance. It increases the probability that water electrolysis will achieve the production efficiencies and rates from that crafted performance.
- This project aligns well with the targets of the DOE Hydrogen and Fuel Cells Program.

Question 3: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project has shown solid data supporting the advancement of the PEM MEA. The impact of membrane thickness on the swelling of the membrane in the hydrated condition is revealed. The 50-µm-thick membrane demonstrates good stability in hydration temperature change. Additionally, the performance of a series MEA with varied thickness is compared. The MEA based on a 50-µm-thick membrane shows the best performance. The optimal ionomer-to-carbon ratio in the system has been found to be 0.05. The novel ink and coating process has been developed, during which the OER catalyst is directly coated on the porous carbon layer by Meyer rod. Characterization of the porous transport layer and cell modeling have revealed the shape of an optimized cell. LBNL is developing a novel fixture that enables the creep study of the membrane and a stress study with the presence of water.
- The project has shown good progress to date. The quarter one (Q1) milestone has been met by understanding the impact of membrane hydration on electrolyzer current density, and short-chain 50-micron-thick membranes have demonstrated current densities over 2 A/cm^2, below 1.9 V, and between temperatures of 50°C and 100°C. The impact of ionomer content on catalyst agglomeration and electrode porosity has been evaluated, and computational modeling shows excellent agreement with the experimentally verified performance. Long-term testing shows relatively stable performance in excess of ~130 hours. The project's future milestones include the following: in Q2, the team will be down-selecting the membrane based on a hydration-state study of mechanical and chemical properties; in Q3, the in operando electrolysis cell will be operational, and two best-of-the-class MEAs will be characterized under two current densities; and in Q4, the go/no-go point of demonstrating 500-hour durability will be achieved. This is the most important milestone because it will allow for the production of hydrogen at $2/kg.
- The improvement in millivolts with the thinner membrane is significant. The project's excellent microstructural analysis is very helpful in correlating the observations. The initial short-term durability data are promising.

- Despite the low funding, the research team has touched on several important parameters affecting electrolyzers and is trying to develop a cohesive understanding. The team has made progress on many fronts.
- This activity is slowly and methodically progressing toward understanding a complex system. Expecting radical advances from this approach undervalues the benefit gained from not missing a key element along the way.
- The project's progress is excellent, but the target is still somewhat far to reach, considering the results presented. However, if proper MEA configuration is found (i.e., thin membrane, catalyst composition, and loading), the project should be able to reach its goals within the time proposed.
- The progress made in fiscal year (FY) 2019 so far has not been as significant as what was achieved in FY 2018. (1) One Q1 milestone was to "understand [the] impact of membrane hydration conditions on electrode performance." While MEA polarization data were presented with membranes hydrated under different temperatures, no deeper analysis was done to check and separate the over-voltages due to membrane conductivity versus electrode performance. In addition, because the MEA tests were conducted at only one temperature (50°C) and not at the targeted 80°C, it may be too early to conclude this study. (2) The delay on the hydration-state study of mechanical and chemical properties (a Q2 task) will postpone the membrane down-selection and further delay Q3 and Q4 tasks. (3) Based on NREL's MEA test results and Proton Onsite's initial data from FY 2018, there is clearly a challenge in maintaining a performance of 1.7 V at 1.8 A/cm^2 for 500 hours. It would be great if the team could come up with potential countermeasures in time to meet the Q4 go/no-go milestone.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The project is effectively leveraging collaboration with other institutions. For example, LBNL is testing hydrated-membrane tensile strength. NREL is developing catalyst ink, evaluating how particle agglomeration scales with ionomer, and helping with catalyst construction. The University of California, Irvine (UC-Irvine) is imaging the catalyst layer distribution in the porous transport layer and comparing it with catalyst on membrane. Combining all these efforts will provide an overarching view of how each component of the cell affects performance. These insights will lead to the optimization of each parameter to maximize cell performance.
- This project well leverages the strengths of the individual partners to characterize the performance and material properties of the elements within this complex system. By utilizing the Energy Materials Network (EMN) nodes as a project backbone, the project may have results that are more effectively disseminated across the EMN network, thereby accelerating research progress.
- The project demonstrates good collaboration along MEA fabrication (Proton OnSite), MEA stress testing (LBNL), novel ink development (NREL), characterization of MEAs (the National Fuel Cell Research Center [NFCRC] at UC-Irvine), and cell modeling (LBNL). It would be great if there were a page that clearly stated the collaboration framework and the shared duties.
- The collaborations within the project team and with HydroGEN appear to be close and productive.
- The team is well selected and working well together, as evidenced by the high productivity.
- The partners' efforts are well integrated into the project.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work is generally good and is working toward achieving the planned targets. Parallel efforts shall be made to consider various strategies and prepare back-up options for addressing the durability challenge. This will be critical for the project go/no-go decision, as the testing cycle (500-hour durability) is very long.
- The proposed future work is well organized and clearly shows the duty-sharing of all collaborators. The optimization of the cathode for the electrolyzer is also important. It is suggested that the team also include further optimization of the cathode (e.g., lowering the precious-group-metal loading on the cathode) in

future study, since the cost of the electrolysis stacking system is also an important aspect, in addition to the operational efficiency.
- This is very good future work, although the team might focus more on reducing catalyst costs and doing lifetime testing. It is not clear if there are any plans to study the effects of start–stop cycling that might occur due to intermittent renewables.
- In general, the proposed work will suffice within the concept of this proposal. It would be beneficial to evaluate the X-ray testing outside of the Ohmic region, should the OER become interesting. It would also be beneficial to identify more clearly the selection criteria for the down-selected materials. Efficiency and durability tend to be inversely related, so the balance between the two should be clarified. That clarification may reveal a need for additional endurance or durability testing, pending available resources.
- The project seems to have a good plan moving forward, but at this point the researchers are still trying to understand how the different components work together and affect the overall performance. Future plans include collaborating with the following partners: (1) LBNL, to evaluate membrane hydration, thickness, and temperature; to incorporate microscale features, including catalyst connectivity; and to study the bubble formation effect on current density; (2) NREL, to construct electrodes with low-catalyst-loading inks and provide them to Proton OnSite for testing; (3) NFCRC, to do in situ X-ray radiography at operating conditions of 1–2 A/cm^2; (4) ORNL, to do post-reaction analysis to evaluate catalyst migration within the electrodes and membranes; and (5) Proton OnSite, to tune cell design and conduct operational tests of screened catalysts and components received from NREL for down-selection based on efficiency and durability.
- This is a very effective and relevant use of HydroGEN nodes. The durability metrics should be defined.

Project strengths:

- This project benefits from extensive collaboration that will address multiple aspects of cell performance. The project has shown promising long-term performance, and accelerated stress tests are addressing how the catalysts will degrade at low loading under realistic, dynamic conditions. The team expects to reduce the PGM loading by a factor of 10 compared to commercial electrolyzers, but this may lead to increased catalyst degradation.
- The project's strengths include the leadership of Proton Onsite in the field of PEM electrolyzers, as well as its very well-defined approach. The project team has the combined expertise to perform materials science and reach the proposed goals, and it has vision with regard to specific challenges related to durability testing.
- This project is methodically and systematically characterizing the elements of a complex system. With this process, the risk of missing a key performance parameter is significantly lower. This risk has been further reduced by the team's utilizing acknowledged experts to execute this process across an established collaborative mechanism.
- The project team and involved HydroGEN researchers are very capable and have a wide range of expertise to tackle different types of technical hurdles. Proton OnSite's experience in electrolyzer production is very important in promoting the transfer of research results to commercial products.
- The project demonstrates the promising potential for the newly developed MEA. The project also shows integrated collaboration among all participating teams.
- This project has a good approach, with good use of the national laboratories' capabilities; it is showing promising progress.
- This is a very well-organized team doing focused work. The researchers are making good progress.

Project weaknesses:

- The only weakness of the project is its reliance on high-loading platinum group metals (PGMs).
- The project does not have enough funding to make much progress. It is a strength to leverage fuel cell research, but it might also be a deficit, as it brings in the same groupthink.
- It will be difficult to demonstrate meaningful durability data, considering the time given for the project. The project's weaknesses also include the integration of new membranes with novel concepts of catalyst layers and the conflicts with existing and traditional stack/system designs.

- The durability of the 50-micron membrane was tested to only 140 hours. The durability plot on slide 17 lacks current density information (based on slide 9, a best guess would be 1 A/cm^2), as well as catalyst-loading information; it is unclear whether this represents 10x lower loading. The progress toward the 43 kWh/kg goal has not been explicitly reported.
- This project includes limited discussion on how the data products will transition from the laboratory to field systems with large-scale hydrogen capabilities. Endurance and operational life appear to be low priorities.
- The project team does not seem to be responding to suggestions from previous reviews. The speed of the transfer and translation of the project results to Proton OnSite's MEA preparation process is slow.
- This project may be trying to address too many challenges at once, rather than critically attacking a few specific aspects of cell performance. Continued progress will determine whether the scope should be scaled back to address fewer challenges within one project.

Recommendations for additions/deletions to project scope:

- The team should include operational process fluid pressure as a variable when evaluating the bubble formation of current-density limitation. The team should also include endurance testing beyond 500 hours, where feasible, to characterize the persistence of already identified performance gains. The team should clarify the trade space between efficiency and durability when implementing the catalyst and component down-selection.
- It would be helpful to clearly show the pathway that leads to the ultimate goal of proposed hydrogen production. The team may consider including further optimization of the cathode in an effort to lower the cathode precious-group-metal loading.
- The project focuses on PEM electrolyzers that use precious-metal-based catalysts. As the ultimate goal is to reduce PGMs by 10 times, it would be better to add specific targets for catalyst loadings and to report in the future if progress is made in this direction.
- A chart should be included that shows the progress made toward project goals. The team should also define durability metrics and extend the durability testing of promising MEAs.
- The project is inching around some key issues. It might be useful to do a "lean innovation" or agility study to see what can be done quickly to have high impact and reduce costs, instead of waiting until 2025 for PEM electrolyzers to proliferate.

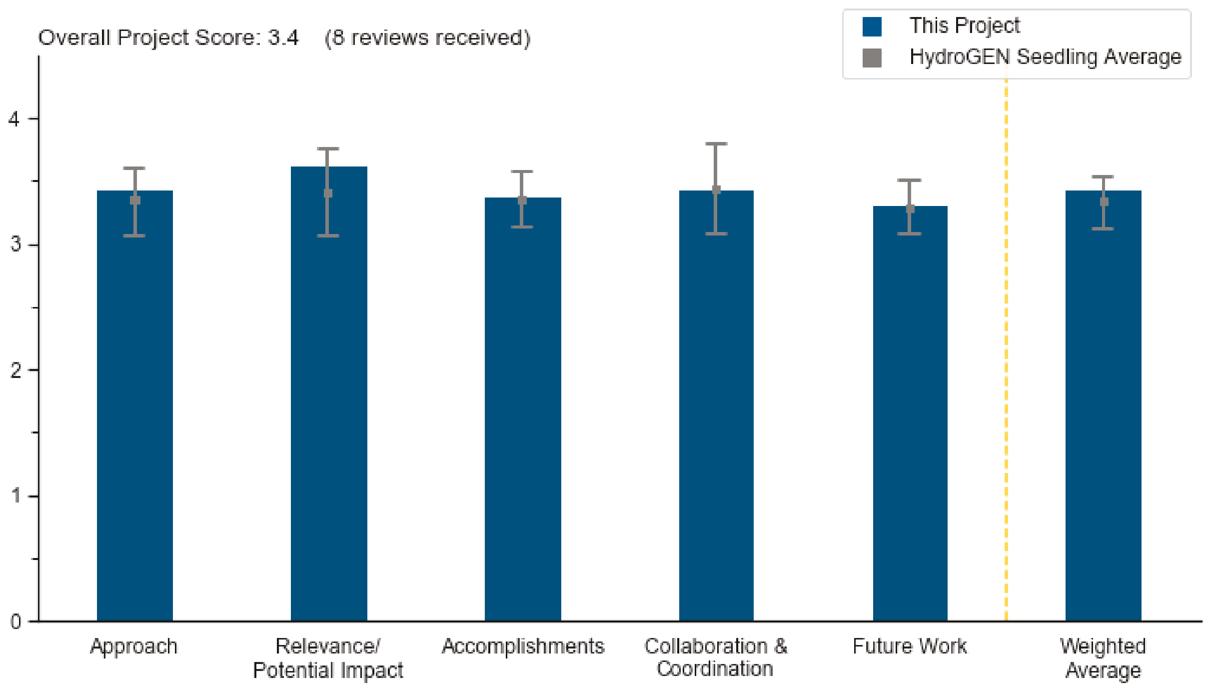
Project #P-156: Developing Novel Platinum-Group-Metal-Free Catalysts for Alkaline Hydrogen and Oxygen Evolution Reactions

Sanjeev Mukerjee, Northeastern University

Brief Summary of Project

The aim of this project is to develop (1) stable, high-conductivity, and high-strength anion exchange membranes (AEMs) and ionomers, (2) stable and active platinum-group-metal-free (PGM-free) catalysts for hydrogen evolution reactions (HERs) and oxygen evolution reactions (OERs), and (3) high-performance electrode architectures that together can begin to achieve the low-cost advantages of AEM electrolyzers. This effort is focused on materials development by tailoring synthesis and composites with supporting efforts in computation and characterization. The project work—and collaborations with the University of Delaware (UD), Advent North America, the National Renewable Energy Laboratory (NREL), Lawrence Berkeley National Laboratory (LBNL), and Sandia National Laboratories (SNL)—strives to enable a clear pathway to achieving hydrogen costs of less than $2 per kilogram, with an efficiency of 43 kWh/kg, via AEM-based electrolysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- This is a great project that uses much electrochemical, materials, modeling, and synthetic knowledge to provide a path to a Pt-free electrolyzer system. Very logical materials were chosen based on fundamental electrochemical knowledge. Appropriate characterization methods are chosen.
- This project intends to tackle all major technical barriers to efficient hydrogen production from an AEM electrolyzer. While OER and HER catalyst development appears to be the center of the project, the team also targets improved AEM material for electrolysis at higher temperatures, which can further improve electrode performance. This strategy of combining multiple opportunities for improvements can be very effective for achieving higher overall system efficiency.

- The project divides the performance conundrum into logical portions for each group in the team to address, according the strength of the specific group. The issues are clearly identified with appropriate measurement techniques to evaluate progress. By appearances, the work this year focused on the Northeastern University (NEU) Center for Renewable Energy Technology's identifying and characterizing three potential HER catalysts and one OER catalyst, UD's characterizing an alkaline membrane, and LBNL's and SNL's modeling work.
- AEM electrolyzers suffer from a lack of suitable membranes and stable, PGM-free anode catalysts. This project aims to produce stable AEMs, stable PGM-free catalysts for both HER and OER, and optimized electrode architectures. The project's success will help to realize the goal of <$2/kg of hydrogen production. The principal investigator (PI) from NEU will focus on catalyst development to produce PGM-free OER and HER catalysts. HER catalysts will be synthesized by embedding metals into nitrogen-doped carbons. OER catalysts will be synthesized from double-layered metal (oxy)hydroxides, supported on Raney nickel. Performance will be evaluated in half cells and full electrolyzers, and in situ Raman spectroscopy and X-ray studies will be conducted to understand the evolution of the catalysts' oxidation state and structure. The collaborators at UD will design new membranes and ionomers, and Advent North America will focus on electrode fabrication. National laboratory collaborators will facilitate MEA preparation and testing (at NREL), small-angle scattering measurements and modeling (at LBNL), and modeling of interfacial phenomena (at SNL).
- PGM-free catalysts are needed to lower the cost of AEM electrolyzers. This effort is well integrated with the HydroGEN consortium network.
- The approach was highly relevant for overcoming the barrier of AEM electrolysis. The project team has identified key barriers and aims to develop active PGM-free catalysts for electrochemical reactions (HER/OER) and stable electrode structures for AEM electrolysis. Although the objectives appear to have been met, the work is quite ambitious and too broad.
- The presentation mentioned only the AEM barrier on slide 3, while the catalyst is also a critical barrier. The approach includes the development of a new catalyst, novel membrane, and novel electrode, which covers the key features of a projected state-of-the-art AEM electrode.
- The metrics defined to reach the proposed performance make sense only if the use of a support electrolyte is initially defined. If it is, the metrics need to be measured under a specific electrolyte support concentration that boosts overall cell performance.

Question 2: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- As the alkaline electrolysis process currently dominates the market, any innovation that decreases cost, increases performance, or increases life reduces the cost of hydrogen production. This project addressed both the HER and OER reactions that generate ions, as well as anionic conduction rates through the membrane. Success in any of these areas has the potential to reduce hydrogen production costs.
- Low-temperature electrolysis will play a key role in affordable, sustainable hydrogen production in the future. Although AEM electrolysis is at an early stage of research and development (R&D), it is a strong candidate among low-temperature electrolysis technologies. The team's efforts align well with the goals of the DOE Hydrogen Production R&D subprogram.
- This project is closely relevant to HydroGEN's mission to produce hydrogen at low cost and through sustainable processes. As the majority of the cost of electrolytic hydrogen production is from the electricity cost, targeting system efficiency improvements is a good strategy and can have significant impact on the success of the DOE Hydrogen and Fuel Cells Program.
- This project is very relevant to the goals of the HydroGEN consortium. The project aims to develop thermally stable AEMs using earth-abundant and cheap transition-metal catalysts. Success will drastically reduce the costs associated with AEM hydrogen production.
- The goal of the project aligns quite well with the DOE's ultimate hydrogen production target. If successful, the project will be revolutionary since all of the catalysts are PGM-free.

- If successful, this project would provide new low-cost materials for electrolyzers. The work is being done at universities, so it is likely to be published. The materials are well characterized and well understood, so they will provide a baseline for more improvements.
- AEM electrolysis is a promising technology to reach consistent investment cost reduction for electrolytic hydrogen. However, AEMs for electrolyzers have poor performance associated with low durability, which makes it very difficult to reach such an ambitious target. However, the authors are proposing some very interesting AEM concepts, and, if linked well with very active catalysts as demonstrated here, such a target could eventually be achieved within the project. Therefore, if properly pursued, this work could have great impact on the field.
- The durability and validation protocols developed by the Energy Materials Network (EMN) should be universal enough to be useful to all electrolyzer projects and allow for comparisons.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has shown good progress toward the overall project goals. For example, the researchers have demonstrated impressive electrolyzer performance for PGM-free catalysts (NiFe/Raney Ni) that exceeds state-of-the-art IrO_2. In situ X-ray absorption spectroscopy (XAS) studies have characterized the evolution of the catalyst's electronic structure as a function of applied potential. Moreover, the team has demonstrated an AEM with almost no change over 1,000 hours at 90°C in 1 M KOH, as measured with nuclear magnetic resonance (NMR). All but one of the remaining milestones have been completed. One milestone was not met because the HER catalysts did not achieve the required target performance, but there is still time for improvements to be made. A catalyst development go/no-go decision point has been met by demonstrating a current density of 500 mA/cm^2 at an overpotential of 150 mV using a PGM-free OER electrocatalyst. Current densities of 800 mA/cm^2 were obtained at an applied voltage of 1.92 V using NiFe/Raney Ni as the OER catalyst and NiCr/C and Ni-cup/C as the HER catalyst. Good thermal stability was observed due to UD's ionomer materials. This met a go/no-go decision point by demonstrating a PGM-free electrolyzer performance of 0.8 A/cm^2 at ≤1.92 V. A molecular model was developed using density functional theory and molecular dynamics simulations to simulate the effects of charging the electrode on the ionomer and mobile species to tie local pH and other resolved quantities to water-splitting efficiency. Small-angle X-ray scattering (SAXS) characterization elucidated the microstructure of the membrane under various hydration conditions.
- The project met its go/no-go milestone target performance for one of the three proposed catalyst systems. The membrane has good temperature stability.
- The project made very impressive progress in the first budget year. Into the second year, membrane material development has already exceeded the planned milestone.
- This project conducted characterization testing of three HER catalysts, compared the performance of an OER catalyst against a traditional PGM catalyst, and started characterization work on an alkaline membrane. A good deal of modeling work was done, some of it not specified within the initial scope of the work. The bulk of the first-year milestones were met, and explanations were provided for the milestones that were only partially successful. Having a clearer discussion on the disparity between the modeling results and experimental results would have been helpful.
- Very good progress has been made on all fronts, despite the large amount of work being done.
- The project has met the AEM and MEA milestone of budget period 1 that was stated last year (0.8 A/cm^2, 1.92 V). There is a significant performance gap between the AEM-based electrolyzer in project PD-156 (0.8 A/cm^2, 1.92 V) and the PEM-based electrolyzer in project PD-155 (1.5 A/cm^2, ~1.76 V [extracted from slide 9]). Because of this, it is recommended that the team clearly outline the pathway from their current status to achieve the milestones noted in the presentation that will lead to the DOE ultimate hydrogen production target ($2/kg H_2, 43 kWh/kg H_2).
- The HER and OER electrocatalyst task has made solid progress laying out a good pathway for the next stage. It would be interesting to see in the next budget year how the combination of those catalysts and new AEMs and ionomers would perform in electrolysis mode. Working with AEM materials with good stability (ex situ) is a significant advantage, as there is no commercial AEM material available now. Catalyst–

ionomer interaction is known to be key in the performance of AEM devices, and thus similar studies including an ionomer stability study with the developed ionomer will be critical in next stage. There is a concern about the use of AEMs with an ion exchange capacity (IEC) of 3.0 mmol/g, which may cause too high of a water uptake (water uptake data is not given in the slides). While AEMs with this high IEC level may enhance ion conductivity and are necessary for meeting the target area-specific resistance, they sacrifice other properties (e.g., mechanical stability, which is equally as important as chemical stability). Typically, these high-IEC AEMs behave like a gel (morphology characterization seen on slide 20) and tend to be partially dissolved in water; this would cause mechanical instability in MEA electrolyzer operation. Although this AEM looks to be chemically stable above 90°C for 1,000 hours in 1 M KOH (by NMR in slide 15), a partial loss of materials due to dissolution cannot be excluded, because IEC measurement by titration and NMR techniques do not count any material loss dissolved into water. On slide 15, NREL's Cl conductivity measurement shows that the PAP-TP-MQN membrane (for which the IEC is 3.0) melted away after the stability test, suggesting that this AEM is (partially) soluble. It is suggested that the team try AEMs with a lower IEC (in the range of 2.5 mmol/g) or adopt a reinforcement strategy for the AEMs to lower water swelling.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- This project did an excellent job collaborating between different institutions. For example, catalyst development and membrane development were equally distributed between NEU and UD. SNL constructed models to simulate the effects of charging the electrode on the ionomer and mobile species to tie local pH and other resolved quantities to water-splitting efficiency. LBNL modeled electrolyzer performance in carbonate electrolyte versus in pure water based on experimental data and conducted X-ray scattering and conductivity measurements of the ionomer.
- The project has excellent coordination among different team members, including two national laboratories. The modeling study done by SNL and the SAXS and carbonate-ion-effect modeling study could provide insight into how future materials need to be optimized. Delivering more solid outcomes and results from these collaborations would serve as an important impact of the project.
- This activity distributes work across multiple academic institutions and multiple governmental laboratories. The integrated test results suggest a high data flow rate between the groups.
- This project involves many collaborators from different EMN nodes, and the coordination with the team seems to be going well.
- This is an excellent team with members who have collaborated successfully before.
- This good team has high productivity.
- Modeling by two national laboratories seems to have helped the progress.
- The project demonstrates good collaboration between the development of new catalysts and new AEMs. However, in slide 19, the LBNL modeling shows that the OER overpotential is significantly higher than the HER overpotential, which does not match the experimental result presented (500 mA/cm^2; η [HER] about 300 mV, η [OER] about 150 mV).

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The project's future work will focus on catalyst development, test station and electrolyzer optimization, modeling, X-ray scattering measurements, and durability measurements. These efforts should result in higher-performing catalysts that will ultimately lower operating costs and achieve the desired <\$2/kg H_2.
- The proposed future work is clearly delineated and organized between the partners. Within the identified resources, this work focuses on further characterizing the catalysts and membrane, refining computational models, and initiating limited durability testing. It would be beneficial to see an effort that includes developing a plan to transition the lessons learned under this project to the industry.

- It will be interesting to see the origin of the effect or role of the added carbonate feed on electrolyzer performance, which the team is proposing to study. The good mechanical stability and low gas permeability of the AEM under hydrated conditions are also important material properties in water electrolysis, which should be addressed in future study.
- The overall proposed future work is excellent. The critical reasoning for the next stage of the HER catalyst plan (Ni-MOx-Nx) should be clearly stated.
- The project team prepared a good plan for fiscal year 2019 activities. It would be beneficial if demonstrations can be made to show how exactly modeling results help the material or process design.
- There is a good plan for year 2. It is not clear when Advent North America will come into the picture; it may be in year 3.
- The proposed future work is very good overall. It seems less optimistic that the membranes will prove durable. The team should perhaps have a plan in case they fail.
- The team must focus to better establish the benchmark to which the final performance is going to be compared. It is also highly important to perform real durability tests to demonstrate the potential for real applications.

Project strengths:

- The team is composed of expert members from each area, and their approaches are well aligned with the DOE goal of sustainable hydrogen production with a PGM-free electrolyzer.
- This project is strategically attacking challenges associated with both the catalyst and the membrane. The results are extremely encouraging.
- This project is very clearly organized and focused on specific elements: computational modeling and characterizing three HER catalysts, one OER catalyst, and an alkaline membrane. The research team consists of solidly proficient institutions that appear to be collaborating quite effectively.
- This is a very good team that is working together and making progress on developing low-cost materials for electrolyzers. The research is based on fundamental understanding, and the results are published.
- The project's strengths include the team's expertise in electrocatalysis and membrane (AEM) synthesis, as well as novel concepts and strong and solid characterization tools.
- The project team consists of PIs with strong and diversified expertise. The team not only pursues performance improvements but also makes strong efforts to understand the mechanism.
- The team identified a catalyst that meets the go/no-go performance milestone.
- The key strength of the project is the combination of non-PGM with AEMs.

Project weaknesses:

- The project has had difficulty in accessing a solid benchmark and has seen complex chemistry during in situ electrolysis testing. There is a challenge to overcome with membrane stability during in situ operation (>5000 hours), as well as a challenge in electrode and membrane integration (ionomer/binder concept).
- It would have been helpful to include a discussion on the disparity between the computational model and test results.
- It is not clear that the alkaline membrane will be effective. It is simply a very hard problem to develop a new membrane.
- Selecting appropriate AEMs and ionomers would accelerate the progress.
- Better correlation between the simulation modeling and experiment is needed.
- There has not been a report on MEA durability yet.

Recommendations for additions/deletions to project scope:

- The project scope is appropriate.
- It would be beneficial to extend the life testing for longer durations, where resources permit it. Characterizing the integrated cell with a range of concentrations of different electrolytes would be helpful

in identifying any potential design sensitivities that would extend into a system design. It would also be beneficial to develop a plan to transfer the lessons learned into practice.
- The team should include a strategy for the fabrication and scale-up of the new catalyst material.
- It is recommended that the team look at alternative alkaline membranes, possibly Fumatec as a baseline and maybe ionomer membranes (from Holdcroft).
- A more judicious choice of AEM and ionomer materials would accelerate progress in the right direction.

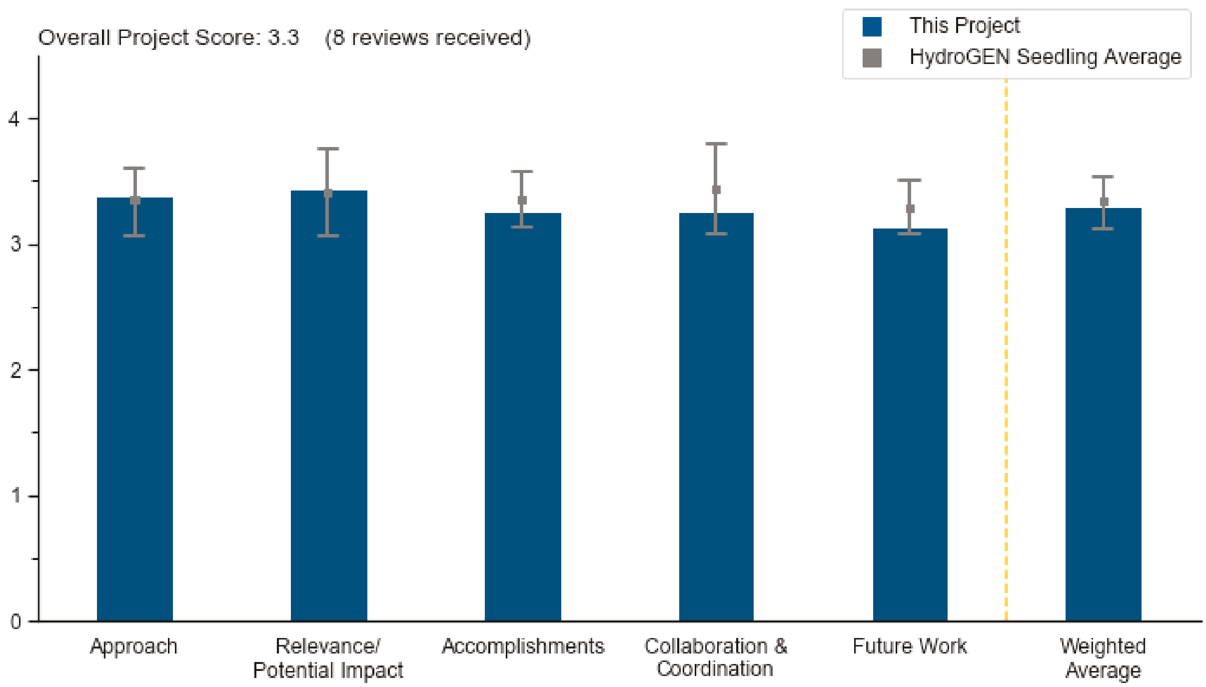
Project #P-157: Platinum-Group-Metal-Free Oxygen Evolution Reaction Catalysts for Polymer Electrolyte Membrane Electrolyzer

Di-Jia Liu, Argonne National Laboratory

Brief Summary of Project

The objective of this project is to lower the capital cost of polymer electrolyte membrane (PEM) electrolyzers by developing low-cost, platinum-group-metal-free (PGM-free) oxygen evolution reaction (OER) electrocatalysts. The project is developing high-activity, high-conductivity, durable metal–organic framework (MOF)-based catalysts via both direct (e.g., solvothermal) and template (e.g., infiltration) synthesis approaches with one, two, or three transition metals. The most promising MOF-based catalysts will then be incorporated in a three-dimensional porous nanonetwork electrode (PNNE) architecture. The goal is to produce durable PGM-free OER catalysts with performance approaching that of current Ir-based PGM catalysts. Argonne National Laboratory (ANL) is partnered with Giner, Inc. (Giner) and University at Buffalo (UB) and is leveraging national laboratories within the HydroGEN consortium.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- This project intends to develop PGM-free OER electrocatalysts to replace Ir-based catalysts in PEM electrolyzers. This is a challenge because there are no commercially available PGM-free PEM anode catalysts that can survive positive potentials. Realizing a PGM-free OER catalyst will dramatically reduce electrolyzer costs. The catalyst of choice is constructed from a Co-containing MOF. This catalyst has shown impressive OER activity in acidic conditions that approaches that of Ir-based catalysts. The electrodes can also be prepared by electrospinning the MOF catalyst to make a porous nanowire-type system. The team is also considering a zeolitic imidazolate framework (ZIF) to create the catalysts. This approach is unique and appears to show great promise. The catalysts are active and stable in acidic conditions, which has the potential to eliminate the need for PGM anode catalysts.

- This project is rated a 3.5 for identifying barriers and addressing them through project innovation, design, feasibility, and integration with the HydroGEN consortium network. This project attempts to develop PGM-free OER catalysts operating in acid electrolyte. The project uses MOFs containing transition metals (Fe, Co, Ni, Mn, etc.) to screen the best OER catalysts in acid with the lowest overpotential (350 mV at 10 mA/cm^2 in this work). The cooperating partners are from computation modeling, characterization, and industrial water electrolyzer technology backgrounds. More fundamental understanding is needed to reveal why this kind of transition-metal-based OER catalyst can exhibit excellent activity and stability—especially stability—in acid electrolyte. More rationale in screening catalysts is recommended. Understanding the role of each addition is of great significance.
- The goal of this project is to develop PGM-free OER catalysts based on earth-abundant metals and their MOF and ZIF complexes for PEM electrolysis operating under acidic media. As PEM electrolysis is at a stage of near-term commercialization (though currently using Ir for the OER catalyst), a successful outcome of this project would immediately bring significant impact to the mission of the U.S. Department of Energy and HydroGEN.
- PNNE is an elegant approach; it eliminates a major source of catalyst corrosion (carbon). The metrics are clearly stated (slide 8).
- There are three methods adopted here to develop efficient PGM-free OER catalysts in acid. Method 1 and Method 2 appear to be appropriate and deliver decent activity and stability in rotating disk electrodes (RDEs) and good performance in membrane electrode assemblies (MEAs). The development of the ZIF-8-derived catalysts in Method 3 lags behind, showing some activities in RDEs. More importantly, this type of catalyst is carbon-based. This is a big concern since at OER, relevant potential carbon corrosion becomes serious and causes rapid degradation of the catalysts. The Co-based catalysts developed in Method 1 seem to contain graphene during the synthesis, but the principal investigator (PI) mentioned that the vast majority of the graphene was removed at the end. These chosen methods for the synthesis of the catalysts match the expertise of the partners in the team. The characterizations in collaboration with national laboratories and the MEA testing methods are appropriate.
- This work focuses exclusively on the OER reaction based on the interactions of the PGM-free catalysts and polymer membrane. This project appears to be at risk of diluting work across too many collaborative entities. While an intentionally catalyst-focused effort, this work provides little discussion on how the work transitions to other scales of integration or will eventually lead to the targeted savings. At some point, this work should transition to industry and have a path to that end.
- The researchers are studying MOFs, which are materials with which they have a good deal of experience. While the class of materials has activity, there is no real evidence given for why these should be active for the OER. In cells, they have very poor current density ($<250\ mA/cm^2$). It is not clear why the in-band valence structure is important. It is good that the project is using Giner to help with the testing.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The ability to create scalable, PGM-free anode catalysts for PEM electrolyzers could be a transformational development that lowers the costs of water electrolysis. The results presented to date are extremely impressive and encouraging for the realization of PGM-free OER catalysts for PEM operation and production of hydrogen at less than $2/kg.
- The goal of this project is to develop PGM-free OER catalysts based on earth-abundant metals for acidic PEM electrolyzers. As PEM electrolysis is at a stage of near-term commercialization (though currently using Ir for the OER catalyst), the development of low-cost, high-activity, earth-abundant transition-metal catalysts could immediately bring significant impact to the mission of DOE and HydroGEN.
- This project directly addresses the problems of expensive anodic OER catalysts. The state-of-the-art OER catalysts such as IrO_2 and RuO_2 could be replaced if robust OER catalysts worked in both acid and base. The biggest problem of current state-of-the-art catalysts for OER in acid is with their stability. If the

stability issue can be solved, PEM electrolyzers can show their advantages of fast hydrogen evolution reaction kinetics and commercialized PEMs.

- This work is very relevant to reducing the production costs of hydrogen by increasing the efficiency of the OER catalysts and/or replacing the PGM-based catalysts with less expensive alternatives. Reducing the dependence on PGM materials is beneficial only with abundant replacement catalyst materials. The dependence on cobalt leaves this activity exposed to questions about catalyst material availability.
- PGM-free catalysts for low-temperature electrolysis (LTE) are needed to reduce capital cost.
- There is an intrinsic risk involved when targeting the replacement of Ir-based catalysts for PEM electrolysis. Iridium seems to be the only stable element that can be used in this environment. Therefore, the potential for impact in the field is very high, but so is the risk.
- The project demonstrated effective hydrogen production with a PEM water electrolyzer (PEMWE) with a PGM-free anodic catalyst with relatively low overpotentials, which shows good progress aligning with the Hydrogen and Fuel Cells Program and DOE research, development, and demonstration objectives. The lack of fundamental understanding of the activity and information about the catalysts will make further progress difficult.
- It does not look like the MOF catalysts work very well, and there does not seem to be a path for them to perform better. Therefore, it is not clear that there will be much important work from this research.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has shown excellent progress by demonstrating the OER performance of PGM-free OER catalysts constructed from Co-MOFs. The team has demonstrated superior stability compared with IrO_2 in accelerated RDE testing in acidic conditions, and co-doping different transition metals into the MOFs has been shown as a way to further improve performance. These multimetallic catalysts show enhanced OER performance above IrO_2 at moderate overpotentials. MEAs constructed from the PGM-free OER catalysts produced a current density of 320 mA/cm^2 at 1.8 V. Ongoing materials characterization using X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS), transmission electron microscopy (TEM), and density functional theory (DFT) are correlating catalyst structure and composition with performance. Structural studies using a variety of analytical tools are being used to better understand catalytic activity and the aging mechanism for PGM-free OER catalysts in the acidic environment, resulting in mitigation strategies for decreasing degradation rates. The team is well on its way to demonstrating the budget period (BP) 2 overall performance goal of >400 mA/cm^2 at 1.80 V in activity and reducing voltage loss of <100 mV after 100 voltage cycles in durability. The team is also currently investigating ZIFs coupled with carbon nanotubes and polymer scaffolds to further increase OER performance.
- In regard to catalyst activity, last year's ANL-a catalyst had the OER overpotential of 354 mV (as seen in the slide on page 9), which is only 21 mV higher than Ir black (100 mg/cm^2) at 10 mA/cm^2, which has already met the go/no-go milestone. However, this year's best-performing catalyst, LM@ANL-b, has a similar overpotential at 10 mA/cm^2 (as seen in the slide on page 11). Some of them (LM@ANL-b, LL@ANL-b) have a lower overpotential, at 20 mA/cm^2, than Ir black. This is attributed to the second and third additions of transition metals. However, the screening method could be more efficient, and the role of each addition could be clarified. Catalyst durability for ANL-a and ANL-b showed only small voltage losses of 24 mV and 22 mV, respectively, at 10 mA/cm^2 after 10,000 voltage cycles from 1.2 V to 2.0 V (slide 9), which is less than Ir black at 100 µg/cm^2 (88 mV). Regarding the MEA test results, the project team has put its OER catalysts in MEA. The project achieved 320 mA/cm^2 at 1.8 V (in the slide on page 12), exceeding the BP 1 goal of 200 mA/cm^2 at 1.8 V and not far from the BP 1 goal of 350 mA/cm^2 at 1.8 V. It is quite promising, and the team should test MEA durability next.
- The BP 1 goal was achieved. Both ANL-a and ANL-b demonstrated current densities ≥300 mA/cm^2 at 1.8 V. These performances approach the BP 2 goals but have not yet reached them. Reaching the BP 2 goals seems quite likely. There is no clear fundamental understanding of the high OER activity of ANL-a and ANL-b catalysts since it is not clear what the two catalysts are. The PI mentioned the team is currently in the process of either publishing or patenting and will reveal the nature of the catalysts afterwards.

- The project has shown promising progress for both ANL-a and ANL-b. Good durability was demonstrated in RDE testing. The project has met the BP 1 target performance in 25 cm^2 cells.
- The team has made solid progress on the development and characterization of PGM-free catalysts (ANL's Co-MOF and porous nanonetwork electrocatalyst and UB's ZIF-8 catalyst). Some of them have shown very good catalytic activity and durability in RDE and half-cell testing under an acidic environment. However, demonstration of those catalysts in a real PEM electrolyzer MEA is still not sufficient. Building MEAs with new catalysts is not trivial, and a delay in the task of MEA development is understandable. The team has to identify what hurdles they face and suggest strategies to meet them.
- The work focused on characterizing PGM-free MOF and ZIF-8, almost exclusively using RDE testing. The parallel work included alternative manufacturing processes to generate the higher-conductivity catalyst support structures. This activity mostly met two BP 2 milestones and is on track to meet the third. This activity provides the appearance of diffusing the work to the point of obfuscating progress.
- The catalysts perform poorly in the electrochemical cells.

Question 4: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- The team has successfully collaborated with Lawrence Berkeley National Laboratory (LBNL) for model simulation and electronic structure calculations. These efforts are modeling the optical properties of the materials in an effort to understand how electronic structure affects electrochemical OER activity. The team has collaborated with Sandia National Laboratories (SNL) for atomic resolution TEM imaging and energy dispersive X-ray spectroscopy (EDX) to quantify local composition and structure. The team has collaborated with the National Renewable Energy Laboratory (NREL) for X-ray photoelectron spectroscopy (XPS) characterization of the catalysts to understand how different catalyst compositions and preparations affect the Co valance state and electronic structure before and after OER testing.
- The team has the following collaborations, which worked out well for the project: (1) computational modeling cooperation at Lawrence Livermore National Laboratory (LLNL) and LBNL, (2) electron microscopy characterizations at SNL, (3) electrode optimization and catalyst characterization at NREL, and (4) industrial partner Giner, which specializes in water electrolyzer technology.
- The team has established good collaboration with other HydroGEN participants, including LBNL (for modeling study to gain insight into the origin of catalyst stability and conductivity), LLNL (for modeling study about charge transfer in OER catalyst), SNL (for scanning transmission electron microscopy [STEM] morphology study of catalysts), and NREL (surface analysis of catalysts). All of these could help the team's effort.
- There is effective collaboration with other national laboratories for modeling and with Giner for in-cell performance evaluation.
- The team is strong and appropriate for what was proposed for implementation. The collaborations with national laboratories are great. The whole collaboration nicely covers all the necessary aspects, including synthesis, characterizations, modeling, and RDE and MEA evaluations. However, there appear to be some disconnections between the catalyst synthesis, performance, and characterizations. The characterizations do not present a clear picture of the catalysts and, together with modeling, do not provide plausible causes accounting for the high OER activity.
- It is good that ANL is working with Giner. The team might also consider working with the fuel cell researchers at ANL (Meyers or Stamenkovic). Research into the prior work on MOFs done by the PI showed surprisingly poor oxygen reduction data in the publication. It was astounding that a group from ANL could be doing oxygen reduction measurements on Pt in sulfuric acid. It is surprising that the work was even published. It does not give much confidence in the alkaline OER data.
- This project has seven collaborating entities focusing on advancing the catalyzed OER. There exists a risk that good work has been spread too widely and is limiting evolving the work to the next scale. At some point, in situ membrane testing needs to replace RDE testing so the project can evaluate the scaling potential of the sub-cell-scale innovations.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The future plans seem appropriate for realizing high-performance, PGM-free OER catalysts for PEM electrolyzers. The stated future plans include synthesizing and evaluating the OER performance of multimetallic MOF catalysts and the potential use of atomic layer deposition for surface doping; evaluating the OER performance of electrospun nanowire-type MOF catalysts; exploring new materials with performance targets in full cell testing; continuing the exploration of ZIF-based catalysts; pushing the performance target higher to 400 mA/cm^2 for the full electrolyzer cell; and continuing to improve fundamental understanding of the structure–function relationship of PGM-free OER catalysts using computation modeling and advanced characterization tools through collaboration with HydroGEN.
- The proposed future work appears to be reasonable and nicely covers all of the work to be conducted, especially the MEA testing and the durability.
- The project has an excellent plan.
- The stated goal of continued focus on catalyst performance in the next fiscal year has merit. However, not identifying a path toward commercialization exposes this project to questions as to how well it aligns with the stated goal of cost reduction. If the goal of this project is to reduce costs, industrial-scale manufacturing processes and integrated cell and stack testing will need to enter into the picture at some point. Those processes may not fit within the project resources, but developing a plan provides answers to difficult questions.
- The planned work seemed to have a lack of focus. The current synthesis methods are already quite efficient and can be used to prepare high-performance catalysts. The key point is to push the MEA performance and to try to scale up the catalyst synthesis. Additional efforts are recommended to understand why those transition-metal-based catalysts can show such high activity and durability in acid.
- In spite of the good progress made in catalyst activity and durability in RDEs, the proposed testing and demonstration in PEM electrolyzer MEAs has been slow. The team should address how to avoid corrosion issues in the catalyst system's carbon matrix under the acidic media of a PEM electrolyzer.
- It may not be worth researching this material any longer.

Project strengths:

- One of the major strengths of this project is in the catalyst development. Both the ANL and UB teams are good at PGM-free catalyst development, and the catalysts developed in this project indeed exhibit promising OER performance in practical PEMWE. This is probably the toughest part of the project since it is not easy to develop PGM-free catalysts for the OER in acid, given that only limited PGM-free materials are stable in acid—and even fewer under such high potentials. In addition, carbon cannot be used to achieve high electrochemical surface area (ECSA) because of the carbon corrosion issue, and not too many alternative supports are stable at such extreme conditions while ensuring high ECSA. It seems like ANL-a and ANL-b, especially the former case, coped with all these issues and delivered decent performance in PEMWE.
- The team has demonstrated a low-cost transition-metal-based OER catalyst. It shows excellent activity and stability in acid. The best, LM@ANL-b, has ~350 mV overpotential at 10 mA/cm^2 (as seen on the slide on page 11). The durability is also supreme. ANL-a and ANL-b showed only small voltage losses of 24 mV and 22 mV, respectively, at 10 mA/cm^2 after 10,000 voltage cycles from 1.2 V to 2.0 V (from the slide on page 9), which is less than Ir black at 100 µg/cm^2 (88 mV). The MEA performance is very encouraging (350 mA/cm^2 at 1.8 V).
- The project has demonstrated excellent activity of PGM-free materials in a non-alkaline environment that is comparable to IrO_2. The future plans seem to be appropriate, and the collaboration is sufficient to understand the underlying structure–property relationships that allow for such impressive OER performance.
- The project's strengths include its ambitiousness, the expertise in MOF synthesis and characterization, and the PEM electrolysis expertise from Giner.
- The project focus is on a narrow, but very important, issue in hydrogen production using PEM electrolyzers. The catalysts developed from this project look very promising, at least in half-cell testing.
- This project focuses exclusively on the replacement of PGM catalysts for the OER.

- This is a strong team; excellent performance has been demonstrated.
- The team has experience with MOF-based catalysts.

Project weaknesses:

- The biggest concern is the lack of information about the catalysts being developed. The presentation did not deliver a clear idea of what the catalysts are, including the element, morphology, active sites, etc. It is understandable that materials may be under publishing or patenting, but this makes it hard to judge the potentials of the developed catalysts. The characterizations are not closely related to the catalyst performance and do not reveal a clear picture of the catalysts. In particular, all of a sudden the STEM shows that the ANL-a has a protective layer of conformal TiO_2 coating that is 1–2 nm thick. This is rather surprising, as this is the first place mentioning that ANL-a contains a TiO_2 layer. In addition, such a thick protecting layer will make active sites inside electro-inactive. This issue needs to be addressed.
- It is difficult to translate RDE results into single-cell testing. There is a short supply of cobalt, the base element of the catalyst proposed here, perhaps even worse than iridium. There may be competition with batteries. Intrinsic low current densities are associated with catalysts for OER other than iridium.
- There is a lack of understanding of transition-metal-based OER catalysts in acid. For example, it is not clear why the stability is better than with Ir black. The screening of the catalysts needs more rationale. The role of the second and third addition metals should be identified.
- The team has very poor electrochemical data in this presentation and a recent history of publishing poor data, despite being at ANL with some of the best fuel cell researchers in the world.
- There appears to be no path toward scaling the innovations or realizing the stated project goal of reducing the cost of hydrogen production.
- More comprehensive demonstration of the developed catalyst at the PEM electrolyzer MEA level is suggested.
- The low current density compared to conventional LTE catalysts means higher electrolyzer capital cost.

Recommendations for additions/deletions to project scope:

- This project would benefit from a plan that addresses how the innovations will meet the stated project goals of reducing the cost of producing hydrogen. At a minimum, this plan should include how to implement the innovations beyond a sub-cell level and how to deliver the stated goal of reducing the cost of hydrogen production on a larger scale. Evolving the catalyst testing beyond the RDE level and implementing more endurance and cell-level testing of the developed catalysts will identify viable catalysts for further scale-up. The characteristics and properties of those catalysts can be fed back into the modeling and catalyst development efforts to further this iterative process.
- It is recommended that the team add the necessary information of the catalysts developed and make sure that carbon is not the essential part of the catalysts; ideally, there should not be any carbon in the catalysts to be assembled in the MEA. The team might try other transition metals such as Mn, Fe, and/or Ni for catalyst development.
- The team should change the target of 1,000 A/cm^2 at 2 V to 1,000 A/cm^2 at 1.6–1.7 V. This can be accomplished by playing with membrane thickness. MOFs will have stability issues at such a high voltage.
- An investigation of mechanisms of transition-metal-based OER catalysts in acid is recommended. This can lead to more efficient catalyst screening.
- More effort on characterization and a demonstration of the developed catalyst at the PEM electrolyzer MEA level is suggested.
- The performance of the ANL cells is well below that published by the Asahi Kasei Corporation. (Yasuhiro Nakajima, Norikazu Fujimoto, Shinji Hasegawa, and Taketoshi Usui. "Advanced Alkaline Water Electrolyzer for Renewable Hydrogen Production." *ECS Transactions* 80, no. 10 [2017]: 835–41.) At 1.75 V cell potential, Asashi Kasei reports current densities on the order of 600 mA/cm^2 at the system level, while this team reports 200 mA/cm^2. There is no clear path to meeting the state of the art for alkaline, never mind for acid electrolysis.

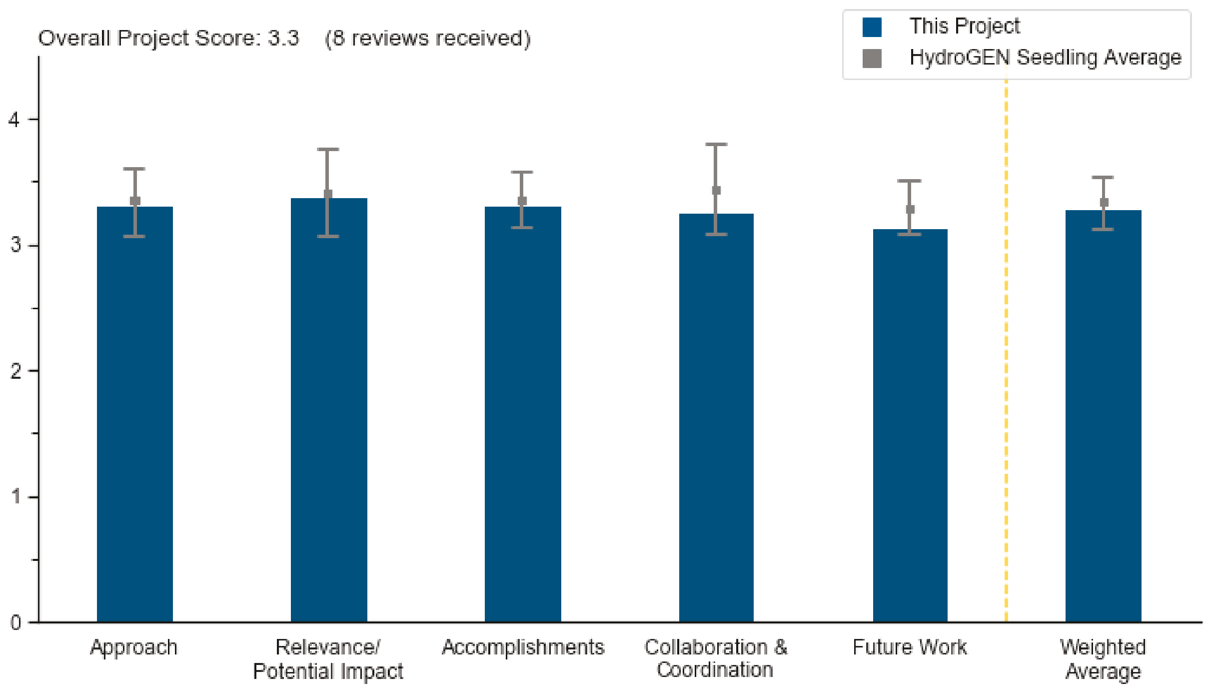
Project #P-158: High-Performance Ultralow-Cost Non-Precious-Metal Catalyst System for Anion Exchange Membrane Electrolyzer

Hoon Chung, Los Alamos National Laboratory

Brief Summary of Project

The primary objective of this project is to develop low-cost, active, and durable platinum-group-metal-free (PGM-free) oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) catalysts with high performance in an anion exchange membrane (AEM) water electrolyzer. The HER and OER catalysts being developed are based on Ni-La alloys and $LaSrCoO_3$ (LSC)-based perovskite materials, respectively. The catalysts and electrodes will be carbon-free, and a pure water feedstock (i.e., no added electrolyte) is targeted. In addition to utilizing HydroGEN Consortium national laboratory capabilities, the project team will partner with Pajarito Powder, LLC (Pajarito) for catalyst scale-up activities.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- A key challenge with AEM electrolyzers is how to eliminate salt or alkaline solutions and split pure water. This project aims to develop PGM-free OER and HER catalysts that demonstrate high activity in the absence of alkaline solution. This will eliminate the cost and complexity of electrolyzer systems with an anticipated goal of <$2/kg of hydrogen. The main goals of this project are to reduce the overpotential and costs associated with traditional HER and OER catalysts. The team's plan centers on designing high-activity, PGM-free OER and HER catalysts for water splitting in the absence of alkaline electrolyte. This project will use AEM cell design for water electrolysis in the absence of alkaline electrolyte. Using water instead of alkaline electrolyte will allow the use of stainless steel current collector to stainless steel, which is estimated to eliminate 75% of the cost compared to polymer electrolyte membrane (PEM) technology. Finally, the team hopes to replace the Nafion membrane with a hydrocarbon membrane. The approach involves synthesizing PMG-free HER and OER catalysts to promote water splitting. The HER catalyst is based on a NiLa system, and the OER catalyst is based on a perovskite catalyst. The perovskite OER catalyst shows impressive performance compared to IrO_2. Electrolyzers using the perovskite OER catalyst can reach a maximum current density of ~240 mA/cm^2 in water at 80°C, with stable performance at over 100 hours. This performance can be boosted to over 450 mA/cm^2 with 0.1 M NaOH electrolyte.

- The project aims to enable low-cost hydrogen production via the development of non-PGM-based OER and HER catalysts for use in AEM electrolyzers. The catalyst materials, LSC-derived perovskites for OER and LaNi alloy for HER, are not new to the research community. The investigation of catalyst–ionomer interaction and the behavior of the catalysts in AEM electrolyzers can provide valuable knowledge for improving the design of catalysts and membrane electrode assemblies (MEAs), with higher efficiency and lower capital cost.
- This project attempts to develop LSC-based materials for operation in alkaline-free water electrolysis systems. The project team added an organic cation (butyltrimethylammonium [$BTMA^+$]) in the electrolyte to promote the OER in perovskite-based catalysts. It is worthwhile to explore those substitutes for alkaline electrolyte. The ionomer–catalyst interface is worthy of exploring.
- The project is taking a very ambitious but decisive approach to use deionized (DI) water for electrolysis operation. This intrinsically limits performance but has a decisive impact on durability. If the project team manages to solve the issues related to AEM conductivity, it would lead to a very important impact on the field.
- The team proposes to develop PGM-free, Ni-La alloys for HER catalysts and LSC-based perovskite materials for OER catalysts for AEM electrolysis. Los Alamos National Laboratory (LANL) will develop the catalysts, and the project's industrial partner will work toward the scale-up production of catalysts. Phase I was focused on catalyst development, while Phase II is more focused on catalyst–ionomer interaction.
- This project has improved its approach since last year. There now exists a clear and logical path for development, supported by solid rationale and cost justification for the work on PGM-free catalysts, water-based process fluid, and alkaline membranes.
- The team is studying a low-performing, non-precious-metal catalyst. Their method is to benchmark against iridium catalysts, but there seems to be something wrong with their iridium baseline, as the cells on slide 8 perform very poorly. As a reference, the authors might look at figure 3 in the following paper by Asahi Kasei Chemicals, Co. (AKC): *ECS Transactions*, 80(10), 835–841 (2017). (There might be some better references out there, but this seems reasonable.) AKC shows performance at the system level, with 600 mA/cm^2 at 1.7 V/cell. Chung reports a cell with iridium at 250 mA/cm^2, in a small cell. It seems that LANL should benchmark project results against a reasonable standard. (This was an old problem in fuel cell catalysts that has been fixed.) The following paper might also be useful for methods (although stationary drying cannot be used for the preparation of electrodes; rather, rotational drying is used): https://doi.org/10.1002/adma.201806296
- The project makes good use of HydroGEN nodes.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- This project is extremely relevant to HydroGEN's goals of inexpensive hydrogen production. One main problem with PGM-free OER catalysts is low activity or dissolution in neutral or acidic conditions. This project demonstrates a perovskite oxide-based OER catalyst that demonstrates excellent water-splitting activity and stability in alkaline-free conditions. The continued improvement of performance is on track to meet the goal of <$2/kg of hydrogen.
- If every milestone is met, this project can simplify the overall system and minimize carbon in the MEA to improve longevity. The bipolar assembly and MEA represent the highest costs of a PEM stack (35% and 18%, respectively). If met, the milestones can reduce 75% of this cost and enable lower-cost catalysts. This project did not use PGM-based catalysts, which may help reduce the cost of catalysts. Ionomer–catalyst interfacial studies can reveal an ionomer-poisoning effect on catalysts; approaches can be devised to address this issue.

- Enabling a water-recirculating alkaline electrolyzer to generate hydrogen nearly as efficiently as a PEM electrolyzer significantly simplifies the wetted-materials issue for electrolysis systems. If the reaction pH is significantly increased, less expensive materials may be used in the process stream. Recirculating pure or nearly pure water can impose known and well-understood challenges that have well-established mitigation options. Replacing PGM catalysts with a more readily available catalyst material reduces cost and eliminates risks of a supply shortage.
- Compared to a PEM electrolyzer, an AEM electrolyzer can offer significant cost reduction by allowing lower-cost bipolar plates and electrocatalysts. AEM electrolysis offers a number of advantages over alkaline electrolysis based on a strong KOH solution. Overall, AEM electrolysis is less mature than those two hydrogen production technologies; however, it could offer significant impact if successfully developed and adopted commercially.
- The project aligns well with HydroGEN's mission to develop an electrolytic process for low-cost hydrogen production. The use of non-PGM catalyst materials and the improvement of their performance can lead to higher system efficiency and lower stack cost. The potential to use only water feed also simplifies the system design.
- The project is high-risk and has a challenge in reaching significant cell performance, but there will be an extreme impact if the team can obtain performance by tuning electrode and AEM structure.
- There is promise of lower capital cost in the long term, but there is a lower technology readiness level than with PEM and alkaline technology.
- It is unclear why the project attempts to use useful materials and develop electrochemical methods when the approaches are really outdated compared to work being done in the fuel cell community. It is not certain that the methods and results are very good or will have much staying power.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- From last year, the team has demonstrated significantly increased electrolyzer performance with a five-fold increase in current density compared with fiscal year (FY) 2018 results. The project has demonstrated impressive OER performance with a PGM-free, perovskite-oxide-based catalyst in both three-electrode and electrolyzer configurations. The team has also evaluated the performance of several ionomer binders to optimize electrocatalytic OER performance. Water electrolysis in the AEM cell reached 243 mA/cm^2 at 1.8 V and 80°C and showed good stability over 100 hours at 100 mA/cm^2. Continued progress is required to meet future milestones, including synthesizing a new NiLa(Zn) HER catalyst that produces 50 mA/cm^2 at 200 mV overpotential for use in an electrolyzer device. The FY 2019 go/no-go performance of 100 mA/cm^2 at 1.8 V has been exceeded, with a maximum performance of 243 mA/cm^2 reached at 80°C. The team is on track to meet the goal of obtaining a PGM-free HER catalyst with degradation similar to Pt.
- The current density with AEM achieved 119 mA/cm^2, 175 mA/cm^2, and 243 mA/cm^2 at 60°C, 70°C, and 80°C, respectively, exceeding 100 mA/cm^2 at 1.8 V. It is worth noting that the project team exceeded last year's record of 119 mA/cm^2. By changing the electrolyte environment from water to 0.1 M NaOH, current density can be brought to 452 mA/cm^2. At 100 mA/cm^2, 1.8 V for 100 hours, the catalysts show almost no degradation in AEM. The team also developed a gas diffusion electrode (GDE) electrochemical cell approach, which successfully identified the AEM ionomer effect on OER performance, demonstrating the merits of using perovskite plus a benzyl trimethyl ammonium hydroxide (BTMAOH) electrolyte.
- Compared to Phase I when the team focused on the evaluation of catalyst performance by rotating disk electrode (RDE), the team has made significant progress in Phase II and has shown good performance and durability of the catalysts in AEM electrolysis (with pure water and no added salt). Furthermore, by developing a novel GDE electrochemical cell experiment, the team has identified the effect of AEM ionomer on OER performance and studied a diverse range of catalyst–ionomer interactions.
- This project demonstrated improvements in both OER and HER activity using non-PGM catalysts. Two budget period 2 milestones were met, with expected progress made toward the two remaining milestones. Testing was completed at the RDE stage and evolved into single-cell testing for further characterization. Significant progress was made in identifying the influence of the catalyst–ionomer support on catalyst activity.

- The project is on track to meet the planed performance milestones for Phase II. It was very impressive that the project achieved additional improvement on OER catalyst performance and showed stability over 100 hours. It would be very beneficial for the project team to conduct deeper material characterization and analysis to understand the mechanism behind these improvements.
- The project team has made good improvement with the water-feed system.
- The project team has improved catalyst performance and studied interactions with ionomers, but the electrochemical performance is very poor.

Question 4: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- This project has demonstrated good collaboration with the other institutions. Sandia National Laboratories is working on AEMs and ionomer synthesis and has planned in situ X-ray photoelectron spectroscopy (XPS) to characterize catalyst–ionomer interactions. National Renewable Energy Laboratory (NREL) is working on AEM water electrolysis testing and materials characterization, using XPS/ultraviolet photoelectron spectroscopy (UPS) to analyze fresh and tested AEM electrolyzer electrodes. Lawrence Berkeley National Laboratory is planning for in situ X-ray characterization.
- This project evidently made effective use of the HydroGEN nodes based on the progress since last year. The group includes two major partners, collaborating with three national laboratories on four network nodes. The analytical and modeling tools, along with the characterization testing from the network, influenced catalyst and membrane design.
- The project team has excellent cooperation with five nodes, consisting of catalyst development, catalysts and organic interfacial study, and MEA fabrications. Two teams have been added on characterizations.
- The project team consists of a good combination of experts from different areas. The project also effectively leverages multiple nodes available at HydroGEN. As this is a fundamental research project, working with multiple nodes can bring synergistic effect for all participants.
- This is a good use of HydroGEN nodes, especially the NREL in situ testing.
- The collaboration between the project team and the HydroGEN nodes seems to be strong and effective.
- The project team needs to increase relations toward electrode fabrication and single-cell testing partners.
- There is no clear evidence in the presentation of collaboration with Pajarito.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The proposed future work is centered on (1) understanding the phenomena that occur at the catalyst–ionomer interface using in situ and ex situ XPS and x-ray absorption spectroscopy (XAS); (2) conducting GDE electrochemical cell studies to evaluate how catalyst–ionomer interactions impact catalytic activity; (3) modifying catalyst composition based on catalyst–ionomer interaction studies to further improve performance and stability; and (4) optimizing catalyst–ionomer ratios to maximize electrolyzer performance.
- The team proposes to better understand the ionomer–catalyst interface by using in situ and ex situ ambient pressure XPS (AP-XPS), XAS, and GDE electrochemical cell technique. It is essential to understand the degradation mechanism brought on by the ionomer. The team also proposes to develop a new category of catalysts and optimize the combination of catalysts and ionomer. This is a good direction to push the performance.
- The project team has a clear plan to achieve the planned milestones for Phase II. Deeper analysis and understanding of catalyst–ionomer interaction will provide valuable insight for future catalyst layer design. Perovskites are fundamentally non-conductive materials. The project team shall consider strategies to address potential ohmic loss at higher current density (i.e., 1 A/cm^2) in the absence of carbon.
- With identification of catalyst–ionomer interaction as a potential reason for poor durability of AEM electrolysis in Phase II, in the next step, it would be logical to think about mitigating strategies by modifying catalysts and/or ionomers.

- The project team needs to better define the tasks to reach better cell performance when using DI water. It is not clear what the specific tasks are for tackling difficulties in ionomer integration during electrode manufacturing.
- The Pajarito effort is very important. Presenters are asked to include who will do what on future Proposed Future Work slides.
- The proposed future work is more of the same research. It is unclear why the project team is studying catalyst–ionomer interaction for a poor catalyst.
- The future work focuses on catalyst–ionomer interface issues without suitably addressing the membrane or ionomer–membrane interface issues.

Project strengths:

- The team developed a series of PGM-free, perovskite-based OER catalysts that show promising performance (with 119 mA/cm^2, 175 mA/cm^2, and 243 mA/cm^2 at 60°C, 70°C, and 80°C in AEM, respectively, and almost no degradation at 100 mA/cm^2, 1.8 V for 100 hours). The team also demonstrated the significance of electrolyte in base and tried to understand the interfacial interaction.
- The project has a strong collaborative network focusing on the integrated cell-level work for an alkaline-based electrolysis system. Utilizing pure water, rather than a chemical solution, degrades performance but also has the potential to reduce the operating and capital costs of a production system.
- The project addresses important barriers for achieving low-cost hydrogen production with an AEM electrolyzer, especially with an emphasis on catalyst–ionomer interaction. Based on current progress, it seems there is a high chance that the team can achieve the planned milestones.
- This project has successfully identified PGM-free OER catalysts that demonstrate high current densities in the absence of alkaline electrolyte. Continued progress should provide fundamental understanding of the catalyst–ionomer interface and lead to even higher system performance.
- This is a new concept for Pt-free catalysts. There is interest in looking at the interaction between the catalyst and the ionomer.
- The project is well organized and has demonstrated solid progress with good scientific understanding.
- The project team has demonstrated progress with a challenging materials/operating system.
- The project team's strengths include its experience in PGM-free catalysts.

Project weaknesses:

- More attention should be paid to the alkaline membrane that enables the anionic communication between the OER and HER catalysts. It does not benefit this activity if the highest-performing catalyst–ionomer combination is incompatible with the anionically conductive membrane.
- The project's weaknesses include a lack of expertise in electrolyzer testing (single-cell), electrode manufacturing, and the not very clear path toward solving the triple-phase boundary in the electrode (with DI water operation).
- The project team has three weaknesses: (1) they have poorly performing catalysts, (2) they benchmark their performance to poor results for standards, and (3) their electrochemical methods are poorly validated.
- Evaluating the cost of the proposed MEA is necessary. The cost of the perovskite and electrolyte also needs to be taken into consideration.
- The project has a low-current-density target of 100 mA/cm^2 that translates to a high electrolyzer capital cost.
- While substantial progress has been made, the performance of the OER catalyst developed in this project is still lower than catalyst materials reported from other projects and previous literatures.
- The contribution from the industry partner is less clear until Phase II.

Recommendations for additions/deletions to project scope:

- The project uses mainly electrochemical testing methods. It could be beneficial for the team to consider more diversified tools—for example, more surface-sensitive and in situ material characterization approaches—to gain additional insights.
- The authors should get some advice from fuel cell researchers on how to do better electrochemical measurements. The team should also focus on developing a reasonable benchmark for the standard materials used in alkaline electrolyzers.
- The project team should continue utilizing the Energy Materials Network to leverage existing work and focus efforts on unaddressed issues. For this project, this holds true for the gas diffusion layer interface questions and the AEM properties.
- It is recommended that the team define clear mitigation strategies of the problems that were identified in Phase II in order to move forward.
- The increasing current density should be the major emphasis.
- It is recommended that the project have a cost analysis of materials and MEAs.

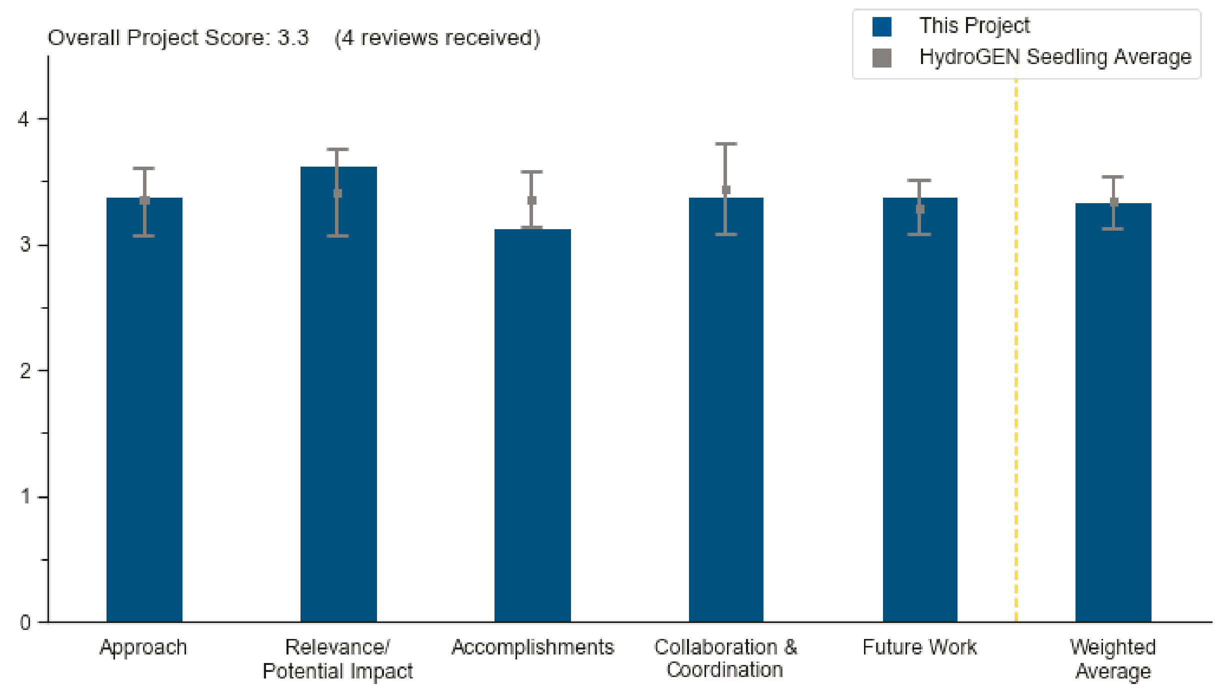
Project #P-159: Scalable Elastomeric Membranes for Alkaline Water Electrolysis

Yu Seung Kim, Los Alamos National Laboratory

Brief Summary of Project

The objective of this project is to develop stable, high-performance, and economically affordable alkaline anion exchange membranes (AEMs) for water electrolysis operation. A low-cost synthetic method based on acid-catalyzed condensation reaction (Friedel–Crafts alkylation) will be developed to fabricate the styrene-based triblock copolymers based on polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene (SEBS) to replace the prohibitively expensive metal-catalyzed reaction route. The project team, which also includes Rensselaer Polytechnic Institute (RPI) and Proton OnSite, aims to develop economically viable elastomeric ionomers having conductivity at least equivalent to polyaromatic electrolytes, with much-improved mechanical properties.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The project focused on developing low-cost hydroxide exchange membranes for alkaline water electrolysis. The team addressed three key barriers: membrane durability, hydroxide conductivity, and mechanical property. Through rationally designed modification of chemical structure and fabrication method, the team successfully demonstrated the membrane (SES25-TMA-1.7) that met the durability (0% loss of conductivity after 300 hours in 1 M NaOH at 80°C), conductivity (42 mS/cm at 30°C), and mechanical property (2091 MPa × %) milestone. In addition, through the collaboration with HydroGEN, the team observed the formation of acidicphenol, which could be the durability-limiting factor for alkaline electrolyzer. This finding would guide further improvement of the overall device durability through ionomer modification. However, more membrane characterization data—for example, the gas permeability of the membrane—at budget period 1 (BP1) would be helpful. Additionally, the developed AEM electrolyzer model showed that the overpotential from oxygen evolution reaction (OER) was much larger than that from hydrogen evolution reaction (HER), which deviated from experimental result.

- Alkaline electrolysis suffers from a lack of suitable, commercially available AEM membranes. This effort is exclusively focused on developing stable and scalable AEM membranes for eventual commercial production. The approach is to use evaluate different membrane chemical structures than what is used with state-of-the-art fuel cell membranes. The hope is to prevent degradation of typical AEM membranes by preventing phenyl degradation. The innovation here is developing a method for scalable synthesis and membrane-casting to make it more cost-effective. The specific technical barriers and challenges this project will overcome are membrane stability in alkaline electrolyte, hydroxide conductivity, mechanical properties, and AEM performance and durability. The membrane chemical structure is not new, but the team is developing methodologies for preparing the membrane in a scalable method so that it can be cost-effective. The project's approach centers on producing membranes using styrene–ethylene–styreneblock copolymers that are synthesized by an inexpensive acid-catalyzed route. The added benefit is expected to be a reduction in cost through the elimination of the expensive metal catalysts used in state-of-the-art membrane synthesis routes.
- This project has a clear objective to advance the alkaline membrane material technology, with all work focused toward generating and characterizing that material. In particular, this work evaluates the fabrication processes of membrane materials, then characterizes the hydroxide conductivity, water content, and material toughness. To complicate the project results, this project utilizes a non-traditional definition of toughness (stress times strain), rather than the traditional definition (area under the stress–strain curve).
- The selected block co-polymer synthesis route has multiple benefits.

Question 2: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- This topic is relevant to HydroGEN and extremely important for the alkaline hydrogen evolution field. Commercially available AEM membranes are limited to a few suppliers, and membrane supply and stability are issues. This project will further commercialization of AEM membranes, which are limited in the open market. Moreover, success will bring AEM electrolysis to the same technology readiness level as polymer electrolyte membranes (PEMs). AEM electrolyzer anode catalysts do not need iridium and can be orders of magnitude less expensive than PEM catalysts. Moreover, the flow field can be made from stainless steel, rather than more expensive titanium. These benefits will lower the system cost and allow production of hydrogen at or below $2/kg.
- Alkaline water electrolysis typically uses platinum-group-metal-free catalysts and low-cost stack components, and therefore the capital cost of hydrogen production is significantly reduced. However, the critical drawbacks of alkaline electrolysis are the conductivity and durability of the hydroxide exchange membrane (HEM). This project directly addresses these critical drawbacks by demonstrating a low-cost synthetic route to high-performance and durable HEMs. The improvement of stability and hydroxide conductivity of HEMs enables the pathway to low-cost hydrogen production in alkaline conditions.
- The higher pH of the alkaline electrolysis chemistry, compared to the acidic chemistry, enables a wider range of wetted materials. This significantly reduces the cost of the components within an electrolysis system. The alkaline membranes traditionally lack the durability or performance required for commercial high-pressure electrolysis systems. Generating a high-pH polymer membrane with sufficient durability and performance to compete with the acidic polymer membranes at the cell level would merge the mechanical lessons from the high-pressure PEM systems with the low-cost materials from the alkaline systems.
- The promise of reducing electrolyzer capital cost is appealing, assuming that the current density of PEM electrolyzers can be matched.

Question 3: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has shown good progress. All fiscal year (FY) 2018 milestones have been met, and now the team is looking at the chemical structure to try to improve conductivity and water-uptake properties. The project has met membrane conductivity requirements, and strain testing has shown good structural stability. The team is trying to further improve mechanical properties through crosslinking within the chemical structure. The secondary electron spectrum (SES) copolymer showed no chemical degradation over 300 hours in 1 M NaOH, with good conductivity and mechanical toughness. An AEM electrolyzer model has been developed to predict system performance and improve understanding of how pH at the catalyst–ionomer interface can impact HER and OER performance.
- The project team successfully demonstrated the membrane (SES25-TMA-1.7) that met the durability (0% loss of conductivity after 300h in 1M NaOH at 80°C), conductivity (42 mS/cm at 30°C), and mechanical property (2091 MPa × %) milestones. The team also demonstrated a crosslinking strategy to improve the mechanical property further. The XL100-SES25-TMA-1.7 membrane has conductivity comparable with SES25-TMA-1.7 but exhibits a high tensile toughness of 6055 MPa × %. The project also identified a limiting factor that affected the durability in alkaline water electrolysis. These results help guide the future improvement on HEMs, as well as the ionomer.
- The project down-selected to a preferred membrane, synthesized and characterized an ionomeric binder, and demonstrated polyolefinic SES co-polymer with chemical stability and high ion conductivity. From the presentation materials, it remains unclear what milestones pertain to BP1 and BP2. This complicates the ability to evaluate progress.
- The project has shown successful polymer synthesis with promising properties.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The major project partner, Los Alamos National Laboratory (LANL), worked on the identification of performance and durability limiting factors for AEM electrolyzers while RPI focused on polymer membrane fabrication and characterization. The team planned to collaborate with an industrial partner (Proton Onsite) to demonstrate electrolyzer performance. The team worked closely with the Lawrence Berkeley National Laboratory (LBNL) to carry out comprehensive studies on the SES membrane, as well as AEM performance modeling. To validate the improvement of the membrane in alkaline water electrolysis, NERL would be involved to perform the AEM performance evaluation. The overall collaboration is efficient.
- The project has good collaboration across the HydroGEN nodes. For example, LBNL is working on X-ray scattering characterization, microelectrode studies, and AEM performance modeling; Sandia National Laboratories (SNL) provided a baseline AEM for comparison; and the National Renewable Energy Laboratory (NREL) is evaluating AEM performance.
- There is good collaboration with RPI and Energy Materials Network (EMN) nodes. LBNL, SNL, and NREL collaboration will be very important for performance and durability validation.
- The presentation materials suggest that collaborative activity occurs just within the national laboratories. There is solid evidence of strong utilization of the EMN nodes, including LBNL, NREL, and SNL, to fabricate and characterize materials.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The project's future plans seem reasonable for achieving a target AEM performance of 1 A/cm^2 at 2 V with less than 0.2 mV/h degradation during a 300-hour electrolysis test. The future plans involve optimizing ion exchange capacity, block size, cationic group, and crosslinking density of SES membranes to improve performance. The project's future plans include completing AEM electrolyzer degradation studies compared with optimized membranes produced in this study. In FY 2020, the team will down-select the most promising materials based on performance, optimize the electrolyzer operating conditions, and begin scaling the synthesis of membranes and ionomers.

- The future work consists of further developing the anionic polymer and conducting performance and durability testing on ionomers and AEM electrolysis membranes. As the target does not specify the process fluid (pure water versus solution), the target membrane electrode assembly performance may or may not be relevant. It would also be helpful to have a list of BP2 milestones to compare predicted progress to actual progress.
- The team planned to focus on the crosslinking SES and full device testing for the year 2019. Down-selection of AEM and ionomer, as well as scale-up fabrication, would be carried out in 2020. The planned work would help advance the proposed technology.
- Data at 1 Am/cm^2 and >1,000-hour durability test is highly anticipated.

Project strengths:

- This project heavily utilizes the strengths of the EMN to rapidly develop a viable anionic polymer for use as a solid polymer electrolyte in an alkaline electrolysis system.
- This project has shown good progress toward developing a scalable and stable AEM membrane. Good collaboration with other national laboratories has allowed for characterization of membrane structure and performance.
- The major strength of the project is that it has demonstrated a low-cost synthesis approach for durable and conductive HEMs.
- The project's strengths include its interesting approach to polymer synthesis.

Project weaknesses:

- The presentation material does not clearly define the use of a nontraditional definition of mechanical toughness. Traditionally, toughness is the area under the stress–strain curve. Applying a direct multiplication of the stress and strain inaccurately inflates the results. Currently, the alkaline membrane durability is a major limiting factor to the implementation of a high-pressure alkaline electrolysis system. It would be beneficial to standardize the nomenclature and testing processes so that materials can be consistently characterized. This permits an accurate assessment of the suitability of a material for a particular application.
- The project's weaknesses include the lack of cost evaluation of the proposed technology and yield comparison to prove the benefit of the proposed synthesis method.

Recommendations for additions/deletions to project scope:

- It is recommended that the project team do a cost estimation on synthesis and compare it with the state-of-the-art approach. A gas permeability test of the membrane is recommended for membrane characterization. More details should be provided on how modifications of the ionomer can help solve the effect of pH on durability.
- The project team should continue the effective use of the EMN nodes and standardize measurement processes and nomenclatures to enable consistent comparison of results across the network.

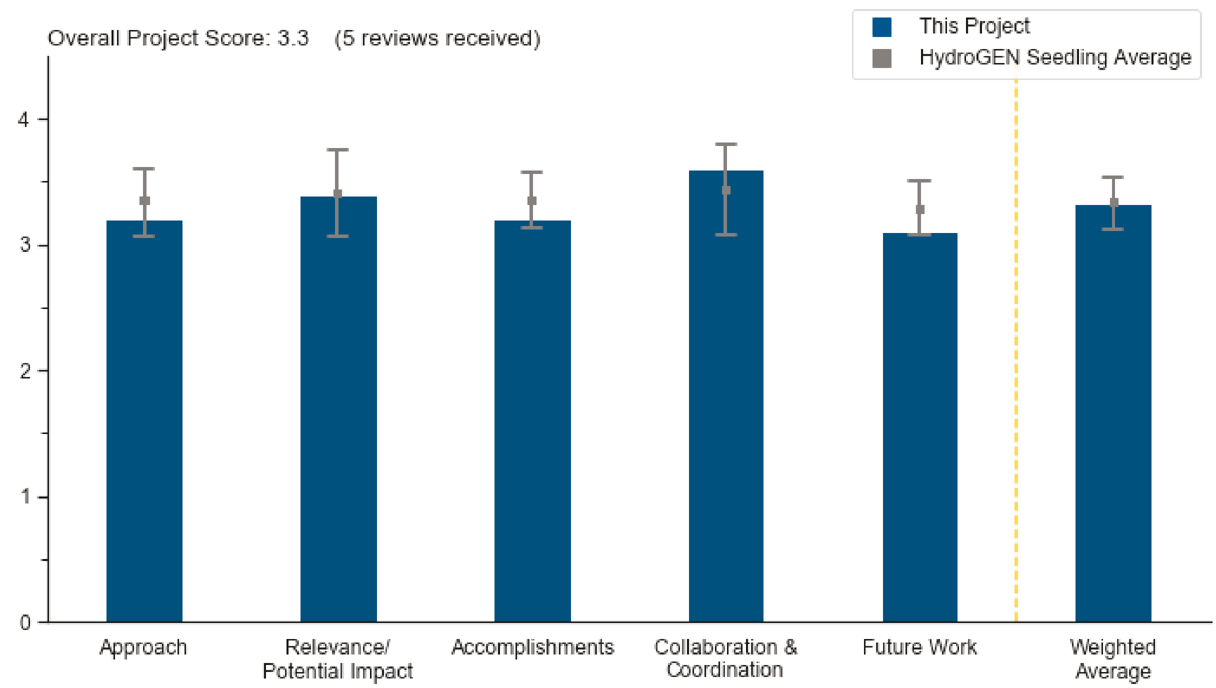
Project #P-160: Best-in-Class Platinum-Group-Metal-Free Catalyst Integrated Tandem Junction Photoelectrochemical Water-Splitting Devices

Charles Dismukes, Rutgers University

Brief Summary of Project

This project will identify the best technical approaches to fabricate both high-performance (HP) and high-value (HV) platinum-group-metal-free (PGM-free) catalysts for photoelectrochemical (PEC) cells without compromising system efficiency. Next-generation devices must eliminate PGMs, even though they perform well, because of cost and sustainability limitations. Using recently developed low-cost HP catalysts, the team will examine the optimal pairing of these materials with established HP and emerging HV photoabsorbers. Cost–benefit analysis of full HP and HV devices and their individual components will enable the preparation of a hybrid product that will significantly advance the state of the art and that has the potential to deliver on all U.S. Department of Energy figures of merit: cost, performance, and stability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The focus on demonstrating improvements to an HP and HV integrated system is a well-conceived plan. The developed designs show a nice synergy between node capabilities and local expertise. Much of the effort to date has focused on the integration of components, and now with demonstrated success here and as the project further matures, it may be useful for the group to think strategically about how to improve both efficiency and durability. This is true in particular with respect to durability; the group should think about how they intend to understand the limiting features and overcome them. A clearer strategy here for the HP and new HV system may be warranted.
- The team has proposed an approach that explores two potential systems: an HP device based on III–V semiconductors and an HV one that uses inexpensive light absorbers. The approach leverages novel

electrocatalysts developed at Rutgers University (Rutgers) and looks at how they may be integrated through interfacial and protective layers with light absorbers. The HP devices are aligned with possibly reaching the DOE performance targets of 20% solar-to-hydrogen (STH) efficiency, and the HV with the $2/kg cost goal. Although these two systems may seem reasonable, it is unlikely that any of the systems would satisfy both performance metrics. The approach for the development and integration of protective coatings and electrocatalysts is appropriate, and the principal investigator (PI) has a proven track record with the materials proposed. The project is well integrated with the HydroGEN network, and the team effectively leverages HydroGEN resources that have complemented project developments. This includes partnerships with the National Renewable Energy Laboratory (NREL) for light absorber development and on-sun testing. The approach to developing HV devices involves the exploration of multiple possible light absorbers but lacks a clear rationale for the choice of materials. The hybrid organic–inorganic perovskites (HOIPs) system demonstrated is quite promising in terms of efficiency and cost, but it needs to be encapsulated to withstand being submerged in electrolyte. It seems clear that a photovoltaic (PV) electrolysis approach is more appropriate to this system.
- Developments utilizing $LiCoO_2$ oxygen evolution reaction, Ni_5P_4 hydrogen evolution reaction, and a TiN diffusion barrier are notable and may have good promise.
- There is a good balance to proving low-cost catalysts can operate in these PEC system configurations on high-cost/HP devices while simultaneously trying to develop them in inexpensive systems.
- The project's approach is effectively addressing the important issue of finding a balance between performance, durability, and cost.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- This project shows a very nice synergy between the participants (i.e., NREL III–V nitrides and Rutgers' work in PGM-free catalysts) in the demonstration of new PEC devices. The new device architectures do have good potential to advance the field. Although much of the focus has necessarily been on integration thus far, there are already promising results. As the project continues to mature, to maximize this impact, it will be necessary to identify techniques for improving efficiency and durability. The team has suggested several routes for the former, but the latter appears somewhat less well developed. While durability is a very challenging problem, it will be necessary to identify strategies to understand and mitigate degradation in the project systems if maximum impact is to be realized.
- The project supports and advances progress toward DOE Hydrogen and Fuel Cells Program (the Program) goals and objectives and also supports the HydroGEN Consortium mission. The HP thrust is making progress toward the DOE's technical targets for PEC efficiency and stability, while the HV approach is attempting to address costs. There is good leverage of HydroGEN resources available to the project.
- The project partly supports the DOE hydrogen goals, as it provides a path for the development of either high-efficiency STH electrodes that are stable for prolonged periods of time or HV devices that may produce hydrogen at a reduced cost. The project also enhances the HydroGEN network, as the team may be able to provide a protocol for the synthesis of high-efficiency electrocatalysts, which may be leveraged by others in the PEC community, thus leading to integrated PEC systems with earth-abundant electrocatalysts. It is unlikely that the project will have a direct impact on the $2/kg DOE goal, given the significant barriers: (1) the III–V-based photoelectrodes explored in the HP devices are too costly, and (2) the HV devices have very limited efficiencies (perhaps with the exception of the HOIP system).
- Achieving the three factors of efficiency, durability, and cost is crucial for reaching the DOE goal of $2/kg of hydrogen. Therefore, this project is very relevant, and the potential impact is high.
- The project's relevance and potential impact is satisfactory.

Question 3: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has shown adequate progress toward meeting most of the targets. The $LiCoO_2/ZnSnN_2$ photoanode work is not complete. The team has made good progress toward the integration of NiP_2 electrocatalysts with HP photoabsorbers. The achievement of HP devices capable of performing unassisted water-splitting at an STH efficiency of 11.5% is promising, but it is still far from the 20% STH required by the Program. The durability tests on a Ni_5P_4/TiN/$GaInP_2$ device are encouraging, but the fact that the photoelectrodes needed to be periodically etched to sustain activity is concerning. The team was able to rapidly evaluate $ZnSnN_2$ light absorbers and discard this materials system because of its poor performance. The incorporation of HOIP light absorbers with high efficiency can lead to high-efficiency HV devices and thus should continue to be explored. Although the quality of the $SrNbO_2N$ films obtained is high, their performance is quite low, and thus continuing to explore them seems unjustified.
- The go/no-go metrics were fairly aggressive, and NREL validated the data gathered at Rutgers. The accomplishments in the HP thrust are outstanding, but the HV is showing only fair progress. It was a good choice to move on from the $ZnSnN_2$ material that was not showing any promise. The $SrNbO_2N$ should either quickly show it can achieve several mA/cm^2 or be abandoned. It was a prudent move to include the HOIPs node to bring into this project some low-cost materials that have the potential to generate photocurrent and photovoltage.
- The project has made substantial progress in the HP system, having met the targets for both efficiency and durability. The decision to forgo the nitride system and move toward an alternative HV structure, taking advantage of node capabilities, is reasonable.
- Overall, the project team has achieved great accomplishments. If they were successful in making the low-cost approach with $ZnSnN_2$ work, the score would have been higher. However, given the limited resources, the team made the right decision in discontinuing this subtask.

Question 4: Collaboration effectiveness

This project was rated **3.6** for its collaboration and coordination with HydroGEN and other research entities.

- This is a highly collaborative effort, which has benefitted from several node capabilities in metal–organic vapor-phase epitaxy (MOVPE), III-V semiconductor & semiconductor characterization (referred to as the PEC node in the presentation), High-Throughput Experimental Thin Film Combinatorial Capabilities (referred to as the HTE node in the presentation), and HOIPs. There are strong, demonstrated interactions with nodes, participation in HydroGEN activities, and contributions to HydroGEN's Data Hub.
- The project shows close, appropriate collaboration with other institutions, specifically the HydroGEN Consortium, with appropriate use of nodes, contributions to the benchmarking and protocols (2b) project, and the HydroGEN Data Hub. The project's partners are full participants and well coordinated. There is evidence of significant interaction and collaboration.
- There are good collaborations within the team, as well as with the capability nodes, that are clearly well reflected in their accomplishments.
- The project team shows good collaboration with NREL.
- The team effectively leverages nodes at NREL that directly enhance the project activities.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project's proposed future work is on a good track.
- The project's proposed future work is generally effective but could be improved; it contributes to overcoming some barriers, meeting some end-of-project goals, and potentially to advancing the materials research mission of the HydroGEN Consortium. The HP targets and tasks are outstanding. Focusing on short-circuit stability testing, pushing on efficiency with next-generation III–V tandems, and validating

both with on-sun testing is precisely what this project should be focusing on to meet DOE technical targets. The future work for the HV is only fair because of the partial focus on exploratory materials that have yet to prove their worth (e.g., $SrNbO_2N$), which is partially abated by the perovskite work.
- Focusing on improving the performance of HP III–V devices seems appropriate, especially given that only 11.5% STH has been demonstrated. The on-sun testing seems premature, especially given that the efficiency targets have not been met. Spending valuable resources on understanding the behavior of under-optimized photoelectrodes under real-world conditions seems unjustified. The team should consider demonstrating a device with a ~>20% STH target before engaging with the on-sun testing. Continuing to work on p-$SrNbO_2N$ photoabsorbers also seems unjustified, given that the current densities obtained were less than 500 uA/cm^2. The team might benefit from investing the resources granted toward HOIP devices, which are significantly more promising.
- The proposed future work seems reasonable but is vague in many instances. For the HP device, there are proposed approaches to improving the efficiency, but more clarity on understanding degradation and improving durability would be beneficial. Regarding the new HV system, the goals are still focused on demonstrating half-cells with the alternative anode materials, but if this can be accomplished, then it is unclear what the associated targets are for efficiency and durability.
- Dropping the least promising subtask is making the proposed future work more promising, with more focus and concentrated effort.

Project strengths:

- This project is making remarkable progress in the HP thrust, with a low-cost catalyst that has shown protective abilities in addition to being an excellent hydrogen evolution catalyst. The interaction with the rest of the HydroGEN nodes and 2b team is another notable strength.
- The project team has demonstrated integration of Ni_5P_4/TiN with $GaInP_2$, reached >10% STH with HP devices, and rapidly screened $ZnSnN_2$ properties, concluding that it had no promising performance properties.
- This is a very competent team, fully leveraging their assets of non-PGM catalysts and surface coating. The very effective collaborations are clearly reflected in their very successful accomplishments.
- The key strengths of this project are the unique device designs that combine expertise of all participants, the strong interaction with nodes, and the focus on demonstration of both an HP and HV device.
- The project team has identified a promising HV device based on HOIP photoabsorbers.
- The project's strengths include the use of new materials.

Project weaknesses:

- There are not many weaknesses. If there was one, it was that not much attention seemed to be paid to understanding why $ZnSnN_2$ did not perform well. However, presumably it was a strategic choice to save resources.
- It is not clear whether the device will work if the pinholes during manufacturing are not avoided. This may indicate a design that is not robust.
- The project's efficiency levels are far from DOE targets, and there is not a clear path to achieving them. Continuing the work on $SrNbO_2N$ is unreasonable based on the poor performance of this photoabsorber. On-sun testing is premature, given the lack of high-efficiency PEC materials.
- The project's largest weakness may be the lack of clarity on strategies for understanding degradation mechanisms and improving durability in the fabricated devices.
- Little progress has been made in the HV thrust.

Recommendations for additions/deletions to project scope:

- The team should consider focusing all their efforts on the most promising HV material, HOIP. For the HP materials, a clear set of tasks and a timeline should be defined to reach the 20% STH target set by DOE.
- Completion of the proposed work is strongly recommended.
- The scope of the project seems reasonable.

- The HV thrust that relies on the HTE node should be re-scoped. While the HTE node might be an appropriate tool for validating theoretical predictions of physical properties of a combination of various elements, to date it has been unable to provide a material that could reasonably be called a photoelectrode.

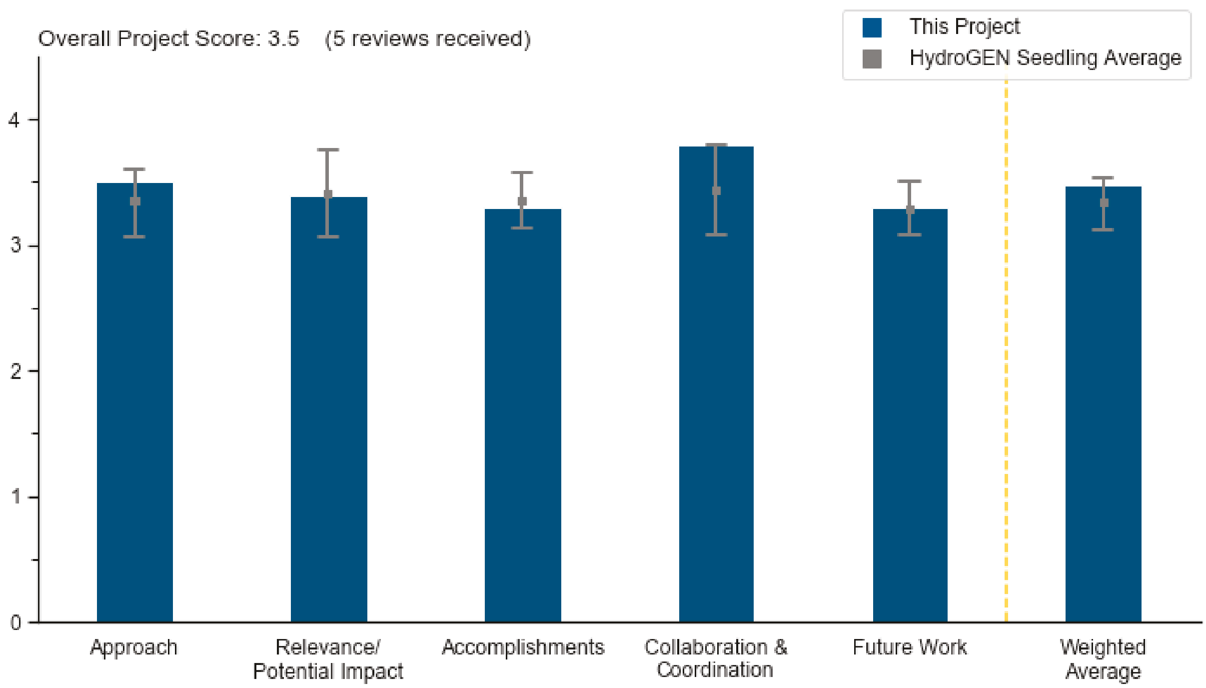
Project #P-161: Protective Catalyst Systems on III-V and Silicon-Based Semiconductors for Efficient, Durable Photoelectrochemical Water-Splitting Devices

Thomas Jaramillo, Stanford University

Brief Summary of Project

The overall goal of this project is to develop unassisted water-splitting devices based on III-V materials, creating pathways to improve performance in terms of efficiency (>20% solar-to-hydrogen [STH]), durability (two weeks), and cost (<$200/m^2). Two distinct water-splitting schemes are being pursued: Scheme 1 (tandem III-V/III-V) aims to develop high-efficiency devices with tandem III-V photoabsorbers (e.g., $GaInP_2$/GaInAs), and Scheme 2 (III-V/Si) targets cost reduction while maintaining high efficiency by growing InGaN on crystalline Si. Both schemes will be coupled with thin-film, semi-transparent hydrogen and oxygen evolution reaction catalytic/ protection layers containing reduced or zero precious metal content that can enhance durability while maintaining high efficiency and enabling low material costs.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach is sharply focused on critical barriers and validating technology innovation and is difficult to improve significantly. The barriers have been clearly identified and are being addressed through project innovation. It is a well-designed project that is highly integrated with the HydroGEN Consortium network. The budget period 1 work scope was used to validate the approach and technology innovation.
- The principal investigator has proposed Scheme 1 using III-V/III-V and Scheme 2 using III-V/Si to overcome the barriers. This dual approach is excellent, as the first one aims for the high-efficiency devices and the second one for utilizing existing Si-based technologies.

- The team has proposed an approach that combines the development of high-efficiency III-V photoelectrodes and earth-abundant, protective electrocatalytic coatings to reach a >20% STH that is stable for prolonged periods of time. This is in line with U.S. Department of Energy (DOE) desired targets for photoelectrochemical (PEC) devices.
    - The approach for the development of protective coatings is appropriate, and the principal investigator has a proven track record with the system proposed. Preliminary results are encouraging, although the protective layers ultimately degrade in a limited number of hours.
    - The fundamental approach proposed to understand degradation is likely to lead to useful insights that may assist in the development of more stable protective coatings. Despite the need for such fundamental studies, it is likely that the time required to understand degradation mechanisms will go beyond the timeframe of the current project. Thus it is unlikely that the project will have a significant impact on the ultimate objective of the DOE Hydrogen and Fuel Cells Program (the Program), independently of the project's self-evident scientific merits in the context of the broader PEC community.
    - While focusing on III-V semiconductors is reasonable in the context of the STH efficiency target, it is difficult to justify that the $2/kg goal can be achieved with the current approach. The team's approach to this economic target is to develop III-V/Si tandems, but the potential cost benefits of such an approach are not quantitatively addressed to fairly evaluate the validity of the approach.
    - The project is well integrated with the HydroGEN Consortium network, and the team effectively leverages resources from it that have complemented project developments.
- This is a well-designed project that targets ambitious PEC goals of demonstrating 20% STH, with on-sun testing for two weeks, via incorporation of protective catalysts on III-V systems. The use of these transition metal-based catalysts on III-V- (and Si-) based systems offers a promising route forward on a challenging problem. The team is pursuing a few device structures in parallel, with the ultimate goal of demonstrating a Si/InGaN system that achieves these goals. The utilization of Energy Materials Network (EMN) capabilities and collaborations is strong as well.
    - Most of the project objectives are concrete (e.g., unassisted water-splitting devices that can achieve >20% STH efficiency and operate on-sun for at least two weeks). However, the objective to provide a path toward electrodes that cost $200/m^2 via earth-abundant, protective catalysts and novel epitaxial growth schemes is not. It is not clear what constitutes "providing a path."
    - The part of the approach that seems the least well developed is the in operando characterization for in-laboratory stability studies. This is an admittedly challenging problem, and the research community certainly stands to learn a good deal from these measurements. However, what is less clear is, even if specific degradation modes are identified, what can be realistically done over the project time frame to overcome limitations.
- Overall, the approach is well-balanced, addressing efficiency, durability, and cost. One minor comment is that MoS_2-based surface protection has a disadvantage in achieving surface protection and catalytic activity simultaneously because of the edge active nature of the material as a catalyst.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- There are strong potential impacts in (1) the demonstration of stabilization of III-V surfaces via earth-abundant, protective catalysts, (2) the potential offered by the InGaN/Si device, which, if successful, may offer a path to high efficiencies with inexpensive processing, and (3) the plans for multiple-week on-sun testing. The team is making substantial progress toward the ultimate project goals, and whether they are ultimately met or not, the project will help us to learn many new things.
- The project aligns well with the Program and DOE research, development, and demonstration (RD&D) objectives, has the potential to advance progress toward DOE RD&D goals and objectives, and is aptly leveraging and contributing to the resources and framework of the HydroGEN Consortium. The varied tasks appropriately address the most important performance metrics of the PEC system, namely efficiency, durability, and cost. For example, working on a transferrable, protective catalytic coating on an efficient but too costly III-V that could eventually be applied to the low-cost InGaN/Si system is an effective way of parallelizing the research activities to ensure continued progress.

- This project addresses the crucial factors for the DOE goal, achieving efficiency, durability, and cost simultaneously. Therefore, it is very relevant, and the potential impact is very high.
- The project supports the Program goals as it provides a path for the development of high-STH-efficiency electrodes that are stable for prolonged periods of time and produce hydrogen at a reduced cost. The project also enhances the HydroGEN Consortium network, as the team may be able to provide a protocol for the synthesis of high-quality, protective electrocatalytic coatings to other teams in the network and synergistically accelerate a path toward more stable PEC devices.
    - It is unlikely that the project will have direct impact on the $2/kg DOE goal, given significant barriers to obtain (1) III-V-based photoelectrodes with significantly reduced costs to outcompete alternative technologies such as Si-based photovoltaic-driven electrolysis, or (2) a high enough STH to offset the higher cost from the III-V semiconductors. The team is far from the 20% STH target, and even if this is reached, it is not clear how this may offset the high cost from III-V semiconductors.
- The work directly supports the Program goals.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project is effective, contributes to overcoming most barriers, and provides data that considerably supports the accomplishments toward impactful go/no-go criteria. The durability results are impressive for a III-V photocathode, and progress toward the go/no-go criteria is supported by unambiguous data.
- The accomplishments to date are impressive overall, with project milestones met or very nearly met. If the InGaN/Si device is the ultimate target for efficient, durable, and low-cost PEC devices, then there are still several steps to be taken to achieve project goals in this structure. At present, the team is still working on demonstrating rectifying behavior in this system and will strategically need to move toward PEC devices and assessment of efficiency and durability.
- The team has made good progress toward developing Scheme 1 and 2 photoelectrodes, protective coatings, and analytical techniques to assess degradation mechanisms.
    - The achievement of >5% STH unassisted water-splitting devices was aligned with the initial targets, but these devices were based on Scheme 1 photoelectrodes, which are expected to be significantly more expensive than Scheme 2 photoelectrodes. Also, the operation of these photoelectrodes was sustained for only a limited number of hours, and it is unclear how long-term stability may be achieved.
    - The STH achieved initially is far from the project target of 20%, and despite trying different material systems, no significant breakthrough has been reached.
    - The preliminary plans and results on the in situ flow cell for Raman microscopy are encouraging for better understanding of degradation mechanisms.
- Progress on most of the important tasks is on track, steadily moving toward the DOE goals. One minor comment is that the progress in improving the durability is slightly lagging behind the rival approach. It is hoped that this is not due to the choice of protection scheme.
- The team is making adequate progress toward the goals. Unassisted water splitting is showing improvement but is far from the PEC goal.

Question 4: Collaboration effectiveness

This project was rated **3.8** for its collaboration and coordination with HydroGEN and other research entities.

- The project has close, appropriate collaboration with other institutions, specifically the HydroGEN Consortium, with appropriate use of nodes, contributions to the benchmarking/protocols (2b) project, and the HydroGEN Data Hub. Partners are full participants and well coordinated. There is evidence of strong coordination with the HydroGEN nodes, as well as the 2b project. There appears to be regular, meaningful interactions between this project and the nodes.

- The team effectively leverages nodes at Lawrence Berkeley National Laboratory (LBNL) and National Renewable Energy Laboratory, which directly enhances the activities of the projects. The new collaboration with LBNL for the in situ Raman spectroscopy is well suited.
- The team demonstrated very well-coordinated efforts that are evidenced in robust progress in improving the efficiency and durability of three types of devices based on III-V and nitride.
- The effort synergizes nicely with EMN nodes and capabilities, which are integrated throughout most tasks on semiconductor epi-layer fabrication and characterization, corrosion analysis, and on-sun benchmarking.
- The project has excellent collaboration.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The incorporation of in situ Raman surface observations is an appropriate path to enhancing the understanding of corrosion phenomena. Also, the use of on-sun testing is important to translate the performance under the artificial conditions applied in the laboratory to a more meaningful and relevant set of conditions an actual PEC device would encounter.
- Given the steady progress made toward DOE goals, continuing the current tasks with an additional in operando corrosion study seems a rational choice.
- The principal investigator has clearly identified the remaining challenges and barriers. The mechanistic understanding of the stability will be of value to the research community.
- A specific set of tasks that will be explored for the optimization of Scheme 1 and 2 photoelectrodes were missing from the presentation. This is particularly important because the performance of the devices tested to date is far from the project target, and the time and financial resources to achieve the required improvements are very limited. A more specific set of tasks and a timeline for research and development activities that directly tackle the pain points of the tested devices would be useful at accelerating the path toward a high-efficiency device. The proposed in situ characterization work is well aligned with the objective of improving the stability of these devices. The on-sun testing seems premature, especially given that the efficiency targets have not been met. Spending valuable resources on understanding the behavior of under-optimized photoelectrodes under real-world conditions seems unjustified.
- The future work as presented was somewhat vague. A fair number of steps remain ahead to achieve the ultimate goal of 20% STH efficiency, and the specific barriers and next steps to overcome these barriers were not clearly outlined.

Project strengths:

- There is a strategic focus on goals and the potential to make a fair amount of headway in (1) stabilization of III-V surfaces via protective catalysts, (2) fabrication of InGaN/Si tandem, and (3) collection of on-sun data via collaboration with EMN nodes.
- All of the personnel, from the principal investigator to the graduate students, are highly skilled and knowledgeable in materials synthesis, characterization, and PEC water-splitting phenomena. The intellectual rigor they apply to the project is obvious.
- The project has demonstrated protective electrocatalytic coatings with long-term stability, as well as >10% STH PEC devices based on III-V tandem electrodes. There is strong integration with the HydroGEN Consortium network and collaborations among team members. There is a clear path to identify degradation mechanisms through in situ spectroscopy.
- The principal investigator has been demonstrating the leading role in the PEC community with extraordinary scientific contributions, and this team is showing itself to be a role model for the HydroGEN Seedling projects by being engaged in the great collaborations.
- The strong team is the strength of this project.

Project weaknesses:

- It is difficult to find a weakness. If any, the late introduction of the in operando corrosion study may delay development of a mitigation strategy.

- The only weakness of the project is the slow progress the InGaN/Si task seems to be making. There is not much time left in the project to prove a tandem structure can split water spontaneously and then to optimize the performance.
- STH achieved in Scheme 1 devices is far from the project target, and a clear path to efficiency improvements has not been presented. On-sun testing is premature, given the lack of a high-efficiency PEC materials system.
- A clear path to improved performance, particularly with respect to durability, will need to be identified.

Recommendations for additions/deletions to project scope:

- This project has shown very robust progress toward the DOE goals, and the principal investigator continues to contribute to the PEC research community. The continuation of the proposed work is strongly supported. The in operando corrosion study should be given higher priority to accelerate development of an effective protection method.
- The team could leverage Si/InGaN tandems developed by other HydroGEN teams to surpass one of the project's technical milestones without spending resources to develop an alternative fabrication approach for an equivalent materials system.
- The project scope is reasonable as is.

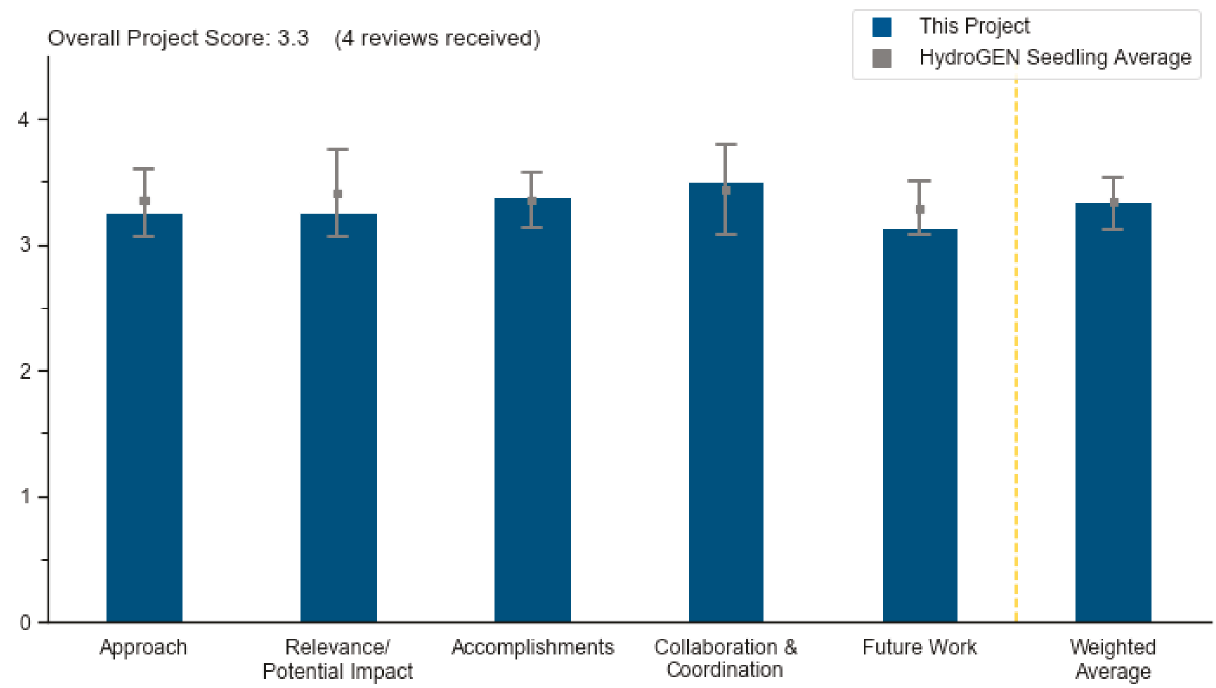
Project #P-162: Novel Chalcopyrites for Advanced Photoelectrochemical Water Splitting

Nicolas Gaillard, University of Hawaii

Brief Summary of Project

The overarching goal of this project is to create a chalcopyrite-based, semi-monolithic, tandem hybrid photoelectrode device prototype that can operate for at least 1,000 hours with solar-to-hydrogen (STH) efficiency >10%. The performance of previously identified wide-bandgap chalcopyrite materials will be improved through alkali doping to passivate copper indium gallium selenide (CIGS) defects, and next-generation chalcopyrites (e.g., Ga-free) will be developed. The photoelectrochemical (PEC)–electrolyte interface energetics and stability will be improved by investigating alternative buffer materials and protective layers. Also, novel fabrication methods will be developed for creating the semi-monolithic chalcopyrite-based tandem devices.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- This project targets the development of chalcopyrite-based PEC tandem devices that are inexpensively manufactured via solution processing and bonding techniques. The ultimate goals are listed as achieving improvements in STH efficiency from 4% to 10% and improvements in durability from 350 hours to over 1,000 hours. There is a clear vision, a target device design, and a set of objectives that must be met to achieve the goals. A potential concern may be that for the most part, the initial set of milestones focuses to a large extent on proof-of-concept demonstrations for more well-studied materials, rather than the new chalcopyrite materials targeted by the effort. The efforts working with the new chalcopyrites appear to be relatively new, and as such, many of the critical goals of this project are backloaded, coming toward the end of the project. There may be several issues to overcome once the team turns to the new widegap and interface materials systems of interest, especially once the project moves toward PEC devices and the characterization of their performance.

- The team's approach thoroughly explores the implementation of chalcopyrite-based PEC systems by combining experimental and synthesis methods for chalcopyrite photovoltaics (PV), with tandem device integration through transparent interfacial layers and protective catalytic coatings to enhance stability. Printable chalcopyrites are interesting from an economic perspective, as they may lead to low-cost PEC materials. In terms of efficiency, it is unlikely that the chalcopyrites explored are capable of reaching the U.S. Department of Energy goal of 20% STH efficiency. The approach is missing a clearly articulated path to reach high efficiency. The team is well integrated and leverages complementary expertise from principal investigators (PIs) from multiple universities and HydroGEN nodes.
- The project's approach is effective and contributes to overcoming most barriers and validating technology innovation. The PI has identified four key barriers and is addressing each of them through innovative approaches. It is a well-designed project and is integrated into the HydroGEN network.
- Chalcopyrites have shown great promise in PV. The project explores its PEC applications. The project team has planned adequate tasks related to synthesis, interface engineering, and device integration. The proposed "printing" technique can help realize the cost targets.

Question 2: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- Most of the project aspects align with the DOE Hydrogen and Fuel Cells Program (the Program) and DOE research, development, and demonstration objectives, and the project is adequately leveraging and contributing to the resources and framework of the HydroGEN consortium. The strength of the project is exploring the materials space of the chalcopyrites and investigating novel, lower-cost synthesis approaches to these materials that can generate high current densities. Unfortunately, these materials continue to struggle in generating a sufficient photovoltage in a PEC configuration, which makes them unlikely to meet the STH efficiency target. Another weakness is that these appear to be economical only under very high solar concentrations (25x), which is an unlikely scenario for a functional device because of mass transport issues under concentration.
- From the technoeconomic standpoint, there is high potential impact, should the project be successful. This is especially true if it turns out that it is possible to inexpensively print the widegap chalcopyrite materials and use the proposed exfoliation and bonding approach to build a multijunction device. These goals are fairly ambitious, but even demonstrating progress on individual technical barriers (even if ultimately they cannot all be overcome) will offer valuable steps forward for PEC water splitting.
- The project partly supports the Program's goals, as the exploration of inexpensive, printable chalcopyrite materials may lower the cost of PEC materials, but it is unlikely to match the efficiency targets required. The materials presented have demonstrated a PV efficiency of only ~10%, which is anticipated to drop when integrated into a PEC device. The project also enhances the HydroGEN network, as the team may be able to provide new light absorbers, which may be integrated in PEC devices with multiple components from the community.
- The potential impact of the work is high owing to the possible compatibility with industrial manufacturing.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project has met its milestones for the first year and is currently working toward second-year milestones. The group has successfully identified alternative chalcopyrite materials ($Cu(InAl)Se_2$, $Cu(InB)Se_2$) that may exhibit fewer defects during synthesis or manufacturing, but the group now needs to turn the focus to demonstrating the printing of the new materials. Similarly, the group has successfully demonstrated the exfoliation and bonding approach for more standard materials (e.g., CIGS) but will need to start developing this for the new materials of interest.

- The project has been effective; it contributes to overcoming most barriers and provides data that considerably support the accomplishments toward impactful go/no-go criteria. There has been considerable progress in this project on many fronts, despite the lack of a single, high-efficiency PEC device. The accomplishments on modeling, ink printing, surface treatments, and transparent conductive binders are significant and could be applied to other material systems if the current set is unable to meet PEC water-splitting targets.
- The team has shown promising integration of modeling with synthesis activities in the context of chalcopyrite PV. The transparent conductive binders show promising performance, both in terms of their optical properties and their electrical conductivity, and these materials may be leveraged for other energy applications. The WO_3/Pt protective layer shows reasonable performance over hundreds of hours, although the performance progressively degraded over time.
- The team is making adequate progress toward the goals.

Question 4: Collaboration effectiveness

This project was rated **3.5** for its collaboration and coordination with HydroGEN and other research entities.

- There is close, appropriate collaboration with other institutions, specifically HydroGEN, with appropriate use of nodes, contributions to the benchmarking and protocols (2b) project, and the HydroGEN Data Hub. The project's partners are full participants and well coordinated. This project is very well integrated with external collaborators (including the University of Nevada, Las Vegas, and Stanford University) in addition to HydroGEN nodes and the 2b team.
- Several collaborations with Energy Materials Network (EMN) nodes are detailed. While some of these seem critical to the project itself, the specific synergies with other collaborations were somewhat less clear. For example, combinatorial development of tunable buffers to improve the interfacial properties supports a critical goal of this project, which is to improve interface stability and performance in the integrated systems. On the other hand, it was less clear how some aspects of the theory and modeling results are to be integrated into the future work and help with specific programmatic goals.
- The team leverages effectively nodes at Lawrence Berkeley National Laboratory, the National Renewable Energy Laboratory, and Lawrence Livermore National Laboratory, which directly enhances the activities of the projects.
- There is good collaboration with the EMN node experts.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project's proposed future work is effective; it contributes to overcoming most barriers, meeting most end-of-project goals, and advancing the materials research mission of HydroGEN. The tasks of modeling, interface engineering, and hybrid device integration will likely continue to make good progress over a broad scope of PEC-related areas. There should be some emphasis placed on making actual devices that can perform unassisted water splitting.
- The planned future work is a logical continuation of ongoing efforts, and it is good that the group will move toward working with the widegap alkaline chalcopyrite materials. If the group wishes to demonstrate a more efficient, more durable chalcopyrite tandem-based PEC device by the end of the project, it may be strategic to push on PEC devices and the actual production of hydrogen sooner rather than later.
- The proposed subtasks in task 1 are not directly aligned with developing a material capable of achieving 20% STH efficiency. It would be useful to explicitly describe a path for chalcopyrites to reach that level of efficiency and align tasks in that path. On task 2, it is clear that the WO_3 protective layers need improvements, but it is also unclear whether the team has a well-defined path to achieving those improvements. The future work on task 3 seems well aligned with the ultimate project goal of developing monolithic devices, and thus it is appropriate.
- The proposed tasks are in line with solving remaining barriers.

Project strengths:

- The strengths of the project include its clear vision for an inexpensive chalcopyrite tandem PEC device, with a good deal of attention being paid to achieving manufacturability via low-cost printing and exfoliation and bonding approaches.
- The project has demonstrated a good match between theoretical calculations and synthesis, a robust synthesis method for chalcopyrites, and promising transparent conductive binders.
- The project's strengths include the possible use of "print" technology to make the electrodes.
- The PI and assembled team are highly competent and are making excellent progress by integrating theory, synthesis, and characterization.

Project weaknesses:

- The efforts working with the newer material systems appear to be relatively new, and as such, many of the critical goals of this project are backloaded. There may be several issues to overcome once the PIs turn to the new widegap and interface materials systems of interest, especially once the project moves toward PEC devices and the characterization of their performance.
- The protective coatings degrade continuously over time; better understanding on the degradation mechanisms is needed. There is no direct path for achieving DOE target STH efficiency.
- A major weakness of the approach is the poor stability of the elements used in the electrode. For example, Cu is very easily degraded and leached out by water.
- The chalcopyrite materials set has yet to be incorporated into a device that demonstrates unassisted water splitting.

Recommendations for additions/deletions to project scope:

- The project team should envision a faster path toward a monolithically integrated device with maximum achievable efficiency. The team should perform detailed technoeconomic analysis on that design.

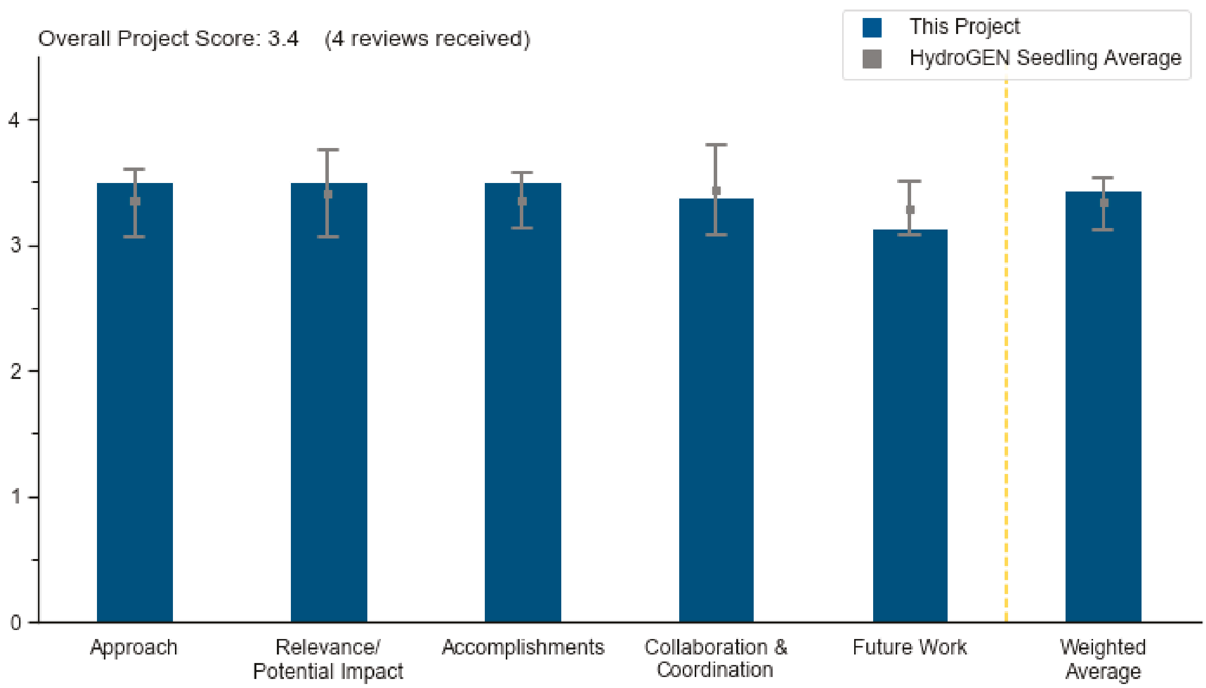
Project #P-163: Monolithically Integrated Thin-Film/Silicon Tandem Photoelectrodes for High-Efficiency and Stable Photoelectrochemical Water Splitting

Zetian Mi, University of Michigan

Brief Summary of Project

This project seeks to establish a low-cost and scalable platform for high-efficiency and stable photoelectrochemical (PEC) water-splitting devices and systems. The improved performance of the top photoelectrodes is required to realize high-efficiency, unassisted solar water splitting, and a functional wide-bandgap tunnel junction that can be fabricated on a silicon platform is a critical component of a silicon-based tandem solar water-splitting device. The tandem photoelectrodes being developed in this project use silicon as the bottom light absorber and newly developed low-cost photoelectrodes made of Ta_3N_5, BCTSSe, or InGaN as the top light absorber. As silicon and gallium nitride are the two most produced semiconductors, the technology being developed will be scalable and lend itself to low-cost manufacturing.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The team has clearly identified a target of high potential impact. The approach to reliably generate Si/GaN-based tandem photoelectrodes has the potential to lead to high solar-to-hydrogen (STH) while, at the same time, lowering the manufacturing cost of photoelectrodes.
    - The protection strategy for the photoelectrode seems appropriate, and its implementation is relatively straightforward. Results on N-terminated GaN electrodes are encouraging.
    - Growing high-efficiency GaN directly on Si has the potential to significantly lower the cost of III-V photoelectrodes.

  - The project is well integrated with the HydroGEN Consortium network, and the team effectively leverages resources from it, which have complemented the developments of the project.
  - Integration of co-catalysts could have a big impact in the performance of the ultimate devices. This can be done either through collaborations in the HydroGEN Consortium network or with other projects in the program. This could help further enhance the stability of the photoelectrodes and ultimately lower the overpotentials required for water splitting.
- This project is focused on developing Si/InGaN tandem photoelectrodes that exhibit 10% STH efficiency and 1,000 hours of operation. There is a clearly defined goal and target device design, with appropriate attention paid to manufacturable processing routes. The project vision is built on some potentially promising developments showing stability of N-terminated GaN nanowires (NWs). Overall, this is a worthwhile and potentially impactful effort.
- The approach is effective and contributes to overcoming most barriers and validating technology innovation. The project effectively identifies relevant barriers in durability, device configurations, and synthesis and targets them with innovative approaches. The project is well designed, feasible, and integrated with the HydroGEN Consortium network.
- Barriers of materials durability, device configuration, and manufacturing have been clearly identified. Use of GaN NW tunnel junction on Si is notable, especially the role of Ga-terminated versus N-terminated NWs.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- This project is critical to the DOE Hydrogen and Fuel Cells Program (the Program). It has potential to significantly advance progress toward DOE research, development, and demonstration goals and objectives and is significantly leveraging and contributing to the resources and framework of the HydroGEN Consortium. This material set is extremely promising since it demonstrates high efficiency, durability, and the potential for low-cost synthesis. Using Si as a substrate is game-changing in high-STH-efficiency devices, and if the initial durability results can be extended to 1,000 hours or more, this is a significant advance in PEC water splitting.
- Monolithically integrated Si-based systems offer the potential for low-cost PEC water-splitting systems, and the demonstrated stability of the N-terminated InGaN NW systems is promising. Thus, overall, relevance and impact are high.
- The project has a high potential for the water-splitting community, especially on the search for stable photoelectrodes.
- The project supports the Program goals, as it provides a path for the development of high-STH-efficiency electrodes at a reduced cost. The project also enhances the HydroGEN Consortium network, as the team may be able to provide high-efficiency photoelectrodes to other teams in the network and synergistically accelerate a path toward cost-effective solar hydrogen technologies. However, it is unlikely that the project will have a direct impact on the $2/kg DOE target, given significant barriers to obtain (1) III-V-based photoelectrodes with significantly reduced costs to outcompete alternative technologies such as Si-based photovoltaic (PV)-driven electrolysis, or (2) a high enough STH to offset the higher cost from the III-V semiconductors (the 15% target is not high enough, and there is not a direct path toward achieving higher efficiencies).

Question 3: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has made impressive progress toward demonstrating stable GaN-based photoelectrodes, and the robustness of the N-terminated GaN electrodes is an important step toward long-lasting PEC devices. The achievement of 10.5% STH unassisted water-splitting devices based on Si/InGaN is encouraging, and there is clear space for improvements. The results on the efficiency improvements over time are also encouraging for the long-term stability of the device and may point toward directions to overcome major degradation challenges.

- Progress is effective, contributes to overcoming most barriers, and provides data that considerably support the accomplishments toward impactful go/no-go criteria. Clearly, this project is making progress toward fairly aggressive performance targets. The project has demonstrated a good efficiency with the current device configuration. However, one of the laboratory partners should corroborate the STH efficiency that was a go/no-go metric. Also, two-electrode durability results should be shown to confirm the durability that is inferred by all of the other measurements shown.
- The team has demonstrated InGaN/Si tandem photoelectrodes, and the initial measurements of their stability (300 hours of operation) are promising. Accomplishments to date are good. To move forward from here, it appears that the photoelectrodes' performance (fill factor, current collection) will need to be improved. A clear plan for addressing the current limitations and overcoming limitations was not described in detail.
- The project has shown good progress toward the double-junction photocathode. STH efficiency of 10.5% has been achieved.

Question 4: Collaboration effectiveness

This project was rated **3.5** for its collaboration and coordination with HydroGEN and other research entities.

- The team effectively leverages nodes at Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and National Renewable Energy Laboratory, which directly enhances the activities of the projects. The collaboration with Francesca Toma is particularly notable, as it can provide insights on novel stabilization mechanisms previously unobserved.
- This project is making good use of Energy Materials Network (EMN) resources, and it is clear that the collaborations are making valuable contributions toward project success. This is particularly true for the in situ PEC scanning tunnel microscopy/atomic force microscopy (STM/AFM) group analysis of degradation during continuous performance, the surface analysis, and band alignment measurements.
- The project has good collaboration, specifically the HydroGEN Consortium, with appropriate use of nodes, contributions to the benchmarking/protocols (2b) project, and the HydroGEN Data Hub. Partners participate and are well coordinated. There is evidence of good collaboration and coordination between the principal investigator and the nodes, as well as good interaction with the 2b project.
- The team has good collaboration with the national laboratories. It will be useful if the collaboration is extended to the industry so the team can benefit from the industrial viewpoints.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The proposed future work is effective and contributes to overcoming most barriers, meeting most end-of-project goals, and advancing the materials research mission of the HydroGEN Consortium. The future work to focus on durability testing of the double-junction electrodes with an STH of >15% has the potential to significantly improve on the state-of-the-art demonstration of high-efficiency and durability if the 1,000-hour target can be met.
- The proposed future work is well laid out.
- The proposed detailed studies on the PEC system are important and will likely lead to relevant physical insights on processes that limit the stability and performance of the photoelectrodes in question. The biggest concern is the lack of a clear path toward the 15% STH device proposed. During the Annual Merit Review presentation, the team indicated several aspects of the project photoelectrodes that needed to be optimized, but a more detailed analysis of the most relevant pain points of the systems and a clear strategy on how to address them were lacking.
- The future work targets focus on PEC studies and on the demonstration of double-junction PEC devices exhibiting >10% efficiency and 1,000 lifetime hours. While this is in line with the overall project goals, the work as presented was very vague. A clear set of remaining barriers to achieving the target efficiencies and stability and a pathway to overcoming these barriers were not laid out.

Project strengths:

- The team's approach and the vision to demonstrate Si-based tandem photoelectrons is solid and may offer a path forward. The early results are promising, including the demonstration of the tandem photoelectrode system that appears to be fairly durable. The use of EMN resources is also excellent, particularly the in situ PEC STM/AFM group analysis of degradation during continuous performance, the surface analysis, and band alignment measurements.
- The team demonstrated a path to reduce the fabrication cost of III-V photoelectrodes, a path to robustly stabilize III-V photoelectrodes, and a >10.5% STH unassisted PEC device. The team has strong integration with the HydroGEN Consortium network and collaborations among team members.
- The team has strong material synthesis skills and good interaction with the HydroGEN nodes.
- An overall strength is the possibility that the team may produce a stable photoelectrode.

Project weaknesses:

- The main weakness may be that, after having demonstrated the Si-based tandem electrode system and making some initial measurements, the specific pathway to overcoming the present performance limitations was not made clear. This makes it difficult to assess the overall likelihood of success in reaching the stated project goals.
- There is an unclear path toward $2/kg, particularly in the context of other solar-hydrogen-competing technologies (PV-driven electrolysis). The project does not define the 15% STH target or the further efficiency improvements needed to meet DOE's ultimate cost and efficiency targets.
- Most of the PEC performance (efficiency, stability) data comes from the principal investigator's laboratory, and it should be validated by one of the DOE partner laboratories.
- The project lacks industrial collaboration.

Recommendations for additions/deletions to project scope:

- The scope of this project is reasonable as laid out.
- The team should consider defining a clear set of tasks and a timeline that will be directly aligned with the project goal of 15% STH.

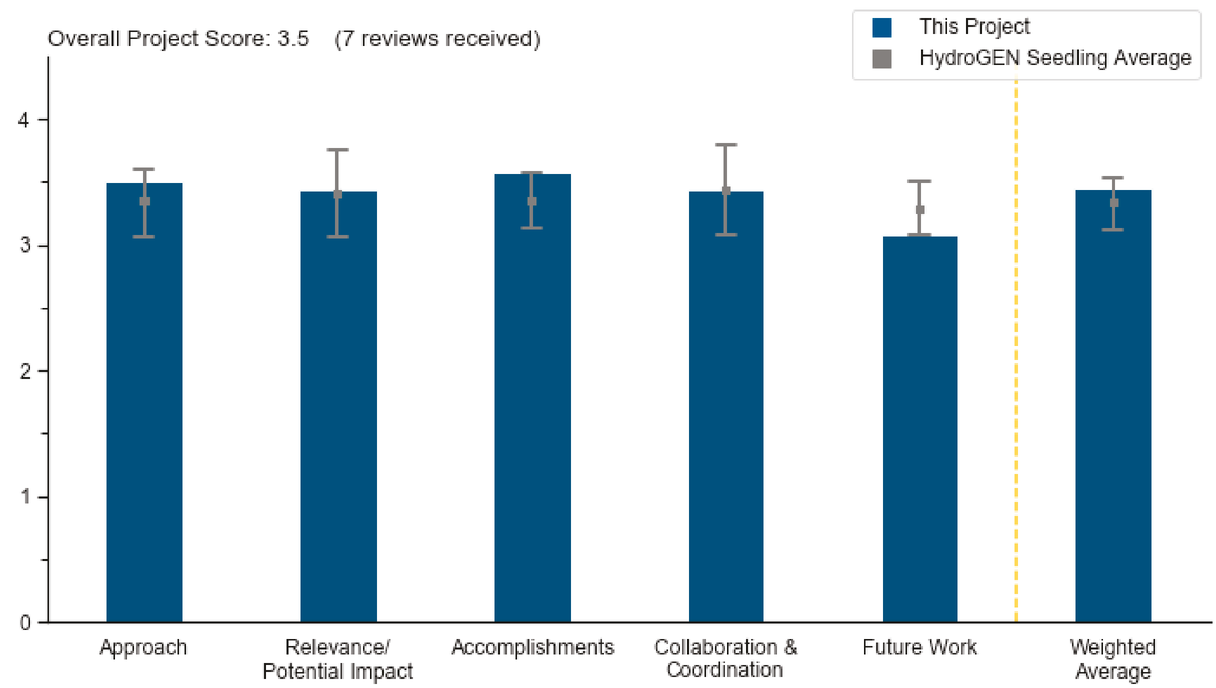
Project #P-165: Accelerated Discovery of Solar Thermochemical Hydrogen Production Materials via High-Throughput Computational and Experimental Methods

Ryan O'Hayre, Colorado School of Mines

Brief Summary of Project

The current state-of-the-art solar thermochemical hydrogen (STCH) material efficiency is approximately 2%, but development of an optimal STCH material could increase the efficiency beyond 60%. This project aims to integrate combinatorial synthesis methods with combinatorial theoretical calculations to rapidly discover new potential materials for use in two-step metal oxide cycles for STCH. The effort builds on prior collaboration between the project partners, which resulted in the discovery of two novel perovskite-based STCH candidates, and leverages the Energy Materials Network (EMN) model of merging high-throughput computational and experimental techniques to accelerate new materials discovery.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- This is a really good project. The team has screened 750+ compounds. The entire periodic table has been considered, as has been done on other multi-university research initiatives in other offices. The admittance criteria for the various elements from the table that are to be considered in the campaign are appropriate. Screening the compositions using pulsed laser deposition and multiple targets to deposit gradients across a surface, thereby accessing a spectrum of compositions, is also a methodology that proved fruitful in other multi-university research initiative works in other offices. There is some risk that the thin-film nature of the compounds produced results in solid-state configurations that are not representative; however, the principal investigator (PI) was aware of this and, by bringing the samples to high enough temperatures, was able to argue successfully that this risk is at a minimum. Furthermore, such thin-film approaches for liquid metals have proven fruitful in the past. Those systems are even more difficult to work with because oxidation must be prevented. In perovskites, there is no such oxidation concern. The optical method of screening for activity using color and color changes is beautiful. The researchers have done top-notch work there, including using off-the-shelf commercial-quality scanners and building five color references into the sample arrays against which to baseline the technique. The choice of analytical technique represents a clear understanding that the activity is obtained from transition metals with electron occupancy in their valiance shells. This is classical inorganic chemistry and materials science at its finest. There is some focus on "super-structures" or "super-patterns" in how the crystals fill space. The project team should be aware that two-dimensional phenomena sometimes do not succeed in filling three-dimensional space.

- The approach in this project is a great complement of theory, synthesis, and characterization and builds off the PIs' previous collaborative success. Targeting lower acceptable maximum temperatures (T-max) is excellent and needed to enable the STCH technology. The project makes use of a well-thought-out methodology in computations of materials properties, which is a really nice component of the project. While the combinatorial pulsed laser deposition (PLD) that enables screening is useful, it may not produce thermodynamic materials, e.g., there is a lack of crystallization.
- The modeling, synthesis, and screening steps used in this project represent a powerful yet nascent approach to exploring and screening candidate STCH materials. Future opportunities to improve the physical tools employed are likely to improve the overall effectiveness.
- The project aims to "integrate combinatorial synthesis methods with combinatorial theoretical calculations to rapidly discover new potential materials for use in two-step metal oxide cycles for STCH." The key barriers are identified as the computational intensity of defect calculations, whether optical evaluation is sufficient (or meaningful), and how thin-film properties may differ from bulk materials. There is significant progress compared to the presentation given at last year's Hydrogen and Fuel Cells Program (the Program) Annual Merit Review (AMR), and there seems to be much greater synergy between the activities undertaken at the various locations. A shortfall in terms of the slide pack is that there is insufficient detail about the project plan to judge progress, resulting in confusion as to what is meant by budget period, year, quarter, or milestones without a Gantt chart or something similar. This makes it somewhat difficult to review progress performance against the scope of work for budget period 1.
- The team has a very good focus on targets and protocol development. The value of STCH from a Program perspective is questionable, however. Perhaps this catalyst screening protocol can be useful for other catalyst development work.
- The project efficiently combines high-throughput synthesis with appropriate modeling to further accelerate the identification of possible redox materials that are able to lower the temperature as necessary to close the thermochemical cycle. The evaluation is based on thin films, which might be different from bulkier materials that are necessary for large-scale hydrogen production, as the material is a reaction partner and not a catalyst. The optical analysis methods are fast and therefore appropriate for the idea of accelerating the process, but they may not be not sufficient for characterization. A similar simplification was chosen for the models, which might not be precise enough to fully predict the materials. However, speed was also in the focus here. The chosen methodology seems to be appropriate for identifying promising candidate materials.
- The Colorado School of Mines (CSM) team takes a combined, experimental, computational go-fast/go-slow approach to identifying new materials for solar thermochemical water splitting. The team also has clearly defined targets of achieving ~75 µmol H_2/g material, with a re-oxidation ratio of at least 10:1 $H_2O:H_2$, with reduction and oxidation temperatures of 1350°C and 850°C, respectively. While these are good targets, there is no clear identification of the materials properties needed (i.e., specific delta H, delta S) to achieve this goal, though the project does identify a wide range of delta H's (2.5–4 ev), which is far too wide. Computationally, the researchers are relying on rapid density-functional-theory-based screening to assess perovskite structure candidates for high activity. Through a down-select method, they have identified key cation components that are "good" for STCH. These are then combined into new structures for detailed analysis, including defect-formation energy calculation. This approach seems fruitful and has resulted in the identification of several interesting new structures. Experimentally, the project takes a colorimetric approach to rapid screening, where combinatorial PLD provides an ability to rapidly produce many compositions simultaneously. Colorimetric results, while an interesting technique, show only redox activity at the desired temperatures; to be significantly useful in assessing materials, thermodynamics are needed to see whether the materials meet the desired reduction thermodynamic characteristics. The "slow"

experimental piece takes an appropriate approach and has delivered interesting results, particularly the ability to form both layered and simple perovskites with substantially different properties. The team is clearly well integrated into HydroGEN, working with both nodes and other teams. The budget is a bit high for the amount of proposed work and the work portion that is being conducted at CSM as opposed to the nodes.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The project seeks a "goldilocks" material that balances stability, temperature reduction, production rate, and kinetics to achieve DOE targets. In the absence of engineering models, the performance of ceria is treated as the "gold standard," and project targets are defined based on a decrease of the peak (reduction) temperature to 1350°C and hydrogen production per gram of active material that must exceed that of ceria. This is well aligned with the Program's goals and objectives, and also supports the HydroGEN consortium mission. The project has strong potential to meet ultimate DOE targets, providing that project metrics are achieved. The most challenging aspect appears to be the steam-to-hydrogen ratio, as the performance of perovskite materials evaluated to date decreases rapidly at lower steam-to-hydrogen ratios.
- This project is highly relevant to Fuel Cell Technologies Office (FCTO) goals. While a clear path to $2/kg of hydrogen is not shown, this is not needed at this stage of research and development. New materials efforts with lower T-max are needed to enable STCH.
- This program advances the DOE goals of STCH materials identification. The experimental work is interesting, particularly the ability to form different structures of perovskites and the use of combinatorial experimental approaches. The computational work seems to have significant overlap with the approaches of other members in the HydroGEN consortium, especially since the computational work has been confined to perovskite structures. It is worth assessing whether it is worth having three projects with such similar computational approaches. While ideas are being leveraged between the projects, there appears to be significant overlap and repetition of work.
- At these early stages of STCH technology development, the fundamental materials focus of this project is extremely important.
- This is good work on catalyst development, notwithstanding the applications to STCH.
- The project aims to accelerate the search of candidate materials and does this very efficiently. However, because of the simplification, it is possible that effects may be missed or underestimated. However, the work will lead to candidate materials and therefore contribute to the goal of $2/kg hydrogen. As with all materials-focused projects, the efficiency of the material is only one aspect in achieving this goal. Without developing technologies, a market introduction will not be possible, and the goal will stay theoretical.
- This is a "get it done" kind of project. Even with all of the best modeling, one still needs to synthesize and characterize the "hits" from the modeling effort. This project can do that at the scale the modeling needs, thereby providing answers about the perovskite class's capabilities. Perovskites continue to hold relevance for the Program; however, the variation in materials properties seems to be occurring in a band or "smear" of values that is just not quite "outstanding." Therefore, a disruptive discovery must occur, or engineering and system design must shoulder any burden of the materials' performance shortcomings, if there are any. Perhaps the layered perovskites reported in this project are one such approach to enhancing the materials properties, but that has yet to be proven. The PI suggests that simple perovskites may be assembled into a layered structure, and that this structure can change the thermodynamics. It is not yet clear that it can do so enough to be disruptive.

Question 3: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- This project represents the "gold standard" in using high-throughput experimental methods to validate, verify, and potentially exploit materials science and related discoveries. It is difficult to imagine better accomplishments or progress; perhaps an improvement would be better integration with the other perovskite works in the portfolio.
- Setting up this multifaceted process is impressive progress. The CSM team is due congratulations for discovering a new layered perovskite.
- The project is on a good path. It continuously improves the rapid screening thin-film technology. It could identify interesting candidate materials that fit the milestones. However, to make substantial statements on their applicability for large-scale hydrogen production, the materials need to be proven in a relevant environment.
- A new STCH compound has been discovered, as guided by simulations, and at least one more new compound was identified. This is excellent. There were questions as to the value of the combinatorial approach, and it would be good to show that this can produce relevant films. The combinatorial method of estimating oxygen content from color is highly qualitative, and the value of this was not demonstrated.
- Significant progress has been made in identifying new materials, particularly in terms of Ce-containing compounds, and in the experimental validation and characterization of the materials. These achievements are made through a combination of work from the DOE nodes and the work at CSM. While the researchers have met one of the go/no-go milestones, namely exploration of five families of materials, they have not met one of the other go/no-go milestones: the production of hydrogen in water-splitting tests at Sandia National Laboratories and CSM.
- The metrics, deliverables, or timing on which the project is to be judged are not clear. However, what is clear is that the project has advanced significantly since the last AMR and is demonstrating good progress toward the DOE goals and the HydroGEN mission. It is good to see that the project now has a maximum steam-to-hydrogen ratio of 10:1, as this is important for enabling the necessary solar-to-chemical conversion efficiencies. The presentation includes data from all partners in a holistic way that suggests the project is moving forward at all levels, although there are still some unresolved questions about the validity and usefulness of the thin-film combinatorial approach.
- The project is accomplishing and meeting milestones, but the project needs to focus on achieving the truly mild reaction conditions. The team could possibly look at Ellen Stechel's presentation from Arizona State University (P-168) for direction on first principle development.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The collaboration appears to be excellent. The team has established the right connections to efficiently integrate the competencies of other HydroGEN partners into the project. This improves the work in all areas, especially in the production of thin films and the analytic description of the identified candidate materials, but also in the efficient modeling of the substances. However, further improved analytics would add value to this.
- There is excellent collaboration with HydroGEN partners, including with the National Renewable Energy Laboratory for simulations and combinatorial synthesis and Sandia National Laboratories for testing. There are really good interactions within the EMN.
- The CSM team has shown itself to be very effective in working with HydroGEN, the nodes, and other members of the STCH materials community. These continued resources are critical to the project's success. There appears to be little-to-no engagement in benchmarking or data-sharing activities such as the Data Hub.
- This was one area that appeared less than fully effective at the previous AMR. It is pleasing to see that the project is now well linked at various partner institutes and that this engagement with the EMN is proving to be extremely valuable in moving the project forward.

- Slide 23 does well in defining which collaborator has contributed to which task, lending a sense of ownership and accountability. The effectiveness of the collaboration is very high.
- The collaboration and coordination with the other partners appears to be very good, judging from the results. However, the presentation did not discuss this point.
- There is good collaboration with EMN and the national laboratories.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The next year of the project is priced commensurate to the first year. The project is pursuing the innovation discovered in year 1 by looking for layered materials and more complex perovskites. The performance targets for these materials in the targeted application (i.e., water splitting) are well defined.
- The proposed work is presented only at a high level, but it seems appropriate and suitably targeted to enable end-of-project goals to be attained. The next go/no-go milestone is rightly seen as a challenging one.
- These plans are well thought out, with aggressive goals.
- The full characterization and advanced study of excellent candidate materials is the right way to go ahead. This is an excellent perspective. However, the proposed Hydrogen Analysis (H2A) hydrogen production models used for technoeconomic evaluation seem not to be appropriate, based only on materials development. The project does not generate any data besides the material that would justify developing the necessary input for the H2A. The team should consider what kind of solar system is appropriate for what kind of reactor, and if existing technologies or models are chosen, how relevant they are for the newly found substances.
- The future work is pointed in the correct direction, but it lacks specificity or a concrete plan. A more detailed plan of how to achieve the goals is needed. Additionally, more specifics are required to help hone the search; for example, it would be helpful to know what the characteristics are of the materials that are necessary to activate the 10:1 ratios.
- The proposed future work is appropriate. Where this project leads and what happens after year 3 was not discussed but is very important.
- It seems the future direction is just a continuation of the current work with the hope that a game-changing material will emerge.

Project strengths:

- This is a really great combination of theory, synthesis, and experiment targeting lower T-max to enable the STCH technology. The goals are highly relevant to FCTO, as new materials with lower T-max are badly needed. There is excellent collaboration with HydroGEN partners.
- This is a great project with a great PI. The experimental methods seem beyond reproach. The campaign seems well planned, and the analysis of results seems very careful.
- This project has leveraged machine learning and experimentation. The key strength of the project is the identification of cations that boost perovskite performance and focus on these materials. Additionally, the ability to make stable materials with similar compositions but layered or simple structures is interesting and potentially important. The multi-natured approach of materials production and analysis, particularly X-ray and thermogravimetric analysis, is good.
- The project's strength is clearly in the combination of fast, combinatory synthesis techniques with fast computing. In this way, it is possible to achieve results efficiently. They might not be the most precise results, but they show a direction in which further development will be promising.
- The project is well scoped and seems to be effectively leveraging the expertise within the EMN.
- The project is doing good technical work; many materials have been screened.
- The project's approach, accomplishments, and team are key strengths.

Project weaknesses:

- As the more complex layered structures and higher-order perovskites begin to be pursued, it will be interesting to see how the team manages the role of the processing parameters in synthesis and preparation. It remains to be seen whether the project will continue to be sophisticated, employing a design of experiments or some such similar and recognized approach for process development, or if the project will adopt an Edisonian trial-and-error approach.
- The importance and abilities of the optical analysis for assessing the detailed thermodynamics of the materials seem to be low; therefore, it is questionable if this is adding to the project or just taking up resources. More detailed plans for year 2 are needed. It seems as if a significant portion of work is being conducted at the laboratories; it will be useful to have a clearer delineation of what is being done at CSM and what the CSM team's contribution is. Importantly, there is significant scope overlap between STCH projects, leading to significant duplication of effort.
- The methodology is focused mainly on acceleration, but it lacks precision. This could result in overlooking some principles that might be important for further development. The work is not sufficient for a technoeconomic analysis (TEA) in H2A. This is the case for all materials-focused projects under HydroGEN. Therefore, the project would be more efficient if the work were concentrated on specific materials developments.
- Some of the concerns raised at the last AMR about the usefulness of the thin-film testing remain unresolved in terms of the validity of the optical assessment. While it is apparent that color is a useful indicator that something is happening, it is less clear what that might be or what exactly the material is.
- The combinatorial method of estimating oxygen content from color has shown limited value and should be critically assessed. The combinatorial PLD enables screening; it may not produce thermodynamic materials.
- Further consideration is needed for hardware enhancements and the longer-term path going forward.
- It is not clear what the proposed value is.

Recommendations for additions/deletions to project scope:

- It would be valuable to have some harmonization of target performance across the HydroGEN projects. Each project has somewhat arbitrarily identified targets, which could benefit from some inter-comparison to ensure that each set is sufficient to meet or approach DOE targets. All of the HydroGEN project presentations should be made clearer in terms of the project plan, performance, and expected timeline.
- The project team should consider incorporating a metamaterial-like pattern in the layered structure, thereby focusing internal lattice potentials to specific layers and encouraging "oxygen hop" through an averaged background potential that is elevated but, by being constrained, not destructive.
- Based on the results from year 1, it seems that the optical analysis is of limited value and should be cut. Additionally, TEA and deep thermodynamic characterization are desirable in the second project period for some materials, rather than leaving this work until the third.
- The project could be improved by additional analytical tasks that would help to better describe the materials. The project would also be strengthened if it could focus on its materials-related work and not on the H2A. Such an analysis that is based only on materials seems inappropriate.
- The combinatorial method of estimating oxygen content from color should be critically assessed, and the clear value should be demonstrated.
- It is recommended that the team really focus on evaluating needs and determining how to screen materials that meet these needs.

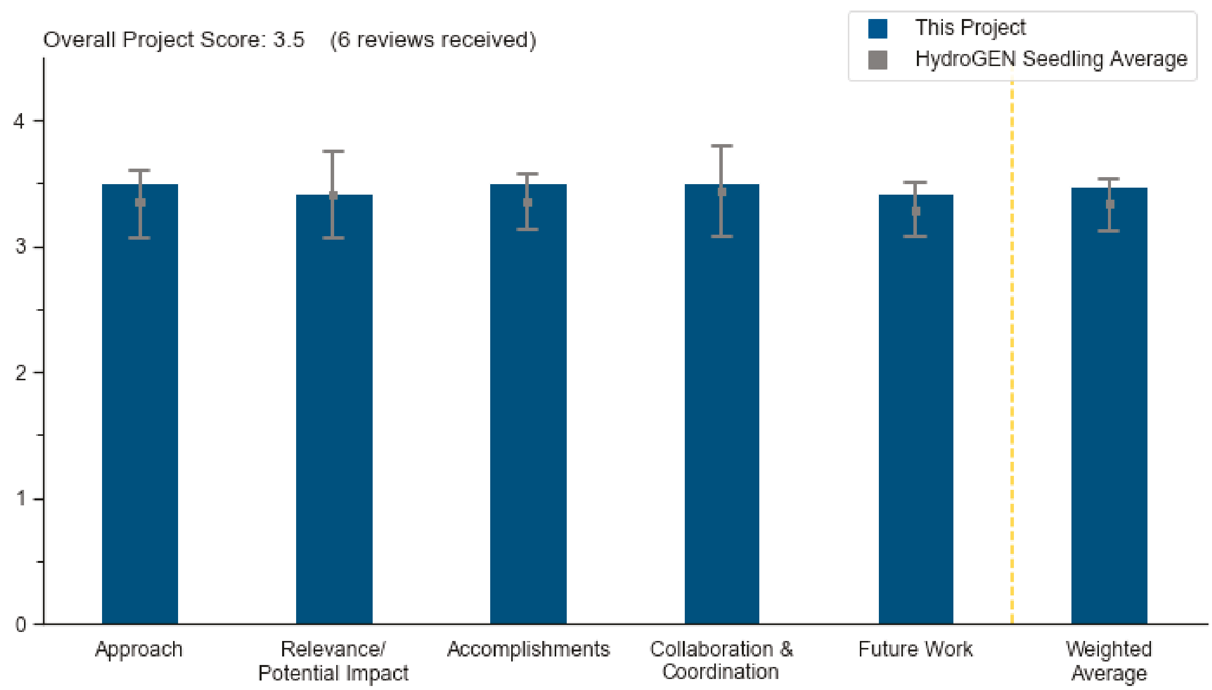
Project #P-166: Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production

Charles Musgrave, University of Colorado Boulder

Brief Summary of Project

The project objective is to utilize machine-learned models coupled with ab initio thermodynamic and kinetic screening calculations to accelerate the research, development, and demonstration (RD&D) of new solar thermochemical hydrogen (STCH) materials. The approach will rapidly screen a vast number of new candidate metal oxide materials for stability, thermodynamic viability, and kinetics. The project will utilize experimental techniques to evaluate thermodynamic and kinetic properties of new materials to provide feedback to the computational thermodynamic and kinetic screening effort.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach of the project to perform the work is excellent. It is innovative to combine machine learning (ML) with *ab initio* simulations to reduce calculation effort while increasing the number of screened substances. However, even ab initio calculations are an approximation of reality. The calculation of each structure is very time-consuming compared to other calculation methods that have a higher grade of simplification but lead to the same hints as to which direction of the search for the best materials. Still, it gives additional insight into the structures; therefore, the higher computational effort is also of high value for understanding the systems.
- This project is the “gold standard” in terms of how high-throughput, computationally aided materials discovery and “proving out” how to proceed. This is outstanding.

- The project has a very solid approach of predictive modeling followed by first principles screening and experimental parametric testing.
- The project aims to "develop and utilize machine-learned models coupled with *ab initio* thermodynamic and kinetic screening calculations to accelerate the RD&D of new STCH materials." This is complemented by experimental validation in thermogravimetric analysis (TGA) and the stagnation flow reactor (SFR) at Sandia National Laboratories (SNL). The main barriers identified are the huge possible compositional space for materials and the vast number of candidates. There seems to be good progress, although some slides are identical to the presentation given at last year's Hydrogen and Fuel Cells Program (the Program) Annual Merit Review (AMR). There is good synergy between the activities undertaken at the various locations. A shortfall in terms of the slide pack is that there is insufficient detail about the project plan to judge the progress, resulting in confusion as to what is meant by budget period, year, quarter, or milestones without a Gantt chart or similar. This makes it somewhat difficult to review progress performance against the scope of work in budget period 1.
- This project seeks to use computation to guide the development of new STCH materials. The use of ML in this space seems novel, but as with all materials applications of ML, the datasets can be very small. The focus on surface versus bulk kinetics is novel and an important part of new STCH materials. The temperature reduction goals seem to be modest. There is a strong need to vet the computations with experiments as a next step.
- The approach to performing the work is technically sound, but the project needs to do more work around the value of STCH, even if amazing catalysts are found.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- This project is brilliant. Consequently, it begs the question of whether this is it for perovskites. Perovskites continue to hold promise in delivering on DOE targets. However, at some point, either a breakthrough combination of elements will be discovered, or the potential of these materials to satisfy the performance requirements exists in a band and that "smear" of capability does not vary as widely as hoped. The materials properties that are available then must be exploited by some process and/or engineering design that makes up for performance gaps.
- The innovation in this project is to use ML models to predict perovskite stability and thermodynamic properties to reduce the solution space for a workable STCH material. In the absence of engineering models, the performance of ceria is treated as the "gold standard." Project targets are defined based on a small decrease in the peak (reduction) temperature to <=1450°C, and hydrogen production per gram of active material must exceed that of ceria (200 vs. 130 µmol/g). This is aligned with Program goals and objectives and also supports the HydroGEN consortium mission. The project has good potential to meet the ultimate DOE targets, providing that project metrics are achieved. The most challenging aspect for successful implementation appears to be the high steam-to-hydrogen ratio, although it is noted that "oxidation will either be operated at H_2O:H_2 ratios of less than 1000:1 or a [techno-economic analysis (TEA)] will be conducted to verify that higher H_2O:H_2 ratios are economically practical with the new material."
- At this early state of STCH technology development, the materials research being carried out by this project team is essential to achieving the Program goal of <$2/kg of hydrogen.
- While a clear path to $2/kg is not shown, this is not needed at this stage. New materials with higher hydrogen production rates are needed to enable STCH. The reduction in maximum temperature is very modest.
- The highly computation-based results give interesting insights into the systems and are an important contribution to HydroGEN. However, the applied methodology is far away from any application of the described materials, and therefore the impact on the $2/kg hydrogen goal is very indirect.
- The development of these catalysts may provide broadly applicable methodology. STCH is not particularly relevant to the development of the hydrogen economy.

Question 3: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- This project should serve as a benchmark of excellence for this kind of work. The team also did a great job on the publications.
- The project is progressing very well. The ML showed very good results, and the calculated systems are promising. The parameter of stability opens up the possibility to synthesis efficiently, promising candidate materials with a very high probability of success. Overall, this innovative attempt seems to be heading in the right direction. Some more proven materials will underline its potential.
- The new descriptor (replacing the Goldschmidt tolerance factor) for perovskite stability is a significant advance and helps reduce the number of calculations.
- The project has had very impressive accomplishments on a complex, multifaceted effort.
- It is not clear on what metrics, deliverables, or timing the HydroGEN projects should be judged. However, what is clear is that the project has advanced since the last AMR and is demonstrating good progress toward meeting the DOE goals and the HydroGEN mission. The various activities are all moving forward, although some accomplishments have been previously reported. The results indicate an improved understanding of some of the underlying drivers of performance, although it is focused more on theory rather than practical demonstration. Conspicuous by its absence is the TEA work that was flagged for the National Renewable Energy Laboratory (NREL); this is mentioned, but no results are reported. Some high-level analysis of necessary performance targets would be valuable.
- This project needs experimental validation to meet the go/no-go decision points.

Question 4: Collaboration effectiveness

This project was rated **3.5** for its collaboration and coordination with HydroGEN and other research entities.

- There is excellent collaboration with some HydroGEN EMN partners, especially NREL for simulations. There appear to be good collaborations with SNL in Livermore, California, and Albuquerque, New Mexico, for STCH testing and materials characterization, respectively.
- The collaboration seems to be appropriate for the structure of the project. The right competencies from HydroGEN are added to the capacity of the project team. The input from the collaborators is necessary and useful. The collaboration is not too broad, so it can efficiently support the project team in achieving its project goals.
- After listening to several of the STCH catalyst presentations, it is clear that there is a strong community and collaboration around this topic. This project, like the others, has strong formal and informal collaboration.
- There is no doubt that the excellent performance of this project may be attributed, in part, to excellent collaborations.
- The project's outstanding collaboration and coordination is evidenced by the impressive results.
- The project reports some nice results from the various project partners, although the tasks do seem a little disconnected in some sense, rather than truly integrated into a cohesive whole. For instance, it is not clear what the status is of Task 4, the SFR work at SNL.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work is exactly what is required to arrive at a firm, defensible conclusion about the potential of perovskites as a materials class. It is a logical extension of the current phase.
- The proposed future work is exactly what is needed to achieve the goals successfully. It concentrates on the key questions of the project and will use the resources efficiently to achieve the goals.
- The future plans are strong, with aggressive targets, but lack a strong connection to experiments.

- The development of first-principle needs makes more sense than screening millions of compounds, but when coupled with Ellen Stechel's work at Arizona State University, the future work for this project looks good.
- Slide 15 suggests that a considerable amount of work is necessary to meet the next go/no-go milestone. This will be dependent on the experimental work being done at SNL, which has either not been started or was not reported at the AMR.
- It is unclear where this project leads, what work should follow this project, or what the pathway forward is.

Project strengths:

- This is an outstanding principal investigator (PI), able to clearly articulate complex campaigns of discovery in easily relatable ways. There is a simple, sound, logical progression of plan and effort. The conclusions are succinct and convincing. On slide 6, the PI did well to articulate the root cause of the systematic error in the correlation plot between the sure independence screening and sparsifying operator (SISSO) and quasi-harmonic models. The magnitude of this systematic error was the same when compared to experiment. The project does well to include various statistical measures of dataset fits to lines and other things. The technical effort is beyond reproach.
- This project takes a novel approach to materials design, incorporating ML and kinetics; it has been highly productive, with some impactful publications.
- The combination of ML and ab initio calculations is innovative and helps with reducing computational effort without losing the depth of the calculations.
- The project is strong theoretically; it seems to be making some good progress at understanding some of the drivers of STCH performance and finding effective ways of predicting properties.
- The project has done good technical work and has a strong record of collaboration and publication.
- The project's approach, accomplishments, and team are all impressive strengths.

Project weaknesses:

- The project as reported seems a little disconnected from the experimental stages, which will be critical for continued progress. This may be intentional on the part of the project lead, but compressing all of the experimental work may prove challenging.
- The final deliverable is purported to be less than 10% loss in hydrogen production capacity between 100 and 200 cycles. While this is certainly an early-technology-readiness-level project, it should have identified the absolute best candidates from the entire class of perovskites. Thus, with 10% capacity loss after only 200 cycles, the material is not adequate, and either a new material needs to be chosen (which should have been chosen in the first place), or a process or engineering design needs to be devised to "save" the material from such a fate. The PI did recognize regeneration as a possibility, although he did admit it is a complex technoeconomic consideration.
- Validation is not the major topic of the project. A closer link to validating efforts would strengthen the project.
- The coupling of the computations to the experiments was not convincingly demonstrated. It was unclear what new materials were actually synthesized and tested. The temperature reduction goals are modest.
- The commercial context, path forward, and ideas for improved hardware and software are unclear.
- The value of STCH is questionable.

Recommendations for additions/deletions to project scope:

- The project is on the right track. The work should be carried out as proposed. A closer link to practical work that could validate the results more thoroughly would strengthen the project.
- It would be valuable to have some harmonization of target performance across the HydroGEN projects. Each project has somewhat arbitrarily identified targets, which could benefit from some inter-comparison to ensure that each set is sufficient to meet or approach DOE targets. It was encouraging to see that this project has a TEA component, but it was disappointing that it has not been made a priority or a necessary component at this stage. All of the HydroGEN project presentations should be made clearer in terms of the project plan, performance, and expected timeline.

- The identification of knowledge and technology gaps should be considered, as should the next steps following the end of this project.
- In future work, it is recommended that the team connect the computational characterization of the material catalytic activity with the first-principle elucidation of catalyst needs.
- The team should develop a stronger coupling with the synthesis teams in HydroGEN.

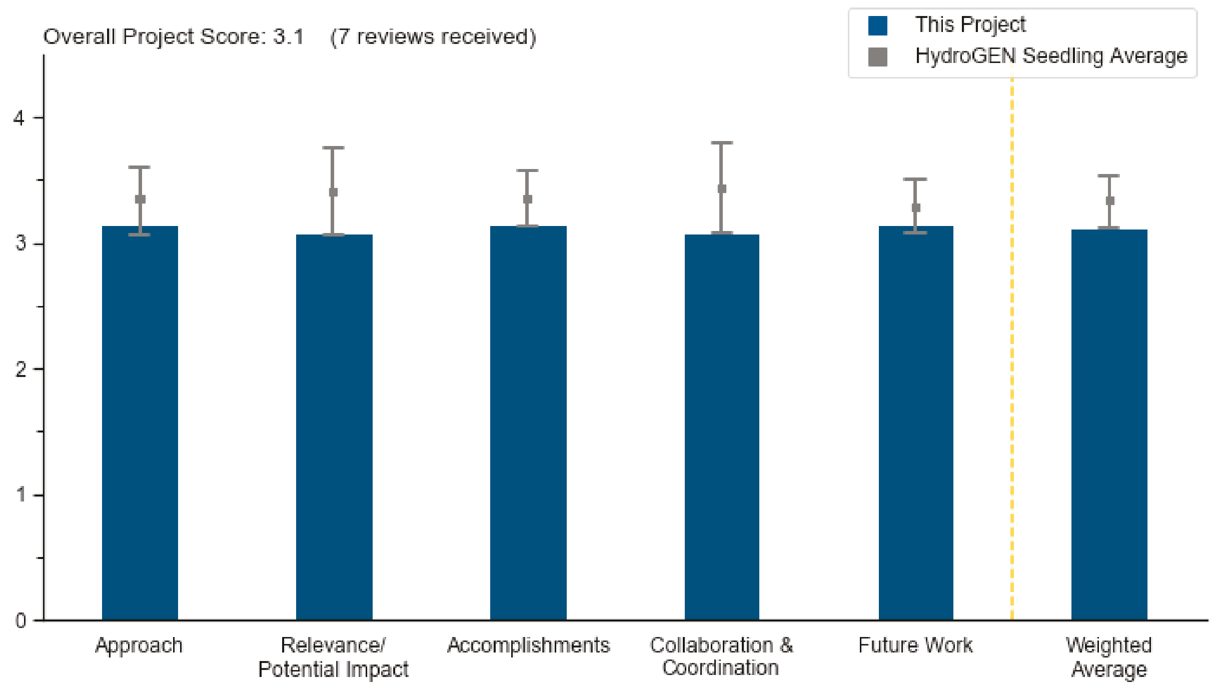
Project #P-167: Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels

Chris Wolverton, Northwestern University

Brief Summary of Project

The project objective is to utilize a computational–experimental approach, combined with materials design strategies to quickly discover and demonstrate novel thermochemical materials with properties superior to the state of the art. The project will investigate what is an enormous compositional space of materials utilizing high-throughput computational and experimental methods to identify promising compounds that show (1) ground state stability/ synthesizability, (2) thermodynamics favorable for <1400°C reduction, and (3) thermodynamics favorable for facile water splitting.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach in this project is a combination of theory and synthesis to target stable and effective materials for solar thermochemical hydrogen (STCH) production; it builds off some previous collaborative success. There is a focus on perovskite-type oxides and a strong link between the simulations, synthesis, and characterization.
- The design map for acceptable materials is a good place to start. Understanding that validating computation using experimentation on simple materials is also a good approach.
- This is a pretty good project. It uses some straightforward, nuts-and-bolts approaches to screening perovskite materials.
- The three-step statement of work is simple and logical, yet extremely challenging.
- The project has a clear strategy to use fast, in silico screening methods built on sound experimental data of model substances. Therefore, the models used are very close to real data and promise to generate high-

quality results that will lead to a fast and efficient identification of promising candidate systems for STCH production. However, the work is still very far away from real applications, and the necessary conditions for use in the field are not taken into account.

- The project aims "to combine high-throughput computational and experimental exploration of oxygen off-stoichiometric oxides and phase change materials for enhancing the efficiency of [solar thermochemical] production of solar fuels." The project as presented is quite loosely formulated, and the barriers are not really articulated. This lack of an articulated focus is compounded by the nature of the slide pack, which has insufficient detail about the project plan to really judge progress. This results in confusion as to what is meant by budget period, year, quarter, or milestone without a Gantt chart or something similar. Also confusing is that the start date of the project has moved forward 18 months from October 1, 2017 (as reported in the 2018 Hydrogen and Fuel Cells Program [the Program] Annual Merit Review [AMR]) to April 1, 2019, in this year's AMR. Thankfully, the year 1 scope of work is well explained, and the experimental work is well described.
- The outlined approach was to use a combination of known computational (density functional theory [DFT] brute force) and new and known experimental (thermogravimetric analysis [TGA] and electrochemical impedance) methods to identify new materials for STCH production. Computationally, the approach is slow, though able to succeed given sufficient time and resources and, of course, the existence of materials with the desired properties. The experimental approaches and innovations are the use of continuous TGA runs, as opposed to stepped runs, to evaluate non-stoichiometry–temperature–pressure relationships. This looks to enable the far faster and more reliable extraction of materials thermodynamics. However, it has a severe drawback in the need to stay within a single perovskite sub-structure; changes in structure between, for example, hexagonal and cubic seem to be a problem for this method, despite occurring at conditions that are critical for STCH materials. No mention or description of electrochemical analysis is made, so its appropriateness, etc., cannot be evaluated. There appears to be almost no integration with HydroGEN. Interactions seem to be present only to check a box rather than as a useful tool.

Question 2: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The objective of this project is to "identify compounds which show: (a) synthesizability, (b) thermodynamics favorable for <1400°C reduction, and (c) thermodynamics favorable for facile water splitting. State-of-the-art currently CeO_2 and Sr- and Mn-doped LaAlO (SLMA) perovskite." The innovation in this project is to compare thermodynamic properties for simple perovskite materials from experimental investigations against predictions from computation. While the performance targets are less explicitly stated than in the other HydroGEN projects (e.g., there is no target production rate), the goals are well aligned with DOE targets and the HydroGEN mission.
- This fundamental materials work is essential to achieving the goal of $2/kg hydrogen.
- As with several of these STCH papers, the work is technically good and could be broadly applied to catalyst or materials development. However, the work around STCH should be evaluated from a Program standpoint.
- The work seems to be very much oriented around basic research. The connection to an application of the results in real hydrogen production plants seems to be very weak. Therefore, the impact in achieving the $2/kg hydrogen goal is low. However, the work is scientifically excellent and might lead to very important results.
- New stable materials with higher hydrogen production rates are needed to enable STCH. A path to $2/kg is not shown, but it is not needed at this stage. The targeted maximum temperature (T-max) is rather high.
- Perovskite materials continue to hold promise to achieve the DOE's cost targets. However, with the new high-throughput computational screening methods (of such high fidelity to experiment), it may well be that the materials discovery stage is either (a) coming to a close or (b) in need of (or currently evolving into) a more complex, super-structure discovery process (the so-called layered perovskites discussed in other projects). Ultimately, it may need to be considered whether the process and the engineering can deliver where the materials may not.

- The project is aimed in the correct direction; however, some self-imposed limitations on experimentation, such as phase-change restrictions, likely hamper the likelihood of success in analyzing STCH active materials. The method of computation seems slow, therefore increasing the challenge of finding the desired materials; this is particularly apparent when compared to the progress made by other projects. The computational work seems to have significant overlap with the approaches of other HydroGEN members, especially since the computational work has been confined to perovskite structures. It is worth assessing whether it is worth having three projects with such similar computational approaches. While ideas are being leveraged between some of the projects, there appears to be significant overlap and repetition of work. This project has not leveraged HydroGEN resources, nor does it seem to integrate well within it.

Question 3: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project presents excellent results by coupling measurements with DFT simulations. A very high number of potential candidate materials could be screened. This is an important input for the DOE goal of identifying the most promising systems for STCH. However, it is very far away from application. Therefore, the main $2/kg hydrogen goal cannot so much be the focus as the actual behavior of the materials. This should be seen as a strength, as the materials alone will never be the key factor of the actual cost of hydrogen. However, their efficiency will be important to designing the right plants.
- The project has been highly productive, with significant progress made in thermodynamic measurements, computation and open databases, and synthesis.
- The team is making good progress toward project goals early on in the project. The validation of 12 perovskites with experimentation is very important for guiding future work.
- For the amount of time that has elapsed, and for the relatively small dollar amount spent, this project has made great progress.
- As noted in other projects, it is not clear how the HydroGEN projects should be judged in terms of metrics, deliverables, or timing. However, here, as elsewhere, there has been good progress in terms of results, and some nice techniques are shown for simultaneously evaluating ΔH and ΔS as a function of δ. Despite the reuse of some slides from the 2018 AMR, the new data presented shows encouraging progress. Missing from the presentation are results from the year 1 scope of work part (b): “validate high-throughput methodology for measuring thermodynamic property using thin film through electrochemical impedance.”
- The team is due congratulations on the seven new predictions for stable double-perovskites with favorable water-splitting thermodynamics. To date, the project has shown that calculated O-vacancy formation energies are in some agreement with experiment (r^2=0.6). Additionally, the project has calculated ~10,000 materials. However, given the vast space of materials available, blind searching would seem to require significantly higher rates of materials calculation. The year 1 project goals were vague, and go/no-go points were not stated; this makes evaluation of the go/no-go decision difficult. The stated scope of work outlined three tasks: experimental measurement of 12 materials, validation of the electrochemical impedance technique, and starting high-throughput screening. The experimental measurement of 12 materials was completed; however, many of the materials studied are already known and therefore do not demonstrate additional progress toward DOE goals. There was no presentation of data regarding electrochemical analysis of materials or proof that this work was done at all. The high-throughput screening was initiated.

Question 4: Collaboration effectiveness

This project was rated **3.1** for its collaboration and coordination with HydroGEN and other research entities.

- The discovery of the layered perovskite STCH compound, the 2018 and 2019 publication, and the invited presentations are evidence of outstanding collaboration and coordination.
- The project has no doubt been able to make such substantial progress in such a short amount of time as a result of its great collaborations.
- There is good collaboration with both national laboratories and universities. There seems to be a strong collaborative community in this part of the Energy Materials Network.

- There are collaborations in HydroGEN nodes: the National Renewable Energy Laboratory for synthesis, Sandia National Laboratories for characterization, and one other seedling (Colorado School of Mines).
- The presentation seems to be strongly focused on the principal investigator's work, and it is difficult to gauge the nature and effectiveness of the collaboration described in slides 19 and 20.
- The project presented its collaboration within HydroGEN. This is appropriate, but compared to other projects, the network seems to be on the smaller side. Maybe a closer integration with HydroGEN and with more partners would improve the position of the project in the framework.
- There seems to be limited interaction with HydroGEN and the nodes, aside from one token high-temperature X-ray diffraction analysis. There is no discussion of interactions with benchmarking or protocols, nor was there discussion of use of working groups or the HydroGEN Data Hub.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The future work plan is strong, with aggressive plans for both the computational and experimental aspects of the project.
- The proposed work is exactly what is needed to achieve the scientific goals of the project.
- This is good future work. The only consideration is that the design map approach and the computational approach have shown great progress. Focusing more narrowly on advancing this work, rather than taking on several new objectives, would be most valuable. From a programmatic standpoint, not much value is seen in STCH. However, that is no reflection on the good work of this project.
- The proposed future work is an obvious extension of the current phase.
- The amount of future work appears to be quite substantial for what is presumably about the halfway point of the project (this is hard to gauge in the absence of a Gantt chart or something similar). It is not clear what go/no-go criteria have been agreed to with DOE for the next review.
- The proposed future work is vague in terms of both goals and methods. It does propose using methods developed in year 1, particularly in the computational area. There is no outline to connect how these works will meet end-of-project goals. Based on the work completed in budget period 1 (BP1), the amount required for BP2 is far too high and should be scaled back significantly to be more in line with the work completed and the apparent time dedicated to the project.
- There is no mention of how the team plans to move its work into initial follow-on applications.

Project strengths:

- It seems like a great idea to use electrochemical impedance spectroscopy to increase the throughput of perovskite candidate characterization. It would be interesting to see whether the colorimetric methods used in other projects correlate well with the electrochemical impedance spectroscopy proposed here. Slide 8 describes and employs some solid physical chemistry. Slide 16 does well to include the Pearson correlation coefficient, which is actually pretty good (0.88). It is important to include this because the R^2 value is not so good (0.63). Slide 17 has a really nice plot to show how most of the periodic table is being considered.
- The project is an excellent blend of theoretical calculation and targeted experimentation. There seems to be good progress in terms of developing methodologies for effectively evaluating thermodynamic properties.
- The project has a closely coupled and strong combination of theory and synthesis for targeting stable and effective materials for STCH. There are very good collaborations with HydroGEN.
- The researchers have corrected their previous assumption that cubic structures can be used to represent perovskite structures, and they have shown that the use of continuous TGA can be useful.
- The strongest part is that the project is starting from the design map (i.e., identifying needs) with experimental validation.
- The strength is the solid experimental foundation of the excellent simulations that lead to a very high number of screened potential materials.
- The approach, results, team, and collaboration are all impressive strengths.

Project weaknesses:

- The project has several weaknesses. Experimentally, no data or proof of electrochemical analysis has been provided, which was a key project component. Similarly, much TGA work was restricted to known and uninteresting compounds. Within the TGA data scope, the restrictions required to conduct continuous scans eliminate significant numbers of materials, particularly those that are likely to be interesting, i.e., materials with slight phase changes. No comment is made about experimental findings in relation to project goals or targets. The DFT work should aim to further identify what "ideal" materials are so that there is a concrete metric during screening. Additionally, methods to either simplify and/or minimize the search space or vastly increase screening speed are needed to achieve the stated goals. There is a clear lack of integration with HydroGEN in terms of using nodes and Data Hub resources. Given the overlap with the other two projects in terms of computational and experiment work proposed and presented, it is worth assessing whether there should be three projects with such similar approaches. This project seems to overlap significantly but is not leveraging the knowledge or method development generated in the other projects.
- The project as reported seems to be more of a single-institution effort rather than an effective HydroGEN collaboration. The go/no-go metrics are not clearly articulated, so it is difficult to see whether the project is adequately defined in terms of material property requirements.
- The project is using TGA as a primary means of generating experimental data. There is nothing wrong with this, per se; however, it takes a long time and is somewhat incongruous with the high-throughput strategy.
- The project seems to be a little more decoupled from HydroGEN than the others in this area. A stronger link to application would help to improve the analysis of the results.
- The targeted T-max is rather high.
- There is a possibility of diluting the impact by doing too much in the future work.
- The lack of a pathway to commercial applications is an area of weakness.

Recommendations for additions/deletions to project scope:

- The project is very well structured. It does not need any additions or deletions. However, a better integration into the HydroGEN framework might improve the excellent work.
- The researchers should focus on accomplishments, but otherwise they are doing great work.
- It would be valuable to have some harmonization of target performance across the HydroGEN projects. Each project has its own targets, which could benefit from some inter-comparison to ensure that each set is sufficient to meet or approach DOE targets. All of the HydroGEN project presentations should be made clearer in terms of the project plan, performance, and expected timeline.
- The budget for the next performance period is not aligned with the work proposed, given the year 1 performance. In particular, the use of electrochemical analysis should be reassessed, as the project has not proven the ability to do this work.

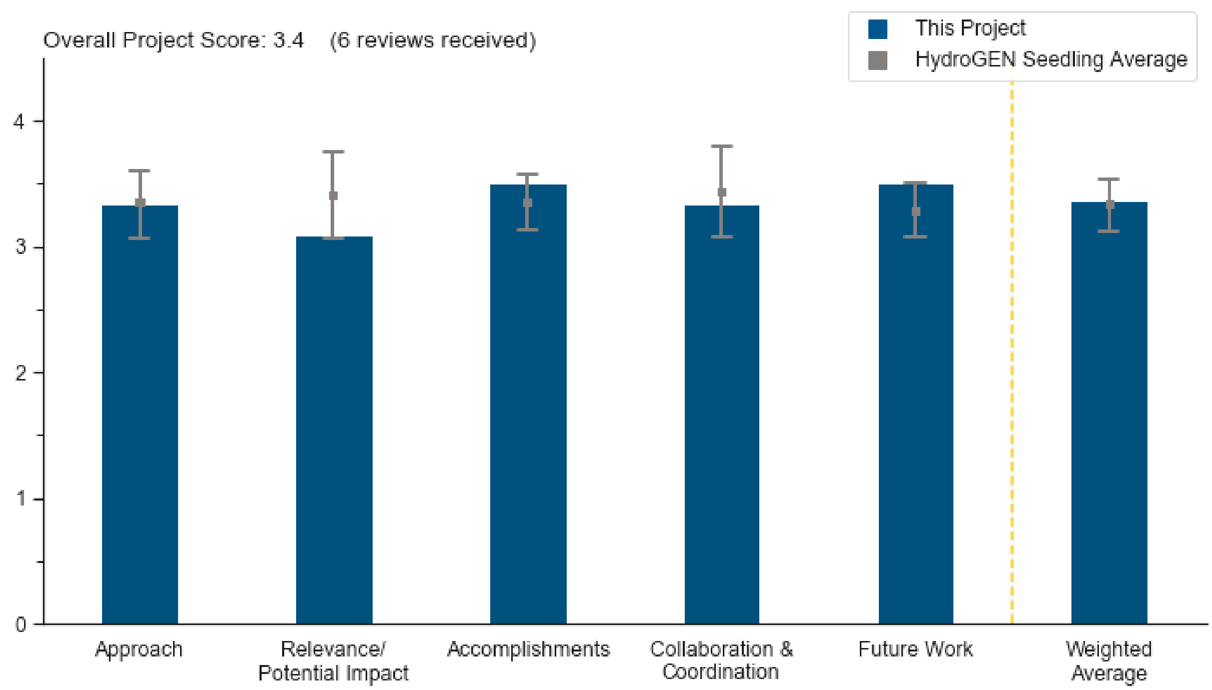
Project #P-168: Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for Solar Thermochemical Hydrogen

Ellen Stechel, Arizona State University

Brief Summary of Project

The project objectives are (1) to contribute to improved solar thermochemical hydrogen (STCH) materials discovery by providing strategies to boost solar-to-hydrogen thermal efficiency and (2) to provide experimentalists with crucial input to synthesize, validate, and perform further testing on promising candidates. The project will apply first principles computational materials design capability to calculate and validate chemical potentials for complex off-stoichiometric redox-active mixed ionic electronic conducting perovskite metal oxides. The end goal is to determine design principles for optimal and discoverable materials that have the potential to perform better than ceria, meet the target efficiency (solar-to-hydrogen thermal efficiency >30%), and approach the ultimate production cost goal of <$2/kg H_2.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The project is strategically focused on thermodynamic principles of the materials used for thermochemical redox chemistry. This is a very promising way to identify promising candidate materials. The work is based on excellent theoretical knowledge, as well as practical experience with concentrated solar radiation. Therefore, it seems that the project is seriously taking into account the difficulties of transferring the results from the simulation into application.
- The project goals are well articulated: "to determine the optimum reduction enthalpy (ΔH) that balances degree of reduction, hydrogen yield, and temperature swing and, given that, strategies to tune the ΔH." Similarly, the barriers are well described, and the project approach is well constructed, with complementary tasks.

- The approach is a well-conceived, simply described, multifaceted body of work.
- This is a theory effort aimed at providing guidance for materials design by first principles calculation of defects at a very fundamental materials level. There was some text mentioning "inverse design," but this was not explained. The key goals are increasing reduction capacity (delta to 0.15) but at only modest temperature reduction, as well as improving uncertainty; these are valuable goals. The question of "how good is good enough" is very important, but the method to achieve this was unclear. It was also unclear how the experimental teams will use the results.
- The first principles approach was appreciated. However, the value of the STCH processes overall is questionable.
- For this project, it was a little bit hard to get the point.

Question 2: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The project has a good balance of theory and experimental work using modeling to reduce the number of candidate materials, as with the other HydroGEN projects. However, this particular project seems the most focused on application of the four oxide discovery projects, and it is perhaps the most robust in terms of considering what is required to achieve the DOE targets. The project arguably "enhances the broader HydroGEN by providing a missing link between computation, experiment, efficiency, and cost of H_2."
- The simulations are valuable to help guide new materials efforts needed for STCH; uncertainty quantification is important here.
- This work is essential to achieving much-needed STCH performance breakthroughs.
- Developing the thermodynamic first principles for materials development should be broadly applicable to DOE and other technical developments. The value of STCH is dubious, but that is a concern for the Hydrogen Fuel Cells Program (the Program).
- As in all other material-oriented projects, the step into application is very big. The results of the project will certainly be important. However, the impact on the $2/kg hydrogen goal will be limited.
- Perovskites continue to hold promise for the Program; however, this project did not do a good job making clear what values constitute success. The targeted reduction capacity values seem very high—five times the state of the art—but the accuracy of the model for the chemical potential is targeted to be +/-20%. If the reduction capacity values approach anything like the multiple the project is pursuing, then it is not clear that 20% would matter; the system would have increased performance by 500%. If the error budget allotted for this work is +/-20% error on a logarithmic scale (as seen on slide 11), then that is perhaps more commensurate with the reduction capacity being targeted, but then the error is just huge. On slide 9, the project claims to provide the missing link between computation, experiment, efficiency, and the cost of hydrogen; however, the cost of hydrogen may be generated only by high-fidelity engineering and technoeconomic models, of which there is little in this presentation.

Question 3: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- As noted in other projects, it is not clear how the HydroGEN projects should be judged in terms of metrics, deliverables, or timing. However, as elsewhere, it is clear that substantial progress has been made since the last Program Annual Merit Review. This presentation is nicely constructed to show that the project has a consistent and logical basis, and the data presented show promise in terms of material discovery, while at the same time recognizing just how tough the problem is in terms of the required performance.
- The project achieved excellent progress. As in all other related projects, the topic is extremely complex, and the work necessary to achieve the final goals will need more time. However, the team showed that the way ahead is very promising and will lead to important results.
- There is progress in achieving the goals, and there are predictions of ΔH for ceria and alloys. It seems that 20% accuracy is aggressive, especially over a range of temperatures and for high delta (reduction capacity)

where vacancies will start to interact. The work did not seem to account for the vacancy–vacancy interaction. It was unclear how close the team was to the go/no-go goal.
- For the dollars spent and the time elapsed, the progress is pretty good. There has been a publication and a few presentations. Perhaps two compounds have been identified as potential candidates.
- This is a good approach that involves defining the need, then finding candidate materials, rather than trying to characterize materials.
- The results to date bode well for future discoveries.

Question 4: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- The project is well coordinated and effectively leverages the appropriate expertise at institutions in the Energy Materials Network (EMN).
- The project is very well embedded in HydroGEN. It presents an excellent collaboration that is absolutely appropriate to achieve the goals.
- Publications from this diverse team are highly anticipated.
- The partnering with Princeton University Dean Emily Carter (outside of HydroGEN) is excellent, but it is unclear how much interaction there is with the synthesis groups. In principle, this can be strong, but this was not demonstrated. It was also unclear how the experimental teams will use the results.
- There seem to be many institutions identified as collaborators, and there is no doubt that some collaboration is ongoing. However, it seems like there might be too many collaborators or that the project is seeking to accomplish too much, and so each contribution is "diluted."
- It is unclear to what extent the team is collaborating with national laboratories on model development. However, this work may be outside the experience of the national laboratories. The collaboration with laboratories on synthesis is good, although it would be good to quickly transfer that work to a commercial materials partner who might accelerate the technology adoption.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The project presented an excellent strategy to continue its successful work. The proposed actions are perfect to achieve the goals within the project.
- It is a good approach to develop models now that candidate materials have been identified.
- The project appears well managed, with a good understanding of where it is and what the next steps need to be.
- The team appears to have a clear vision of its path forward.
- This was brief but directed along the necessary lines.
- The work on (A,A')(B,B')O3 "quinary" perovskites seems interesting, especially if it can consider, respect, or reflect the so-called layered structure that others have observed. The quantification of the thermodynamic and/or kinetic benefits of these higher-order opportunities needs to occur. However, it is not clear that the layer structures or other natural phenomena are of large enough magnitude to be a game changer for perovskites. There is some mention of enhancing and/or refining some of the collaboration. Perhaps this will serve to focus the team's contributions.

Project strengths:

- This is a fundamental materials design project that targets new, badly needed materials for STCH. The key goals of accuracy and increasing capacity are excellent.
- The thermodynamic-based simulation is the clear strength of the project, along with the experience the scientists involved have with the application of the materials under real solar conditions.
- The project team has a successful history of working in perovskite materials and a strong working relationship with Sandia National Laboratories (SNL).
- This is an impressive piece of work that effectively utilizes the multi-institution competencies within EMN.
- The strength of this work is first principle development and comparison with experimentation.
- The project's goals, approach, team, collaboration, and results are all impressive.

Project weaknesses:

- A closer connection to application would improve this project. However, as the materials are the main focus, at least a little more effort on experiments might underline the successful modeling work.
- "Materials by design" is an aspirational goal that many fields have failed to achieve. This approach seems to come with considerable risk, with the uncertainty that propagates through the models and the currently vague nature of the engineered systems required to exploit the as-of-yet unidentified materials.
- The June 30 go/no-go milestone is quite close, and it is difficult to judge how the SNL work is tracking to deliver on this.
- There is no focus on reducing maximum temperature, an important issue in STCH. There seem to be limited interactions with experimental teams, especially in terms of synthesis.
- The value of STCH overall is questionable.

Recommendations for additions/deletions to project scope:

- The project works well. It should be continued as presented.
- The scope is good.
- It would be valuable to have some harmonization of target performance across the HydroGEN projects. Each project has its own targets, which could benefit from some inter-comparison to ensure that each set is sufficient to meet or approach DOE targets. All of the HydroGEN project presentations should be made clearer in terms of project plan, performance, and expected timeline.
- The team should improve interactions with the synthesis efforts in HydroGEN.
- Publication topic plans would provide context and direction at this point.

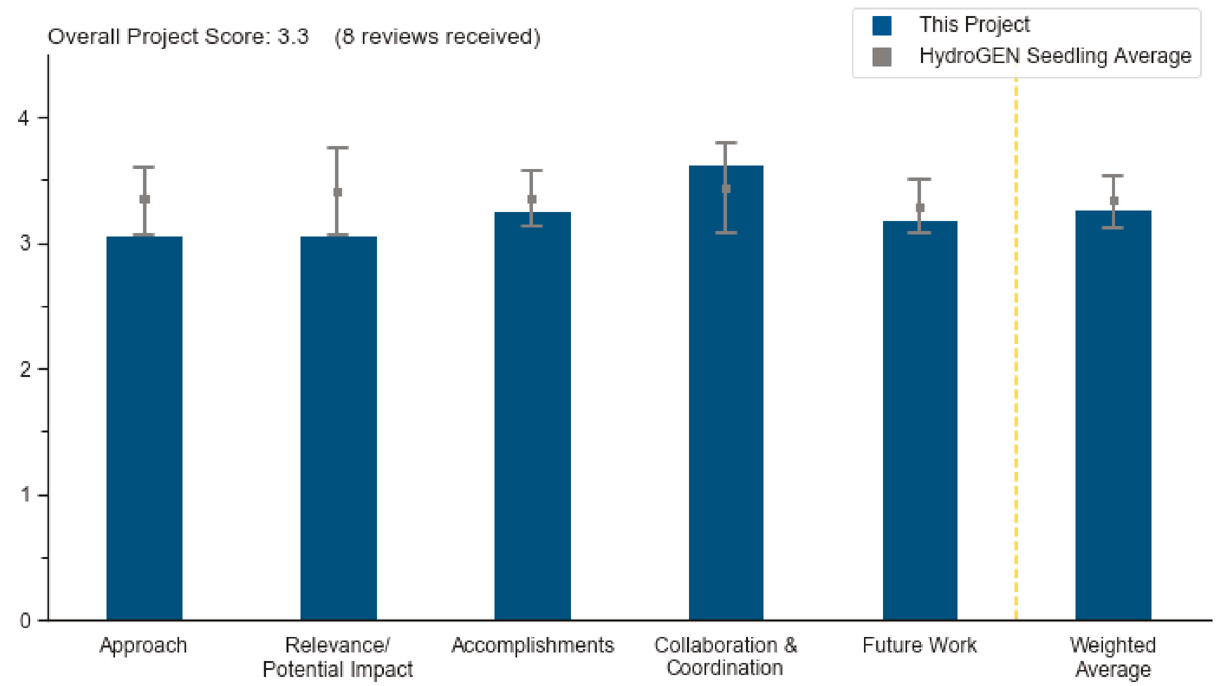
Project #P-169: High-Temperature Reactor Catalyst Material Development for Low-Cost and Efficient Solar-Driven Sulfur-Based Processes

Claudio Corgnale, Greenway Energy

Brief Summary of Project

The project objective is to develop an efficient and low-cost solar thermochemical hydrogen (STCH) process. In particular, this project is focused on the solar-driven hybrid sulfur (HyS) cycle and the development of catalytic materials to decompose sulfuric acid, a critical step in this two-step water-splitting cycle. The project will (1) develop a new catalyst material using the team's demonstrated surface free energy and electro-less deposition technique; (2) design a novel, integrated, direct solar reactor–receiver, based on a demonstrated cavity solar reactor, and (3) perform system and cost analysis on an effective new STCH plant process.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The approach is excellent. The consortium has defined its goals very well. The work performed has led to excellent results in both catalyst stability and reactor design. A comparison with the state of the art would make this work outstanding. Maybe the time limits of the presentation did not allow for this.
- The project vision is well articulated, and barriers and solutions are well explained. The well-designed project has the potential to make significant and worthwhile innovation for the HyS process. It is less clear how this project fits within the HydroGEN consortium network, and while the same (and other) laboratories are engaged as in other projects, the activities and personnel are quite different and perhaps outside the Energy Materials Network (EMN), as such. Despite this, the project is excellent collaborative work that taps into the broad expertise available within the national laboratories. The project is well constructed, with complementary activities.

- The approach of splitting the work up into three levels enables the team to focus on various aspects of the project. The barriers of each of the tasks seem appropriate and well understood. Additionally, by looking barrier by barrier, the team can focus on the individual challenges associated with each. The team is clearly highly capable of achieving the individual tasks and goals.
    - However, it is not clear that the results from each level are passed on and the needs/solutions are integrated. This seems particularly true between level 1 and level 3. Particularly concerning is the fact that the economic model identifies key operating points that are outside of the catalytic operating window, i.e., T = 875°C and P = 35 bar, when materials failure occurs below 900°C. All economic assumptions are predicated on this, and therefore new materials metrics are needed that reflect this analysis. The use of summer solstice data as the basis for economics is dubious and should be clarified or reconsidered. Additionally, the assumption/approach of using a 360-degree tower is troubling, as light distribution is unlikely to be even the entire way around.
    - Similarly, it is unclear how the collaborations move between institutions; the slides attempt to show collaboration by writing names of teams, but it seems that Greenway Energy is mostly coordinating work rather than establishing a tight collaboration. Similarly, the hub members/ consortium seem intimately integrated as project partners rather than stand-alone “helpers.” A more coordinated approach should be taken in which results are more directly passed between partners. This needs to go beyond just biweekly/monthly meetings, or at least the collaborative results need to be more clearly articulated.
- This is an interesting project, and storing condensable SO_2 as a “potential” for, or deferred source of, hydrogen holds great promise as a cost-effective STCH strategy. It just seems like this project is doing too much: catalyst discovery, receiver design, plant layout, cost analysis, etc. Most of the work seems to be phenomenological in nature—or at least there is little in the way of scientific hypothesis presentation and evaluation. Many other projects and programs have looked at silicon carbide. In the U.S. Department of Energy’s (DOE’s) Solar Energy Technologies Office, a concentrated solar power (CSP) plant operator had a project looking at tubular SiC for a solar receiver. The researchers dropped a piece of this material on the floor from two or three feet up, and it fractured. After seeing this, they stopped investigating the material. This project does not state whether it is addressing the brittleness concern. The cost analysis does not adequately incorporate or otherwise represent uncertainty. It simply and flatly states that the cost hits \$2.0/kg H_2, which is exactly the target. It is interesting that the project suggests two significant figures (i.e., \$2.0, not \$2). The level of confidence in that 10-cent place is unclear. On slide 19, the solar plant efficiency is simply stated as 56.4, but the slide does not indicate whether this is the annual or peak average, or whether this is solar to electric or solar to thermal.
- The broader goal of the project—achieve low-cost hydrogen by developing new catalyst materials and integration with novel solar reactor design—comes through very clearly. However, the team’s approach using Pt and Ir catalysts is unlikely to yield the desired goal. Besides, the project’s approach is not consistent with established approaches and many other DOE-supported efforts that are trying to do away with platinum-group-metal (PGM) materials to achieve the same goal. In addition, estimating the cost of hydrogen production is not that meaningful at this time, given the early stage of development of this process, the multiple large uncertainties in the steps, and the use of PGM catalysts. This exact dilemma was part of the reason for the EMN’s creation—to go back to the drawing board and focus on developing new materials.
    - The chosen configuration is very difficult to implement for multiple reasons. (1) Having a process step involving a 900°C reactor mounted on top of a 200- to 400-meter tower comes with its challenges, such as maintenance. (2) Given variabilities in weather and cloud cover conditions, maintaining a reasonable temperature gradient (and hence, conversion efficiency) across both a unit solar reactor and the entire assembly is very difficult. (3) Daily thermal swing is likely to create its own catalyst durability and capacity factor challenges unless 24-hour storage capacity is considered, which will likely have an impact on the net system cost. (4) Controlling the dual-phase H_2SO_4 flow behavior will present additional challenges.
- This project has three components to achieve the goal of developing a new STCH plant process. The project takes a very wide approach to achieve the goal. All three parts seem to be progressing well. The new catalyst level has been successful and met the milestones, but there are concerns about limited stability demonstrated (only 75 hours) and the use of PGMs. Some concerns were expressed on the reactor designs. It is unclear what happens when a cloud goes overhead.

- The basic approach is novel and compelling. However, it is not clear that a centralized tower/heliostat design is optimal. Dish concentrators may lend themselves to lower capital expenses via economies of hardware mass production.
- The project received a lower score because it seems to be evaluating many different parts of this plant vs. having a definite technical target to improve. There should be more work at the Hydrogen and Fuel Cells Program (the Program) level to determine whether STCH processes even have value. CSP is not likely viable across a large geography, and the diurnal solar cycle necessarily requires pairing an intermittent heat source with a chemical process that works better at steady state. Nuclear thermochemical makes sense, but this seems to be trying to fit a square peg into a round hole. Reevaluating the value of STCH at the Program level is recommended.

Question 2: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The HyS cycle is one of the most likely options to attain the \$2/kg production cost. While not necessarily dependent on the discovery of novel materials, as is the case with the metal reduction–oxidation reaction (redox) cycles, considerable work remains necessary in the other aspects of the cycle to enable successful implementation, and this project identifies a number of these. The electrolyzer is necessarily outside the scope of this project but might be worthy of consideration within HydroGEN.
- The relevance of this is exceptionally high because cost-effective hydrogen production must occur as part of a vertically integrated industrial complex. Sulfuric acid is a foundational chemical capable of providing this opportunity. The number of process steps must be absolutely minimized and the energy recuperation maximized, where cost-effective (practical).
- This effort directly addresses the DOE goal of \$2/kg H_2.
- The goal of the project is relevant to achieving an alternate low-carbon hydrogen source.
- The project supports the DOE goals. That being said, only a portion of the budget/project is dedicated to materials development. The other aspects of the project are critical to identify pinch points, but these need to feed back into the materials development to update/re-evaluate the materials' stability and performance targets. This has not been done in a sufficiently clear manner. It is worthwhile to note that the project's technoeconomic analysis (TEA) seems to show that materials development is a lower cost motivator than project location. This should be assessed and explained, as this seems to be the biggest driver of cost savings, and there is no explanation as to where the original/new locations are or why they would save \$0.28/kg H_2. The project leverages HydroGEN resources, particularly for high-temperature and high-pressure testing of the catalytic behavior.
- The project is highly relevant to Fuel Cell Technologies Office objectives, and a cost-viable path to \$2/kg H_2 is shown, but most of this comes from the non-technical location to increase plant capacity factor.
- It seems to be rather difficult to achieve the very ambitious goal of \$2/kg H_2 using an iridium-based catalyst. The material is active, and it is stable for about 70+ hours, but the price of iridium is prohibitive for large-scale applications. Use under the very difficult solar conditions will be additionally challenging because of thermal shocks, frequent cycling, etc. Therefore, cheaper materials must be identified. The splitting of (waste) sulfuric acid is a well-developed industrial process. It would be interesting to compare the new catalyst materials with established ones.
    - The receiver design is interesting. However, it is not fully clear how the receiver will work efficiently on a solar tower with a round field. It is not clear how the receiver can be homogenously irradiated, taking into account that each mirror projects an image of the sun on the receiver that is brighter in the center and less bright at the edge. It is also not clear how the vertical flow of the gas in each fin is controlled such that the whole fin is used. Perhaps this has been solved already but was not presented in detail, probably because of limited time.
- There are serious concerns regarding the physics of the STCH pathway. Trying to pair an intermittent heat source with a continuous chemical process requires massive storage of chemical reagents and starts from behind the eight ball.

Question 3: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The consortium presented excellent developments. The stability of the materials could be improved substantially, and an interesting new reactor design was developed. The main developments in both areas are described, and patents are filed. The presentation described well how the project actions will reduce hydrogen production cost to achieve the final goal. As always, baseline cost can be discussed, but the actions to further reduce costs seem to be appropriate.
- Congratulations are due to the project for outstanding progress on the design and engineering of an innovative process cycle.
- The absence of reporting against a project plan makes it difficult to gauge progress in terms of metrics, deliverables, or timing. However, it is clear that substantial progress has been made since the last Program Annual Merit Review. The presentation shows significant progress in the solar reactor design, flowsheeting, and cost analysis. Perhaps slightly less impressive is the catalyst work, which is less sophisticated than in the other HydroGEN projects. Arguably, PGM-free catalysts are not as critical here, although the replacement of Ir is seen as important in the overall cost reduction. Good progress has been made in terms of long-term stability through use of a BN support rather than TiO_2.
- The progress on each level has been good. The project has successfully demonstrated a new catalyst that meets the requirements, showed an adequate reactor design, and conducted TEA of the reactor process. There are concerns about the cost of Ir and durability.
- The team has clearly identified and met project milestones as originally outlined, and the data appear convincing in terms of catalytic activity and longevity. The team presents system efficiency numbers that achieve the milestones, but these are less substantiated. Based on the data, it is imperative that the milestones and future go/no-go's are based on updated catalytic stability numbers that reflect the required operating conditions of the plant (T = 875°C and P = 35 bar)—harsher conditions than those under which the materials failure occurs. The budget looks appropriate for the work done, but no budget was presented for the second time period.
- There have been significant accomplishments toward catalyst development that exceeds targets. Perhaps this would be useful in nuclear thermochemical.
- It appears from the presentation that the project met its stated milestones. However, it is difficult to verify some of the assumptions that led to the optimistic results. For example, the solar-to-electric efficiency for a similar but simpler and more established tower-based direct-steam design for CSP is about 21%, which suggests even lower solar-to-hydrogen efficiency than the results shown in this project. The presentation material did not make the project resources or funding level clear, which would help in better gauging the accomplishment. The stated funding is for year 1 funding, and year 1 started September 2017.
- For the budget and the time elapsed, the accomplishments are okay; however, there are too many things happening, and so each accomplishment is less than excellent. For example, an interesting catalyst has been identified, but it comprises PGMs. An interesting receiver design has been proposed, but it is built of very risky materials. A cost analysis is complete, but it does not include error bars or some assumption analysis.

Question 4: Collaboration effectiveness

This project was rated **3.6** for its collaboration and coordination with HydroGEN and other research entities.

- This project plays a key role for HydroGEN, as it is the only one that takes the application of the process heavily into account. The exchange within HydroGEN seems to be excellent. The data provided for the Data Hub is of especially high value, as it helps the other HydroGEN projects to get a sense of how their processes might get implemented on solar tower facilities and how flowsheets of such processes would look.
- This is a very diverse and innovative team. The results, patents, publications, and presentations are evidence of outstanding collaboration and coordination.

- There is very good collaboration with HydroGEN partners, including Idaho National Laboratory for testing, the National Renewable Energy Laboratory (NREL) for reactor modeling, and NREL and Savannah River National Laboratory for TEA.
- The project is well coordinated and effectively leverages the appropriate expertise at institutions both inside and outside the EMN. Collaboration is happening and is well documented.
- The collaboration effort of the project team looks excellent, including the use of the HydroGEN Advanced Water Splitting Materials nodes.
- There is great collaboration across national laboratories and universities. It would be good to see a company or end user that would like to develop this technology to buy down risk on the application side.
- It is clear that the use of the nodes is critical to the work of this project. Hydrogen partners appear to do a great deal of work that has led this project to meeting its goals, particularly in terms of materials testing. There seems to be little integration with the 2b benchmarking and protocols team, the cross-cutting project, etc. The use of the Data Hub seems to be as a repository for work but not of great materials-sharing or development data value.
- Collaboration is good, but with so much of the work being delegated, it seems the results should be more robust.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed future work is completely logical. This is the way to proceed. It is very likely that the proposed way will lead to excellent results that help to implement the technology.
- The project appears well managed, with a good understanding of where it is and what the next steps need to be.
- The proposed future work is good and seems to have recognized some of the potential barriers (such as stability and cost) that need to be addressed. There are still open questions related to stability and long-term durability that need to be addressed.
- The future plans reflect the massive body of work that lays ahead.
- This is appropriate; however, materials requirements need to be updated to reflect the operating conditions found by systems modeling.
- The proposed future work all seems appropriate, but it seems to be continuing along the vein of trying to tackle too much. The project should identify the truly enabling aspect of this technology and focus on doing that bit first—and very well—and then tackle subsequent areas.
- The project team should focus on developing non-PGM catalysts and put less effort into system TEA. The new catalysts can potentially be used for other non-solar-based configurations. Since the current catalysts are unlikely to deploy commercially, it does not make sense to spend time on long-term durability tests.
- It is not clear what the next steps would be. Catalyst development is the highest-value target but is worth only a 7¢/kg cost reduction in the waterfall chart.

Project strengths:

- The global view on the whole process is the major strength of the project. The achieved results help with understanding the key components of the process, the active catalyst materials, and the solar reactor. Flowsheeting is used to describe the whole process and can be used for a sound economic evaluation.
- Strengths include very strong catalytic work and modeling/system design across different levels of the project. This project stands out in offering an approach to STCH different from other projects in terms of technology and systems design.
- The team is focused and making excellent progress toward a challenging goal. There are excellent collaborations within HydroGEN, and the team has made efforts to ensure good communication around the different parts of the project.
- The project team all have experience in the respective areas. The principal investigator is ambitious. The chemicals employed are of importance on national and international scales.
- This is an impressive piece of work that effectively utilizes the multi-institution competencies both within and outside the EMN.

- The ability to innovate is the team's most obvious strength. The involvement of commercialization partners is an area of strength that is missing from many other STCH projects.
- A strength is the ability to coordinate diverse skill sets, namely catalyst development and reactor and systems modeling.
- The project has good technical work.

Project weaknesses:

- There is a question of fit to the HydroGEN consortium, but in the absence of an alternative, this project should continue to be funded here.
- The selected materials seem to be too expensive and too rare for an application in the gigatonne range (which will become the hydrogen range). A comparison with the state-of-the-art catalysts would show whether this weakness might be overruled by the improved efficiency. The reactor design needs a deeper description concerning annual operation on a solar tower and flow within the receiver. Probably this was already done, but it was not presented in sufficient depth, probably because of time restrictions.
- If the project moves forward, getting some commercial catalyst and system original equipment manufacturers (OEMs) involved would be helpful. Boron nitride and silicon carbide are both commercially made and manufactured. OEMs should be able to help with understanding thermal cycling's effect on these catalyst supports.
- Better team integration is needed across the levels in terms of updating system results and moving new operating points. The reactor model needs to be updated to include shape factors and consider the implications of hot spots on the feasibility.
- The project team appears to downplay or ignore multiple significant technical challenges, which potentially led to the oversimplification of the technoeconomic model.
- A weakness is the apparent absence of risk management plans that address uncertainties involving the novel reactor design.
- There is a focus on PGMs that may limit applicability, and durability has not been adequately addressed.
- The project is trying to tackle too much all at one time.

Recommendations for additions/deletions to project scope:

- The project is excellent. It is on the right track. The project goals should be kept as they are.
- It would be valuable to have some harmonization of target performance across the HydroGEN projects. Each project has its own targets that could benefit from some inter-comparison to ensure that each set is sufficient to meet or approach DOE targets. All the HydroGEN project presentations should be made clearer in terms of the project plan and performance against the expected timeline.
- The project should focus on material identification, evaluation, and selection for the solar receiver and the design. If there are no materials that can operate with an adequate chemical, mechanical, cost, and risk profile, then that needs to be addressed.
- The value of STCH should be re-evaluated from a Program perspective, and risk should be mitigated by adding an end user. Involving catalyst, support, and OEM companies would buy down development risk.
- Materials stability requirements need to be updated per the system model; they do not account for the harsher operating conditions that are required.
- Non-PGM and durability focus should be increased. Given the emphasis of HydroGEN, the team should reach out to the EMN to better understand the catalysis mechanisms.
- The team should focus on catalyst material development, the basis for subsequent reactor and system studies.

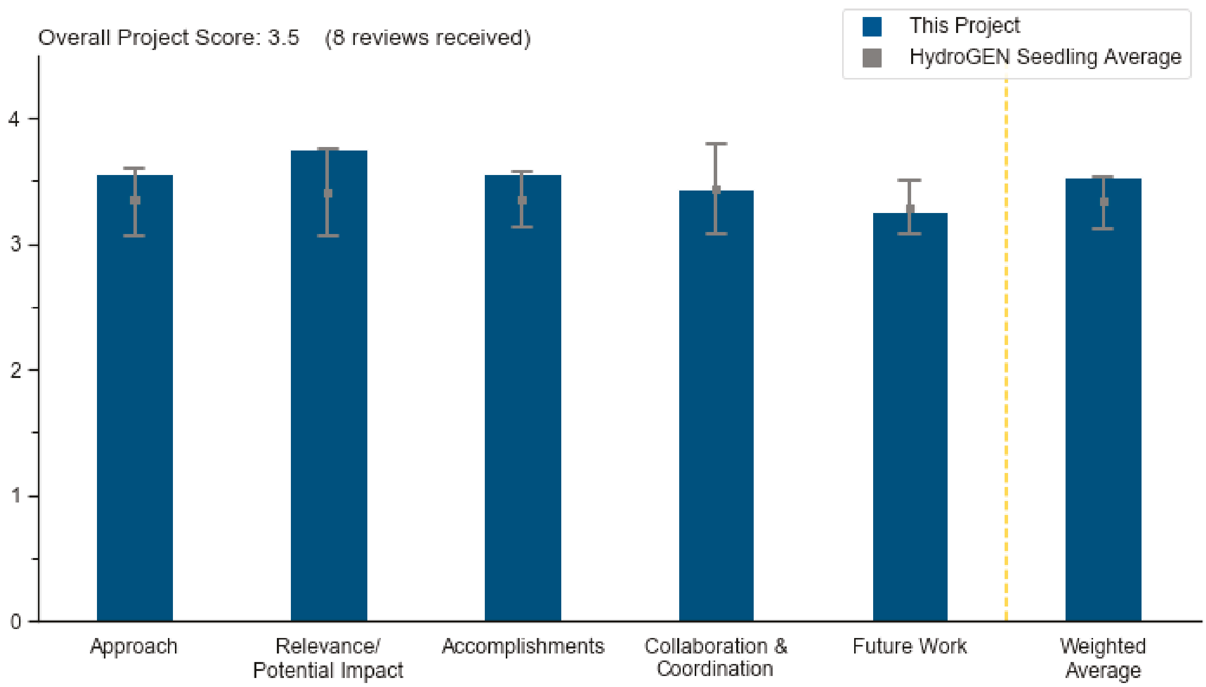
Project #P-170: Benchmarking Advanced Water-Splitting Technologies: Best Practices in Materials Characterization

Kathy Ayers, Proton OnSite

Brief Summary of Project

The project will develop a community-based living roadmap across technologies to assist in maintaining a balanced U.S. Department of Energy (DOE) portfolio. The project vision is to (1) develop a cohesive research and development (R&D) community working together; (2) interact with the Energy Materials Network (EMN) to define targets, best practices, gaps, and priorities; (3) aggregate and disseminate knowledge; and (4) accelerate innovation and deployment of advanced water-splitting technologies. The assembled team of subject matter experts for each sub-area will engage with each sub-community. A consultant from a similar effort in hydrogen storage will convey lessons learned. The project addresses a lack of consensus regarding testing protocols and standards and the need for a large diversity of information for compiling and developing. The project also addresses challenges presented by differences in technology readiness levels (TRLs) between different technologies.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- The development of standards and protocols for benchmarking is critical for providing an "apples-to-apples" comparison tool, which will allow researchers to evaluate and compare the performance of their materials relative to DOE technical targets. The development of protocols for benchmarking durability is challenging, given the goal of predicting long-term durability using a short-term test metric, but it will be of great value in the long run if an appropriate protocol can be developed and validated. The project appears to be well designed and well managed. The project includes non-HydroGEN members, both domestically and internationally, to gather information and feedback to develop the benchmarking protocols; this inclusion could allow the developed protocols to serve as the benchmarking metrics for the entire global scientific community.

- This is a good approach, given that the broad-ranging project covers benchmarking for three diverse water-splitting technologies. The metrics and survey priorities are a logical start to gathering information. Assembling roadmaps will give a high-level overview and enable better communication across the different hydrogen production options. Identifying gaps should allow for more strategic application of funds. Establishing standardized benchmarking protocols for testing should lead to better definitions of protocols and support the overall knowledge transfer.
- Addressing the need for such a database and roadmap is a very good idea. Gathering a community of experts to establish a set of protocols is of great value; the ability to compare developing components and emerging technologies is key to comparing various research groups' results. The searchable library of current protocols, procedures, and data is a great means of accessing the field.
- The approach for the project is reasonable. The team understands community acceptance is of utmost importance when developing protocols and has established methods to listen to the community through meetings and surveys. Identifying gaps and proposing future development roadmaps ensure the continued development of the initially proposed protocols.
- This is a large, intractable project that requires a high degree of collaboration. The structure of a lead principal investigator (PI) (and co-PIs) leading multiple subject matter expert entities is perhaps the only feasible approach. The community must accept the approach, so there must be significant industry input in development of the metrics. Given the wide scope of the project, breaking the project into five tasks, with sub-tasks for each technology, is a practical way to manage the project. A quarterly newsletter is an inefficient way to ensure interaction among stakeholders (or at least awareness of issues).
- The approach is very nice and systematic in terms of looking at different critical issues. There could be more outreach to international organizations in terms of the questionnaires and utilizing work being done by the International Energy Agency, etc. The technologies are all at different TRLs, and so the approach needs to be tailored a bit more for that. The audience of the protocols is unclear, as is how they will be utilized or validated.
- The project team has a comprehensive and well-thought-out approach for developing a framework for testing protocols and accumulating standards for water-splitting materials and associated pathway technologies. The researchers are using their own considerable expertise in conjunction with mechanisms (e.g., survey/questionnaire and in-person workshop) used to elicit input from the larger research community. This said, it is not completely clear how "best" practices will be assessed as such, or what metrics should be used that reflect how effectively the team is facilitating acceptance of community-wide technology.
- This is an ambitious effort, with many moving parts and reliance on building trust networks with various technology development communities outside HydroGEN. Given the limits on budget and time, this effort should focus its resources on (1) developing and documenting protocols, standards, and testing methodologies; and (2) building consensus and acceptance within respective communities for those outcomes. The roadmap and gap assessment activities, if necessary, should be conducted elsewhere.

Question 2: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- The collaborative input and participation of government, industry, and academia are important for a clearer understanding of practical needs for the technology and the current state of the technology. Management and analysis of these stakeholders' responses to surveys, etc., are of significant importance. Care must be taken not to have bias toward one group or technology, so it is key to get the biggest pool of responses for each questionnaire and survey. It is acknowledged that the PI is at the mercy of the participants' schedules and willingness and ability to submit feedback in a timely manner. However, slide 9 shows that a total of only 70 questionnaires were sent, which seems to be a small set.
    - The development and open dissemination of test protocols to interested parties could ensure that measurements, test conditions, etc. are all consistent and directly comparable. The collective results of this project could greatly reduce the time researchers need to develop their own

protocols. Many accomplishments are provided, including holding workshops; developing, disseminating, and collecting questionnaires; developing several standardized tests; and doing calibrations.

- The development and validation of benchmarking standards and protocols that are accepted by the broader scientific community is critical to supporting and advancing R&D progress toward meeting the DOE Fuel Cell Technologies Office (FCTO) and HydroGEN EMN overarching goal of producing hydrogen from renewable energy sources at a production cost of $2/kg H_2. The project does a good job leveraging the capabilities and expertise within HydroGEN to develop and execute benchmark protocols and standards, but the team also recognizes the need to engage the broader scientific community.
- Standardized testing will be critical to helping DOE bring diverse stakeholders together. Testing will also provide realistic input to Hydrogen and Fuel Cells Program goals and give clear, quantitative benchmarks to show whether future efforts are actually making progress toward cost and performance goals. Of great interest is the potential for reduced development cycle timelines and better management of R&D funds.
- This project brings a critical element to the HydroGEN consortium by ensuring that the methods used to discover and validate new water-splitting materials are used consistently across the research community. This type of benchmarking is rare and addresses issues of validity and provenance of data while this sub-field of materials science and engineering is still gaining maturity.
- The project has high relevance. Common frameworks and definitions are required for the clear discussion of ideas. DOE is uniquely capable of organizing this effort. Project outputs clearly benefit that community and the nation.
- This is a well-needed area and activity that FCTO should be doing. The impact could be very large, although that will vary with the technology level—with lower TRLs perhaps benefitting the most.
- A standard and fair comparison for the different water-splitting technologies has been a need in the community for years.
- Congratulations are due to the team, who accomplished quite a bit in the first year.

Question 3: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- There has been good progress to date in engaging both the HydroGEN members and the broader scientific community through the workshop (annual project meeting), questionnaires, and face-to-face discussions to define the needs and developmental pathway for establishing the benchmarking protocols and standards. The node gap analysis is critical to determining whether the required capabilities and expertise exist and are at the appropriate readiness level within HydroGEN, or if there is a need to leverage outside capabilities and expertise within the DOE national laboratory system—those not already involved in HydroGEN—or the broader academic or industrial community.
- This is a large project for which consensus may be difficult to achieve. Nonetheless, it appears substantial progress has been made. Technology roadmaps appear to be key and very useful products of the project. Roadmaps have been drafted but have not yet been finalized. A first round of test protocols has been developed. From the number of protocols, it appears to be a very substantial body of work.
- The project has completed five of six milestones, with a final go/no-go decision under discussion. The draft roadmap has been completed for each technology area and now should have some level of external third-party review from sources not involved with DOE or the national laboratories.
- The accomplishments are documented and are impressive. If participants and the research community contribute to the DOE database, it will be a great asset to all.
- By its very nature, if this project did not collaborate and build trust networks with HydroGEN and the broader technology development communities, it would fail. Thus far, it does not look like a failure.
- The team has made really good progress in the past year.
- The team has an impressive list of accomplishments for the amount of time spent so far on this effort (roughly one and a half years). The list includes the creation, distribution, collection, and analysis of questionnaires for each water-splitting pathway, development of a test framework, analysis of nodes (capabilities) missing from the HydroGEN consortium and needed for materials discovery or validation, a community-wide workshop, definition of an initial set of test protocols across the water-splitting pathways,

and creation of draft roadmaps for these pathways. One element that seems to be missing is publications that bring methodologies and results developed in this project to the wider community. A majority of the items listed on slide 26 are conference presentations and (perhaps) proceedings. However, increased impact will be achieved by even wider dissemination of the team's results through peer-reviewed journal articles.

- The team has made progress in defining and getting input from stakeholders and defining what needs to be done in terms of the protocol development. The maps and initial outputs are promising, as was the workshop, but the exact follow-up is not clear. Also, the pathways are not easily translatable among the different technology pathways, as they exist at different levels.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- A strength of this project is its effort to engage the broader global scientific community to assist in the design, development, and validation of the benchmarking standards and protocols. It was particularly encouraging to see the high level of response from the international community, as shown in the table on slide 9. Developing benchmarking protocols and standards that are accepted by the broader scientific community will go a long way toward accelerating the development of the renewable hydrogen production technologies being pursued by DOE and HydroGEN, which could provide added benefit to DOE.
- The project appears to be have been highly effective in collaboration. A large number of industry experts have been involved, with numerous opportunities for researchers to voice their thoughts. The regularly scheduled meetings, use of questionnaires, and breakdown into technology-specific topics all combine to create a highly collaborative work environment.
- Developing protocols is difficult; the project team seems to engage the HydroGEN and larger community with all the steps along the way.
- Advising about standard practices, as well as having a means to compare disparate results against standards, is very important for advancing R&D. This is an ambitious effort with potential for high impact.
- This group has done a great job engaging, collaborating, and coordinating with many groups in the field.
- The team is doing a great job at collaborating and coordinating the core team's individual areas of expertise to lead community information-gathering efforts in these areas. The team is still in the process of consolidating the different contributions for dissemination on the Data Hub website, and thus the appearance of the site is very rough and provides only questionnaires and results at this time. According to the PI, many of the additional contributions (e.g., test protocols) are available on the primary h2awsm.org site. Consolidation onto the Data Hub will be critical; it will limit user frustration and maximize accessibility. At the least, the Data Hub should contain links to this other information. It would also be good to see a more detailed list of the institutions (outside of HydroGEN and the benchmarking team) that are contributing information used for this activity. This would provide a sense of how large the affected and participating community actually is.
- Outreach to the community has been good, although further international participation would be good, as would ensuring that the protocol audience members are participating. Collaboration with companies that work with similar technologies such as fuel cells, chlor-alkali, etc. would be good as well.
- With the diverse maturity levels, it may be difficult to find sufficient collaboration from industry. It would be helpful to have a separate listing of all external review efforts for each individual advanced water-splitting technology: electrolysis, high-temperature, and photoelectrochemical (PEC). A limited number of partners outside of the laboratories or FCTO were mentioned.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- Developing protocols for evaluating durability and degradation is a challenging but extremely critical task. The assumption is that sub-scale development is focused on establishing benchmarking protocols for components and systems at the pilot scale. Given that this appears to be a two-year project slated to end at the end of fiscal year 2019, it is unclear whether this effort is part of Phase I or work that will be done if the project is renewed. Developing benchmarking protocols for components and systems is as critical as developing benchmarking protocols for materials and should be pursued, whether it is part of budget period 1 or budget period 2 (presumably budget period 2 is the renewal). The node gap analysis identified the need for node expansion in each technology. This appears to be a critical issue, and if so, it is unclear how these needs will be addressed: perhaps this work can be done with existing capabilities and expertise within the six national laboratory partners, or perhaps it will require external collaboration, either within or outside the DOE national laboratory system.

- While the project is ending in September 2019, there are several important items listed as proposed future work. If any or all of these items are completed, this would have to be considered a very successful effort.
- Several milestones are left for 2019, and the list of operational conditions, accelerated testing protocols, and gap analysis will be critical to leveraging existing work to date.
- Development of accelerated testing protocols is particularly noteworthy. A future focus on bench-scale validation is also well considered.
- Future work shows a clear path forward.
- This group and the associated HydroGEN laboratories will be quite busy developing, testing, and validating protocols (at whatever scale). Assessing the capability content of HydroGEN and identifying gaps for future needs should be conducted separately from this project.
- The dissemination strategy, and whether information will reach everyone it needs to, is not clear. DOE might have to drive this. A critical step in this activity seems to be protocol evaluation and verification, which is not budgeted or handled by this group, but it seems the EMN nodes might handle this step—that is not clear or budgeted. This is the main reason for the lower score given. It is not clear how the outputs of the first workshop are being used, especially for subsequent workshops, which are proposed to be annual. The proposed work in terms of approach is fine for the protocol development, aside from the comment regarding validation, which is a final milestone.
- The proposed future work presents a logical sequence of next steps needed to formalize this protocol development. It is curious that the milestones for budget period 2 do not mention specific deliverables associated with disseminating the team's results and accomplishments. It is not clear if there is a plan for this beyond feeding data into the Data Hub.

Project strengths:

- The establishment of benchmarking protocols and standards for materials, components, and systems is critical for enabling DOE to meet its hydrogen production cost target. The engagement of the broader scientific community in developing the benchmarking protocols and standards is a particular strength of this project. This engagement has the potential to have these protocols and standards accepted by the broader scientific community (beyond HydroGEN), which could benefit DOE in the long run by accelerating the development of these technologies.
- The PI, Kathy Ayers, is very well suited—perhaps uniquely suited—to lead this effort. She is a key strength of the entire project. The team of subject matter experts selected and willing to participate is another strength. They collectively represent the cutting edge of the relevant technologies. This group's adoption of the final test protocols will ensure adoption of new standards throughout the community—and the world.
- This project brings a critical and valuable element to the HydroGEN consortium's activities. The approach is comprehensive and well thought out, and it is producing results that further the goals of DOE, HydroGEN, and the larger water-splitting materials community.
- This ambitious effort is heavily predicated on successful engagement with HydroGEN and the larger technology R&D communities. Thus far, the approach appears sound and is producing results, thanks to the strength of the core project team.
- The strength of this project is having identified the need to establish a set of standards for evaluation in a specific technology. The team has systematically engaged the experts; collected and analyzed their thoughts, opinions, and inputs; and produced agreed-upon protocols.
- This is a critical area with a good team across different technologies. The project has a very systematic approach toward establishing roadmaps and benchmarks but can work with others doing similar efforts in related technologies.

- The project involves a diverse group across academia and industry. This is a quantitative effort, with standardized surveys requesting status and updates of the three different hydrogen production areas.
- This is a well-thought-out and much-needed project for the community. The main strengths are in the accomplishments so far, as well as the open communication with the stakeholders.

Project weaknesses:

- In looking at the limited information provided in developing the benchmarking protocols and standards, there appear to be a significant number of properties for which protocols and standards are being developed for new materials being developed for a specific technology. There is a very high probability that a new material will not meet all of the required performance targets. It is not clear whether there is any effort or benefit to ranking which material property is most important at the early stage of development. Such an effort might serve as a guide to help both developers and funding agencies determine whether a material should be further developed and, if so, where the R&D focus should be.
    - Given that this project is still in the early stages of defining and developing the protocols and standards, there are no glaring weaknesses. Critical will be the validation and acceptance of the protocols and standards. The perceived value of the project is extremely high. The more difficult task will be trying to "quantify" the benefit in terms of how it accelerates and reduces the cost of technology development.
- Perhaps the initial questionnaire pool was too small, but otherwise, this is an important project.
- There are no significant weaknesses that need mentioning.
- Protocol validation is critical but not within scope. The effort and the approach are being applied equally among the technology pathways, although the lower-TRL ones should need some more effort than the higher-TRL ones, or perhaps a different focus. Also, the PEC ones, for example, can leverage previous activities, whereas high-temperature electrolysis can perhaps leverage solid oxide fuel cell efforts and low-temperature electrolysis can leverage company efforts. It is not clear how these are being translated and whether the gaps are being identified with that perspective in mind.
- It is unclear how "best" practices will be assessed as such, or what metrics should be used that reflect community acceptance of water-splitting materials and technology. One element that seems to be missing is publications that bring methodologies and results developed in this project to the wider community, thereby increasing its impact.
- This effort should focus its resources on (1) developing and documenting protocols, standards, and testing methodologies; and (2) building consensus and acceptance within respective communities for those outcomes. The roadmap and gap assessment activities should be conducted elsewhere.
- The project could use additional industry or objective third-party input on the effort.
- Frameworks and roadmaps are not yet finalized (they are behind schedule).

Recommendations for additions/deletions to project scope:

- The project scope seemed ambitious but appears to be going exceptionally well, based on the demonstrated accomplishments. No additions or deletions are suggested.
- Once the benchmarking protocols and standards are established and are being practiced, there should be a follow-on effort to evaluate the effectiveness toward accelerating technology development to meet DOE's overall goal in terms of its hydrogen cost target. Developing protocols and metrics for benchmarking material performance typically utilizes commercial analytical equipment for conducting the evaluation; most materials developers either own such equipment or can easily get access to it. For components and systems, standard commercial breadboard-type systems either do not exist or are not readily accessible to many developers, especially those developing components. Component developers often use computer-based engineering systems modeling and analysis to evaluate component performance and its effects on system performance as a means of reducing cost. The team should consider engineering systems modeling and analysis as a tool for benchmarking performance in an integrated system.
- It is critical to consolidate information to the Data Hub, so that all project results are in a single "location." Also needed is a more detailed list of institutions that are contributing information to this activity, as it would provide a broader sense of the community size invested in this research field.

- International reviews of the roadmaps and additional input or review of progress would be helpful, if resources and time allow.
- It appears likely that follow-on work to update, expand, and further validate the frameworks and protocols will be beneficial.
- The project needs to add validation of protocols, which should be done at the HydroGEN laboratories.
- The project should delete the technology development roadmap and EMN capability gap assessment activities.

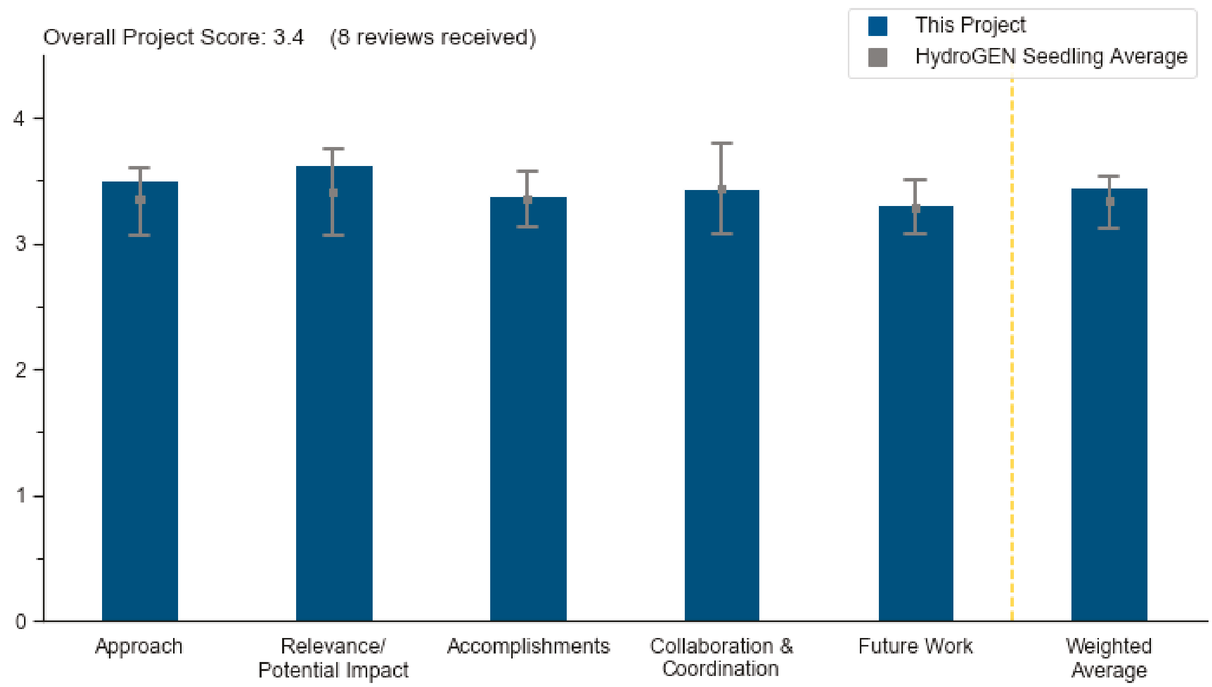
Project #P-175: Intermediate-Temperature Proton-Conducting Solid Oxide Electrolysis Cells with Improved Performance and Delivery

Xingbo Liu, West Virginia University

Brief Summary of Project

This project will develop an intermediate-temperature proton-conducting solid oxide electrolysis cell (H-SOEC) through innovative material discovery, high-throughput screening, and model-informed electrode design. The result will be an anode with extensively broadened reactive sites and highly intrinsic electrocatalytic activity to yield current densities in an H-SOEC of >1A/cm^2 at 1.4 V/cell at 600°C and degradation of <4 mV/1000 h. The team will identify highly active, triple-conducting electrocatalysts and develop conformal coating methods for depositing these catalysts into composite anode functional layers to lower the dominant anode polarization resistance associated with water splitting in H-SOECs.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- There is no need to improve any more. The proposed approaches can effectively fulfill the U.S. Department of Energy's goals.
- This is a strong project with a solid team and several excellent concepts that are being pursued. The project has the very good idea of simultaneous water splitting and hydrogen separation to suppress nickel oxidation, and the coefficient of thermal-expansion-matched anode and electrolyte materials are good ideas if the performance of both the electrolyte and anode materials can be optimized. There are some compelling reasons to consider proton-conducting ceramic electrolytes for electrochemical water splitting to produce hydrogen. Operating temperatures are high enough so that precious metal electrodes are not required, yet not so high that thermal integration is challenging. The electrode-supported electrolyte membrane architecture targeted in this project makes a lot of sense for minimizing resistance (and power

consumption) during electrolysis. A challenge is that the best proton-conducting ceramics (based on barium zirconate) require very high sintering temperatures for densification, which makes it difficult to achieve the targeted porous-electrode-supported, dense-thin-film electrolyte architectures. Another challenge is that the design of electrochemically active and stable electrode materials for operation at 600°C is not easy.
- The researchers are addressing the key issues and, unlike many others in the proton-conducting field, are considering the impact of potential nickel oxidation. They are using experiments and modeling to understand the system. They are proposing atomic layer deposition for the catalyst. It is not clear that this deposition approach can be economically scaled.
- There is a good balance of experimental and modeling contributions to address the project's objectives. There is a worthy objective of increasing the durability of high-temperature electrolysis by moving to a proton-conducting system that can operate at somewhat lower temperatures. One caution is that the approach involves a large number of challenges; the team should make sure to focus on few enough of them that meaningful progress can be made.
- Addressing interfacial conductivity to solve some of the proton-conducting solid oxide electrode issues seems to be a promising approach.
- A triple-conducting backbone electrode offers substantial theoretical advantages for SOEC systems.
- The approaches are logical and appropriate, considering the current stage of development of the technology.
- The presenter answered questions clearly. The project focused sharply on overcoming critical barriers and presented strategies to address the issues.

Question 2: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- Solid oxide electrolysis is a key component of DOE's emerging portfolio of hydrogen production technologies. If this project is successful, a promising materials set for SOECs with potential for improved long-term durability will be identified for the future development of SOEC stack and system technology. Thus, this project has high relevance and a significant potential impact.
- The project brought in a new concept and characterization for achieving high-performance, high-temperature electrodes for efficient and cost-effective hydrogen production. It is critical to the DOE Hydrogen and Fuel Cells Program (the Program) and has the potential to contribute significantly to DOE goals and objectives; the project is significantly leveraging and contributing to the HydroGEN consortium.
- Intermediate-temperature electrolysis is a key enabler for H2@Scale and is very relevant. Since the electrolysis occurs at an elevated temperature, significantly less electrical power is required compared to low-temperature electrolysis, which translates into lower-cost hydrogen. The project is using low-cost materials, resulting in low capital costs. The researchers are trying to decrease the degradation rate, which is a key limiter for high-temperature electrolysis.
- The project aligns well with the Program and DOE research, development, and demonstration (RD&D) objectives, and it has the potential to advance progress toward DOE RD&D goals and objectives.
- The project is likely to uncover important information to guide further development of hydrogen SOEC technology.
- The direct separation and potential electrolysis of hydrogen is highly relevant; this characteristic advantage seems understated.
- The project aligns well with the Program.
- The project is relevant to high-temperature water electrolysis.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- Within the short term of the project period, the team has achieved very good current density under -H-SOEC mode and has produced three papers or manuscripts. This project is on the right track to approach its objectives and make significant progress toward overall DOE goals.
- The project started in fiscal year (FY) 2019. Key research thrusts that have started include developing the system model, exploring the material composition space using high-throughput screening, synthesizing and characterizing new materials, and doing button-cell testing.
- Excellent progress toward the project objectives has been demonstrated through clear and measurable performance indicators; the results suggest that one or more critical barriers will be overcome.
- The project goals are on track, with good progress made on model development. Evaluating conditions (such as water concentration) should be stated on the target table for the various years.
- This project just recently started, so it is difficult to judge progress. Some materials issues have been identified, and good progress has been made to address them.
- Progress has been made toward achieving the overall objectives.
- The project has made sufficient progress.
- The kinetic model development is very good and will be useful in modeling a cell or stack. The project achieved the ~1 A/cm^2 current density at 1.4 V and 700°C. The temperature is very high for an "intermediate" temperature stack. It would be expected to be closer to 600°C. The researchers will need to improve their catalyst. The durability was done at the very low current density of 400 mA/cm^2, so it is not surprising that they were able to meet the durability target. To evaluate the durability, they need to stress the cell by operating at higher currents. The fabrication methods being used are not very amenable to stack fabrication.

Question 4: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The collaboration between West Virginia University (WVU), the Colorado School of Mines (CSM), the National Renewable Energy Laboratory (NREL), and Idaho National Laboratory (INL) is perfect. They all contribute to the project well. If regular team meetings could be scheduled, it would be better.
- This is a strong team, and there appears to be a high degree of collaboration among the team members. There seem to be many moving parts in this project; it will be interesting to see how they all come together.
- There are effective collaborations with partners. Using NREL to do combinatorial studies is interesting. It would be good to see how those studies are being done and the results. Combinatorial studies are difficult to set up to ensure no false positives or negatives are produced. Unless the testing is being done in a relevant environment, misleading results may occur.
- All research thrusts (WVU, CSM, NREL, and INL) are engaged and contributing to the objectives laid out in the plan.
- There has been excellent and effective coordination between the team members.
- It appears that collaboration between partners is well coordinated.
- The interactions between collaborators are reasonable.
- Collaboration appears effective and extensive.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future work seems to be well planned. The proposed tasks are effective for overcoming most of the technical barriers.
- The proposed future work is excellent. If there were a plan for integrating the X-ray photoelectron spectroscopy (XPS) characterization results with the electrode kinetics model, it would be better.

- The proposed future work is a logical continuation of the presented effort. Hydrogen cost and thermal cycling should be part of future testing.
- There is a reasonable outline of the next steps. It would be good to see some modeling added to guide materials composition selection.
- The researchers are focusing on improving the performance and addressing the key challenges. They should consider the manufacturing aspects of how to scale up the cells or work with someone who has experience in stack manufacturing.
- The proposed future work is appropriate to address the identified technical barriers.
- The proposed future work is consistent with the project objectives.
- The FY 2019 combinatorial catalyst-coating task should conclude or be constrained before the start of FY 2020 to avoid changing too many variables going into the conclusion of the project.

Project strengths:

- The project integrates the kinetic modeling, button-cell evaluation, materials screening, in situ XPS characterization, and large-scale testing, allowing for significant achievement. The new design and understanding of a triple-conducting composite anode will significantly boost research in the high-temperature electrolysis field. The use of "environmental" XPS (E-XPS) is also a great addition.
- The breadth of the team and the approach are strengths, as is the extent of progress that has been made in a short period of time. The team is working on an important challenge (durable steam electrolysis systems).
- The project has a strong team. Strong concepts are being evaluated. New materials sets are being established with the potential for high performance and long-term durability.
- The project has excellent kinetic modeling capabilities and a good team. The materials are of interest and have the potential to achieve their technical targets.
- The project has a unique approach that, if successful, is well suited to meet DOE goals and targets.
- The project is focused on addressing the interfacial transport of various species.
- The project's main strengths are the approaches for addressing the technical issues of the proposed concept.
- The team seems to work together well.

Project weaknesses:

- The project has no major weaknesses.
- The durability is in question since the tests run were at a very low current. The button-cell fabrication techniques are not amenable for large cell and stack fabrication.
- The researchers may be biting off more than they can chew, so it may end up being difficult to generalize or build off of the results.
- With so many moving parts, maintaining focus and team cohesion will be a challenge.
- There are several opportunities to get stuck in an "optimization loop" as the project concludes.
- The efficiency of the proposed system is not mentioned.
- The coatings might be more prone to fracturing.

Recommendations for additions/deletions to project scope:

- It is suggested that the team do the durability testing in a lower steam concentration (below 60%).
- The durability tests should be done at a more challenging current.
- The team's materials modeling capabilities should be considered.
- There are no recommendations for additions/deletions to the project scope.

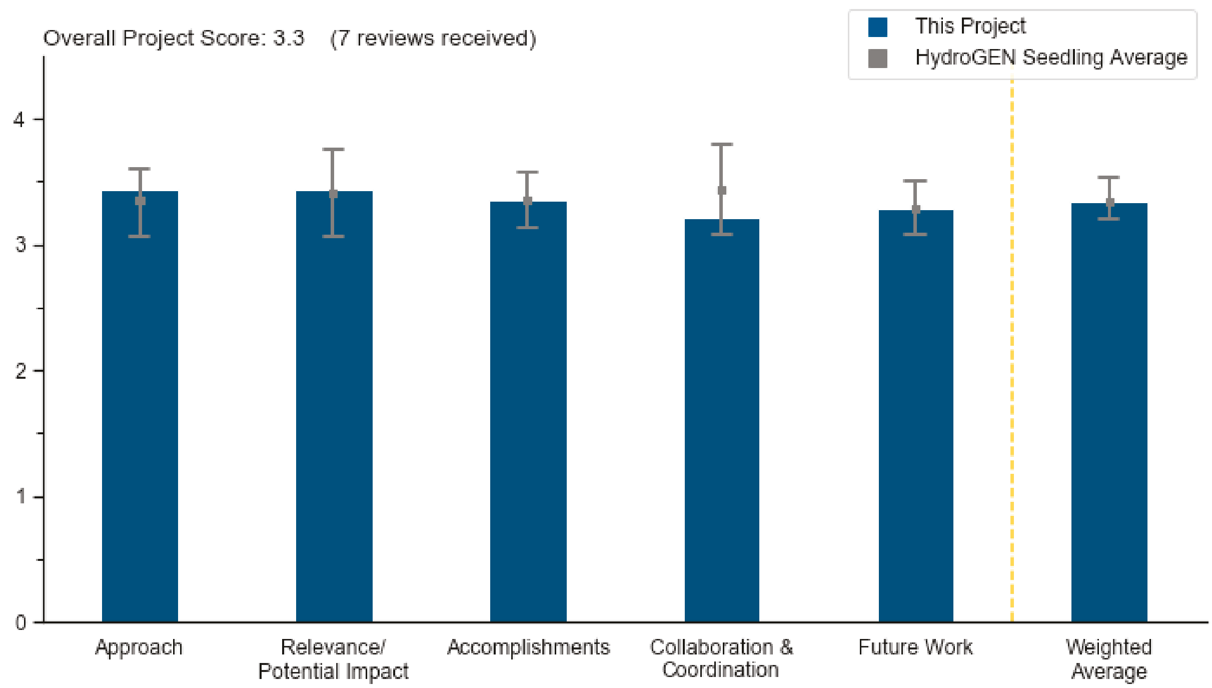
Project #P-176: Development of Durable Materials for Cost-Effective Advanced Water Splitting Utilizing All-Ceramic Solid Oxide Electrolyzer Stack Technology

John Pietras, Saint-Gobain

Brief Summary of Project

This project will develop a high-temperature electrolysis technology that combines a new anode material with a novel all-ceramic stack design. A major innovation and key to the project's effort is the identification and development of nickelate-based materials for the anode in solid oxide electrolysis cells (SOECs). A fundamental understanding of performance degradation and electrode delamination in nickelate-based SOEC materials and interfaces will be developed. Compositions addressing this degradation will be developed to meet specific performance targets: area-specific resistance ≤0.30 ohm-cm^2, current density >1A/cm2 at 1.4 V, stack electrical efficiency >95% lower heating value (LHV) H_2, and stack lifetime ≥7 years. Specific objectives are to optimize the materials and to demonstrate their capability in all-ceramic SOEC cells and stacks by modeling, fabrication, and testing. Results will be validated, and technoeconomic impact will be established.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design, feasibility, and integration with the HydroGEN Consortium network.

- Leveraging a previously developed all-ceramic stack is a viable and cost-effective approach.
- The project follows a solid approach with a promising technology.
- The approaches are appropriate and logical.
- Improving the durability of SOECs is definitely on the critical path to commercial relevance. The team has made a sound hypothesis on how to solve oxygen evolution reaction electrode delamination through chemical composition. There is, however, a lack of modeling to complement (and hopefully expedite) the experimental approach, especially since the compositional space is large. It is recommended that the team engage with other HydroGEN nodes for help.

- The all-ceramic, co-sintered stack approach has been developed by Saint-Gobain over many years, and the issues related to material incompatibilities and sintering shrinkage mismatches have been addressed. There is much value for this stack design if applied to solid oxide electrolysis because pressurization should be easier to achieve. This project aims to use the same concept with a brand new materials set; this seems a bit daunting. For example, co-sintering a ceria-based air electrode with a zirconia-based electrolyte is likely to result in resistive interfaces.
- The approaches are largely effective, but they could be improved; the project contributes to overcoming some barriers. More work needs to be done to demonstrate that layered perovskite is the solution for addressing the delamination issue of oxygen-based electrolyzers. In addition, such materials are very reactive with electrolyte materials, causing potential degradation problems.
- In general, the approaches are excellent. If clearer approaches for achieving target current density were provided, it would be better.

Question 2: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program goals and the HydroGEN Consortium mission.

- Solid oxide electrolysis is a key component of DOE's emerging portfolio of hydrogen production technologies. Saint-Gobain's stack design has some very good attributes for SOEC applications. If this project is successful, Saint-Gobain will be positioned to complete stack and system development and ultimately produce solid oxide electrolyzer systems. Thus, this project has high relevance and a significant potential impact.
- The focus on stability improvement can directly target DOE goals, which will contribute to the commercialization of high-temperature electrolysis (HTE) technology. The work makes a significant contribution to the HydroGEN consortium.
- HTE is a very good platform for DOE to advance through research and development support. This project would benefit from adding a modeling component.
- The project is relevant to high-temperature water electrolysis.
- The relevance and impact of the project are clear.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program (the Program).
- Significant progress has been made, but there are weaknesses that need to be addressed to improve the rate of progress or improve the clarity of the project's objectives and performance indicators. The project contributes to overcoming some barriers.

Question 3: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project started in fiscal year 2019. Good progress has been made to date on milestones.
- The project goals are on track. Evaluating conditions (such as water concentration) should be stated with the various milestones. Hydrogen cost should be calculated for the proposed technology.
- Most project aspects align with the Program and DOE research, development, and demonstration objectives.
- The project has a solid background and a good start, and it should be able to approach the DOE goals.
- Good progress has been made toward cost targets; the approach is unique.
- The project has made progress toward the project goals.
- The work at Boston University is focused on design of rare earth nickelates as air electrodes for SOEC systems. Compatibility issues between the nickelate and doped-ceria phases of composite air electrodes have been identified and are being addressed. However, ultimately, this ceria-containing air electrode will need to be co-sintered with zirconia; this likely will result in a resistive zirconia-doped ceria phase at the electrolyte–electrode interface. There does not appear to have been any work that was performed (or was reported in the presentation) on whether this issue is being encountered or how it will be addressed if or when it is.

Question 4: Collaboration effectiveness

This project was rated **3.2** for its collaboration and coordination with HydroGEN and other research entities.

- Collaboration seems to be proceeding well, with monthly meetings and extensive conversations and discussions.
- The team has a good collaboration history. The current collaborative task arrangement is perfect.
- Collaborations with Idaho National Laboratory and other partners are fairly well coordinated.
- The interactions between collaborators are reasonable.
- The project has been well coordinated.
- It is too early in the project to assess whether there is effective collaboration, but it seems that the only results presented were those obtained by Boston University.
- The project’s engagement with partners and HydroGEN nodes seems light thus far; it is mostly just discussions.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future plans are generally built on past progress and will contribute to overcoming most of the technical barriers.
- The proposed future work is a logical continuation of the presented effort.
- There are no issues with the proposed future work. The team may want to roughly budget more time for short-stack construction for varied compositions. The short-stack construction will likely be difficult, despite the expertise.
- There is a strong experimental plan. The team is encouraged to have discussions with DOE about how to engage HydroGEN modeling capabilities.
- The proposed work can fulfill the project objective. If the work for avoiding the co-firing challenges for the stack were clearer, it would be better.
- The proposed future work is appropriate; more detailed description of the approaches for future work is recommended.
- The reaction between the ceria-containing air electrode with the zirconia electrolyte during co-sintering could be a major death threat to this project. This needs to be assessed and addressed sooner rather than later.

Project strengths:

- The team identified a critical issue with an important hydrogen production technology platform; the researchers developed a hypothesis to address the issue and an experimental plan to test that hypothesis, and they are making good progress on that plan.
- The project develops a complete ceramic system that eliminates many issues on HTE cells while also working on strategies to prevent electrode delamination.
- The project has a clear path to solve the stability issue. The co-firing technique for achieving a stack is promising.
- The all-ceramic stack design has advantages for SOEC applications.
- The project’s main strength is in the approaches to address the identified technical barriers.
- The project has a unique approach and a strong team.
- Some good progress has been made.

Project weaknesses:

- This project has no major weaknesses.
- The initial synthesis and construction of the stack or short stack may take more time than predicted. There are bound to be unforeseen issues with the varied compositions, however small the variation.
- A preliminary cost estimate for hydrogen production using the proposed technology should be calculated earlier in the project.
- There is an absence of modeling to complement the experimental plan. There is relatively minor engagement with HydroGEN capabilities.
- More work needs to be done to demonstrate that layered perovskite is the solution for addressing the delamination issue of oxygen-based electrolyzer. In addition, such materials are very reactive with electrolyte materials, causing potential degradation problems.
- It is highly questionable whether the nickelate or ceria-composite cathode will be compatible with a zirconia-based electrolyte in Saint-Gobain's stack manufacturing process.

Recommendations for additions/deletions to project scope:

- There are no recommendations for additions/deletions to the project scope.
- It is suggested that the team do more durability testing under electrolysis mode. More focus should also be given to the performance demonstrated by the layered oxygen electrode under real operating conditions, on either a symmetrical cell or fuel electrolyzer cell.
- Modeling is suggested to help guide experiments to motivate choices for new electrode compositions.
- The team should evaluate the co-sintering earlier rather than later.

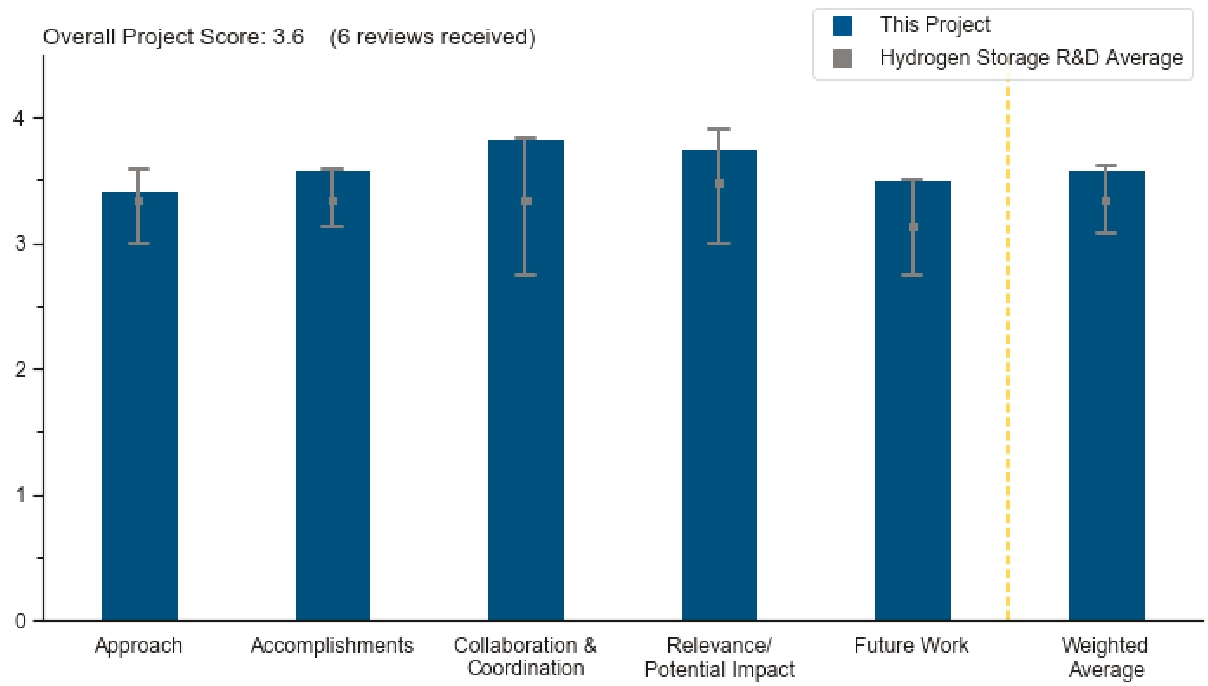
Project #ST-001: System-Level Analysis of Hydrogen Storage Options

Rajesh Ahluwalia, Argonne National Laboratory

Brief Summary of Project

The main objective of this project is to develop and use models to analyze the onboard and off-board performance of physical and materials-based automotive hydrogen storage systems. Specific goals include (1) conducting independent systems analysis for the U.S. Department of Energy (DOE) to gauge the performance of hydrogen storage systems; (2) providing results to materials developers for assessment against system performance targets and goals and for guidance in focusing on areas requiring improvements; (3) providing inputs for independent analysis of onboard system costs; (4) identifying interface issues and opportunities and data needs for technology development; and (5) performing reverse engineering to define material properties needed to meet the system-level targets.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has been ongoing for almost a decade. Its approach is evolving with the needs of the Fuel Cell Technologies Office (FCTO). The project is highly relevant and provides excellent information. Analysis of approaches to hydrogen generation, transport, and storage, both on-site and on-vehicle, is highly informative and fuels discussion.
- This is a comprehensive ongoing project related to onboard and off-board storage of pure hydrogen and liquid hydrogen carriers. The project includes production and conversion of hydrogen (if any). As such, it is an excellent product with a toolset that addresses most hydrogen-related aspects of realistic hydrogen-based energy systems.
- The approach of this project is very strong overall, especially considering the breadth of the project. The project continues to investigate important aspects of hydrogen transport and storage relevant to current

focus areas. There are only a few places where the approach could improve. In the approach for Task 1, 500 tons of geologic hydrogen storage is assumed; however, this storage capacity is available in only a relatively small area of the country. It would be more relevant to include other, more accessible forms of storage in the base case. The approach for Task 3 could be improved by including the packaged volume of the storage cylinders rather than simply including the internal volume.

- The approach is well thought out and relevant to the needs of industry and DOE in understanding the approaches and related cost implications of large-scale hydrogen storage and transportation of hydrogen carriers. It would be beneficial to consider adding an item to the overall cost analysis: the cost of transportation from the cavern storage to the city gate.
- The team involved in this project has a history of adopting excellent analytical approaches with transparent assumptions and logical analyses. The approach toward medium-duty (MD) and heavy-duty (HD) tanks was inappropriate since the internal volumes of compressed natural gas tanks were used to project internal volumes of hydrogen tank capacities, though hydrogen storage tanks would actually be larger in overall size. The MD and HD tanks appeared to be missing the details of the system assumptions, including the additional weight and volume required for the support brackets and container.
- This year, this ongoing project has focused on three aspects of hydrogen storage: bulk hydrogen carriers, geologic storage, and MD and HD storage. The approach is well planned, and the project results are extremely valuable to the hydrogen community. However, with the exception of the MD and HD analysis, it is unclear how the work done contributes to the seven stated critical barriers.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This project continues to make great progress on relevant topics. The comparison of hydrogen carriers is helpful in understanding which materials are suitable and which materials require more scrutiny. With regard to the capital cost of the methanol plants, it would be clearer to include labels on the cost and capacity graph that specify the production method that corresponds to each data point. If the best-case use is autothermal reforming, which is currently not a widespread process, the data could be slightly skewed to favor methanol as a hydrogen carrier. The bulk hydrogen storage study is very well done, and the sensitivity analysis is appreciated. It would be interesting to see how the cryogenic bulk storage system would compare to the analysis presented. The cryo-compressed storage study was similarly well done. It will be interesting to see how the analyses change as data from the Hydrogen Materials Consortium becomes available.
- Methanol is shown to be cost-competitive with compressed gas as a bulk carrier, and salt caverns are shown to be the most economical option for large-scale stationary storage. The project's year-over-year progress is good, and the results are valuable to the hydrogen storage community.
- Accomplishments to date have been detailed and informative. Since the work adjusts to market and industry needs, the progress is quick and accurate. The principal investigator (PI) reaches out to required stakeholders to ensure accurate input into the models.
- The large-scale hydrogen storage and the hydrogen carrier results will be very useful to DOE for planning ongoing programmatic activities. While gaseous hydrogen and methanol appear to be good energy carriers (slide 11), the team should also continue to consider ammonia as an energy carrier. Numerous activities involved in ammonia production may be leveraged to reduce production and overall costs of using an energy carrier. There has been very good progress in bulk hydrogen storage analysis for understanding methodologies and costs.
- The team's accomplishments show great progress toward DOE's goals of understanding large-scale storage costs. It would be beneficial to conduct a comparison of cryo-compression with other storage methods for MD and HD trucks in the future, and it appears that this effort is under way. The advantage of using lower pressure for cryo-compression is the cost reduction that results from using less fiber.
- The inclusion of large production plants for the carriers demonstrates notable progress. The bulk storage analysis is a helpful reference for infrastructure and H2@Scale analysis. The hydrogen storage progress seems to be limited.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- This project demonstrates an outstanding level of coordination with other organizations. Each project topic has received a great deal of outside support and collaboration.
- Collaborations are numerous and effective.
- This is a very well-coordinated project with a good team of collaborators. Yara North America may be helpful as an additional collaborator on ammonia.
- The project makes use of an excellent set of collaborators. The coordination with participating agencies appears adequate for the purpose of conducting analyses. It would be helpful for the project team to list specific industrial contacts, such as truck manufacturers, involved in data collection.
- The project demonstrates a high level of collaboration with national laboratories and Strategic Analysis, Inc. (SA). However, additional industry support would be beneficial, especially for the carrier analysis.
- There is an excellent team in place to support the project. However, the specific ways in which the team supported the project were not always clear. Though the presenters provided acknowledgements at different points during the presentation, the lack of detail in the acknowledgements did not inspire confidence in the results.

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is very relevant to DOE's current focus. The inclusion of MD and HD vehicles to the scope of interest and the prevalence of H2@Scale and its associated projects further enhance the project's relevance.
- This work is highly relevant, which is unsurprising, as the direction of this ongoing work is changing on an annual basis. The project provides an excellent toolkit and great information to assist in informing and guiding decisions.
- The project is extremely relevant to the hydrogen community. It provides important analysis that is otherwise missing from the materials-focused projects.
- The data and modeling tools in this project have evolved to a point where they can provide clear and reliable results for a broad set of topical areas important to industry and to the FCTO.
- The relevance of the project to the DOE Hydrogen and Fuel Cells Program is high; however, the project focus seems to have changed from "Hydrogen Storage Options" to hydrogen delivery and infrastructure options.
- The project elements are very relevant to current needs and to the impact storage costs of large-scale production can have on the price of hydrogen. The project increases understanding of the costs of various large-scale elements such as piping and installation. Perhaps there are other approaches to cavern storage lining or research areas that could help reduce the costs of the different elements that determine the storage volume. It is unclear whether hydrogen losses from permeation are considered as part of the cost of each storage option.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The inclusion of renewable-specific production, storage, and transport scenarios in future plans is good. This project could benefit from exploring Hydrogen Materials—Advanced Research Consortium (HyMARC)-related hydrogen storage materials and anticipated developments. The use of reverse engineering to determine the desirable materials properties that favor hydrogen carriers would be very interesting, and its success may be likely.
- The proposed work is relevant to the needs and continued improvement of the model. The approach continues to expand the reach of hydrogen storage from the caverns to the city gates. Presumably, the

transportation cost from one location to the next will be included. The MD and HD future work is necessary in helping DOE determine a future focus.

- The future work is appropriate to meet the project goals and milestones. In particular, the proposal to determine the desirable materials properties that favor hydrogen carriers will help guide decisions in other projects for years to come.
- The proposed future work follows logical next steps based on the results of the previous work. The choice to take the analysis to the next level and continue to refine the results is effective.
- The proposed future work includes investigation of important details that will help strengthen the project. However, additional areas of work should be considered for future efforts. It is important to investigate competition related to geologic gas storage, since chemical companies are developing storage in similar manners for ethane and other commodity chemicals. As these potentially feasible geologic gas storage formations are limited in number, storing hydrogen underground might be cost-competitive, compared to other substances.
- In general, the future work is good, but potential improvement from the past analysis is likely to be incremental rather than significant. The future work does not seem to include an attempt to identify significant improvements to the key barriers for hydrogen storage.

Project strengths:

- Thanks to its logical approach, effective collaboration, and good DOE guidance, this continues to be one of the best projects in the Hydrogen Storage subprogram category.
- The project manages to focus on the important aspects of each topic and present them succinctly, a difficult feat for a project of such breadth. It is apparent that a great deal of consideration went into each topic.
- The project team and its capabilities are the project's key strengths. The project's breadth of interrelated topical areas allows it to provide valuable information and data for a realistically large-scale hydrogen-based energy system.
- The project strength is the team, which has an excellent history in hydrogen storage systems analysis and development.
- The project team demonstrates great coordination with all national laboratories and other interested parties. The cost analysis and break-even point comparison of technologies are greatly detailed.
- This excellent project addresses the storage, carriers, and alternative storage approaches on MD and HD vehicles.

Project weaknesses:

- Though it is difficult to find any weakness in the project, an investigation of the electrochemical production of ammonia may be beneficial.
- This is a strong project with very few weaknesses. The only glaring omission is the lack of consideration of liquid carriers for the bulk hydrogen carriers section.
- Overall, there are some aspects of the project that lack clarity. It is understood that a great many assumptions are required to perform analyses such as these; however, more detail should be provided to support reviewers' understanding of project decisions. Most of the project is well described, but there are a few areas, such as the methanol plant capacity chart, which could use a few more details.
- The project title, "Hydrogen Storage Options," is misleading, as the effort has been related mainly to hydrogen delivery carriers and infrastructure bulk storage. Also, the project should attempt to include infrastructure companies and other references to validate project results.
- The project team has not clearly communicated information or feedback from its collaborators. It is clear the PI is communicating with industry, but no industry participants other than BMW are listed.

Recommendations for additions/deletions to project scope:

- There should be a systematic exploration of transport and storage performance and cost of hydrogen and hydrogen carriers from renewable sources. This exploration should cover interstate, regional, and local levels of hydrogen production integrated with renewable resources.

  - It would be interesting to compare glass microspheres to CH_3OH, NH_3, and MCH for long-haul hydrogen transport. Glass microspheres flow like liquid and can be reversible and cycle similarly to MCH/toluene. However, these properties depend on material permeability versus temperature and wall thickness. A performance of 10–20 g/l and 10–14 wt.% can be achieved, according to 1995 data.
  - For CH_3OH, NH_3, and MCH, forecasting analysis needs to consider the anticipated demand growth rate coordinated with fuel cell electric vehicle production rate, rate of availability of geologic hydrogen storage facilities, and H2@Scale-based hydrogen demand growth rate. This translates to the large-scale production/conversion facility installation rate.
  - For normalizing cryo-compressed pressure vessels, the term to consider when describing thermal input rate into the cryogas should be watss per kilogram (or maybe watts per 100 kilograms) of hydrogen stored, rather than simply watts (slide 25).
  - The team should consider collaborating with Yara North America on large-scale anhydrous ammonia production, storage, supply, and transport.
  - At this point in the project, it may be useful to consider adding perturbation analysis of hydrogen transport and storage that incorporates realistic failure or disruption scenario effects on specific hydrogen production-to-end-use configurations.
- The hydrogen carriers should be compared to liquid and cryo-compressed hydrogen to complete the baseline. It would be useful to determine whether cost savings from using a previously excavated site (e.g., a depleted salt mine) for geologic storage are possible. The project's work toward critical barriers is very relevant to the hydrogen community. Project barriers should be updated to include additional barriers that match the work being done, as opposed to altering the project to better meet the barriers.
- The project should return to analyzing hydrogen storage options and opportunities, or at least strike a balance between hydrogen storage and delivery concepts. Since SA has, in the past, conducted the cost analysis for Argonne National Laboratory (ANL), the cost analysis could be deleted from the project scope. This could be an opportunity for ANL to focus on the technical analysis and have SA conduct the cost analysis for carriers and other infrastructure concepts.
- It would be interesting to see how bulk underground hydrogen storage compares economically with other chemicals. Considering the limited number of sites appropriate for bulk storage, it would be interesting to determine whether development for hydrogen storage is economically favorable or whether industry would use these sites for other purposes.
- It would be useful to compare conformable hydrogen storage technology using a volumetric storage density metric. Conformable hydrogen storage is improving and, if permeation issues are resolved, it offers a huge on-vehicle storage advantage volumetrically.
- The project team should include cryo-compressed storage on MD and HD vehicles in cost analyses.

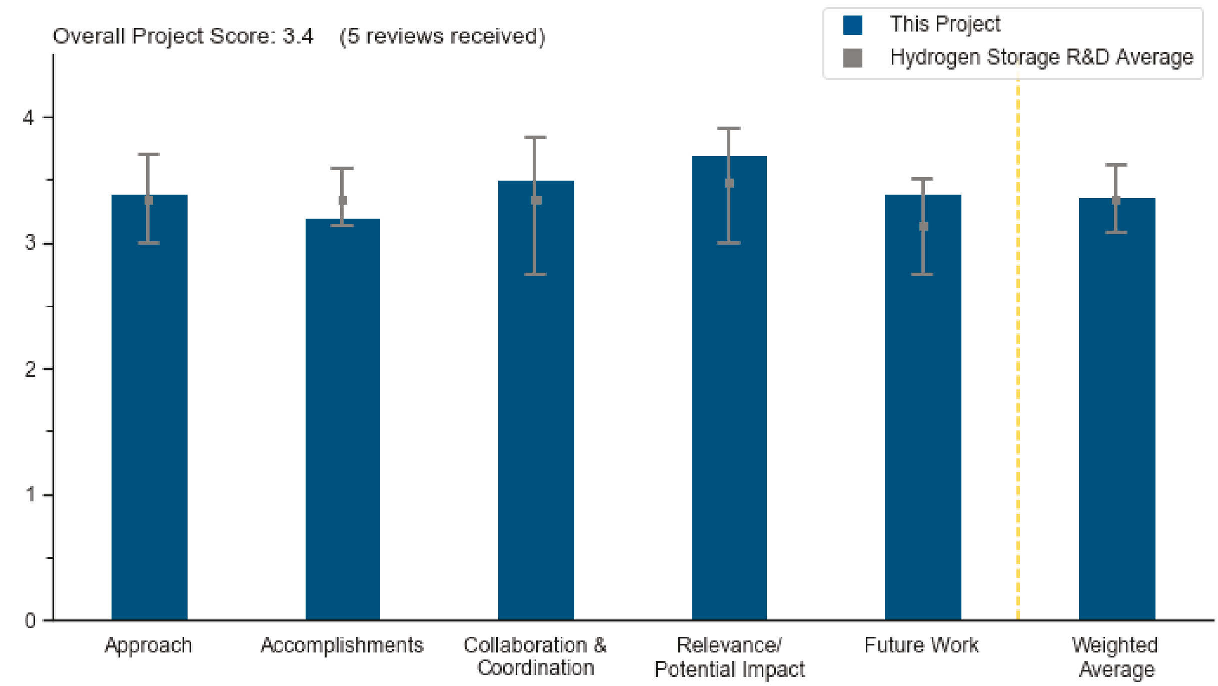
Project #ST-100: Hydrogen Storage Cost Analysis

Brian James, Strategic Analysis, Inc.

Brief Summary of Project

The goals of this project are (1) to conduct independent Design for Manufacture and Assembly (DFMA) cost analysis for multiple onboard hydrogen storage systems and (2) to assess/evaluate cost-reduction strategies to meet the U.S. Department of Energy (DOE) cost targets for onboard hydrogen storage for different types of fuel cell electric vehicles (FCEVs).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project focuses on the cost of hydrogen storage systems, an essential component of fuel cell adoption. This project complements other projects well. This year, the focus has shifted to medium-duty vehicle (MDV) and heavy-duty vehicle (HDV) applications, which matches auto industry trends. Previously calculated values have been updated to reflect changes in carbon fiber price and inflation.
- The approach is sound and addresses project barriers. Updating information and pricing based on new data is essential to staying relevant. Pricing baseline updates prevent the presentation of misleading or outdated information. Comparison of light-duty vehicles (LDVs) with MDVs and HDVs is useful in understanding what learnings can be leveraged and what cost increases can be expected.
- The team involved in this project has a history of adopting an excellent DFMA-based approach with transparent assumptions for economic analysis of hydrogen storage systems. This past year, the approach provided incremental refinements to past analysis and focused only on compressed hydrogen. The approach would benefit from the inclusion of a cost analysis of other projects within the DOE portfolio.
- The approach employs analysis of onboard storage packaging and economy-of-scale pricing for MDV and HDV hydrogen storage. The model updates, which correct for inflation between 2007 and 2016, are

important, although a little late. The general approach enables a clear understanding of storage system cost predictions and shows challenges and alternatives for onboard storage on HDVs.

- The approach is relevant to current areas of investigation and includes the use of a strong industry-developed tool in DFMA.
- This cost analysis could be used to provide recommendations for future research topics and/or targets.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The analysis of MDV and HDV sales trends is excellent. The team has made good progress on its LDV hydrogen storage tank comparison. The team provides a detailed analysis of carbon fiber pricing with updated pricing data. The demonstration of the impact updating 2007 costs to 2016 costs is excellent.
- The project has done an excellent job painting a clear picture for HDV storage configuration options. The project also explains the impacts of component choices and economies of scale on hydrogen storage designs. The suggestion (in slide 9) that the models may overestimate costs also suggests that the project team should revisit the models and seek more input from industry.
- This year's incremental progress includes updates to the carbon fiber price and low-volume LDV hydrogen tank system. These updates are useful and important to establishing a new DOE record for an industry reference. Unfortunately, the cost opportunity updates make only a minor change in the 2015 record after the addition of the inflation adjustment. The medium-/heavy-duty (MD/HD) hydrogen storage system background was provided, but the cost information was not provided.
- Good progress has been made on overcoming identified barriers. The cost model and associated adjustment of the dollar basis appear to be well done. Based on the market scoping, MD and HD FCEVs are a potentially strong market for the creation of American manufacturing jobs. The packaging options could have been a little clearer; the chart provided is very difficult to understand without labels. The reason for lumping cab and roof-mounted options together under MDV is unclear. The team should justify this choice and determine whether the aspect ratio differences justify the assumption that they will be the same mass.
- Initial scoping of MD and HD applications and an updated carbon fiber cost in relation to LDVs are presented. The accomplishments appear to be relatively low, compared to previous years.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The team engages in excellent collaborations with national laboratories and industry. Furthermore, the team leverages two industry experts for additional credibility.
- The project appears to have an appropriate level of collaboration with national laboratories and industry. It is excellent that the project team connects with carbon fiber and component suppliers to ensure the cost estimates align with current material and component costs. Since the tank is the dominant cost for the hydrogen storage system, additional communication with tank suppliers may be useful for validation of estimates.
- The project coordination appears fairly strong. The project draws on a good mix of industry groups and national laboratories. It would be interesting to see how the data would differ if actual material suppliers, not system manufacturers, were consulted in carbon fiber pricing.
- Collaborations appear to be appropriate and well utilized. For this type of analysis, a more formal collaboration with original equipment manufacturers (OEMs) may be appropriate.
- The project's collaboration team is well equipped and well-coordinated to provide the very useful results in this presentation and to extend the analysis and its applications. However, the project does not seem to collaborate with FCEV OEMs of LDVs, MDVs, and HDVs who can likely provide valuable insight on costs and design options for hydrogen storage systems.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is highly relevant and provides critical information for the Hydrogen and Fuel Cell Program in the form of a cost assessment that ultimately feeds into DOE strategies for the commercialization and future success of FCEVs. The project sets itself apart from other DOE projects by providing a cost analysis and assisting other projects in the portfolio with cost projections.
- This work is very relevant and high-impact, as the price of carbon fiber is the main cost driver of hydrogen storage systems. The detailed and thorough analysis presented in this project allows for a strong understanding of this key market's needs for development.
- The project provides excellent go-to information necessary for making critical choices in MDV and HDV hydrogen storage system design. The project also provides sensitivity analysis for all FCEV storage systems. This analysis assists DOE target initialization and evolution.
- Without accurate and relevant cost information and predictions, it would be extremely difficult to understand where the market needs to focus to move fuel cells and hydrogen into the competitive market space. This is highly relevant and has a big impact for researchers and potential users.
- The project aligns with the DOE hydrogen goals. Furthermore, this project is unique in the sense that it takes a very in-depth look at hydrogen storage costs. The impact of the results will most likely be limited to other DOE projects and not the industry as a whole, as OEMs tend to conduct cost analyses independently. In other words, the project may have an impact on policy but not on commercialization. However, the project methodology may be adopted by some OEMs.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work is very strong. The levelized cost of multiple storage methods provides a great tool for comparison. The analysis is a great tool for guiding the development of the forthcoming targets for MDVs and HDVs. The application of the analysis to H2@Scale will be immensely useful.
- The models are now able to investigate levelized costs in cents per mile on all storage tank designs, an improvement that will be very valuable to the Fuel Cell Technologies Office (FCTO) and industry. Hopefully, the inclusion of cryo-compressed hydrogen (CcH_2) storage in that process implies that the team will overcome the industry shortcoming of sparse data on the component costs for CcH_2 vessels.
- Informing DOE truck targets and levelizing costs are excellent next steps.
- The proposed work is a logical next step, based on the results presented, and may contribute to overcoming some of the project barriers.
- The future work outlined for this project seems appropriate. However, the scope of future work should include development of novel concepts or the analysis of related concepts in the DOE portfolio to reduce the cost of hydrogen storage systems. The reverse cost estimation could be very useful in the development of material storage or carbon fiber targets.

Project strengths:

- The project's core strength is its team, which has an excellent history in analyzing and developing hydrogen storage system cost estimates. The connection with key researchers and other technology teams (e.g., fuel cell cost analysis) to provide a comprehensive analysis is another project strength. The project team has the cost estimation skills and technical capability to evaluate novel hydrogen storage concepts.
- The project has built up extensive modeling capabilities and an excellent team over the years. As a result, the team can quickly and effectively help FCTO and industry understand cost impacts and configuration options for hydrogen storage systems.
- The project demonstrates detailed analysis and thorough data reporting. The project team successfully coordinates with industry connections.

- The project has a strong methodology that provides a very close estimate of actual prices. The inflation adjustment was well done and will hopefully continue to provide valuable results as the project continues.
- Strategic Analysis, Inc., has much experience with cost modeling hydrogen storage systems, and the list of collaborators is strong.

Project weaknesses:

- The weakness for the project was the incremental progress for this year. The tools and skill set of this project team should be stretched to consider additional opportunities for cost reductions and/or assessments of commercialization potential for other projects in the DOE portfolio.
- As with any cost project, the estimates are only as good as the assumptions. The cost projections for LDVs (slide 15) may be too low because, presumably, only a one-tank system is considered. In the market today, there are no one-tank systems for LDVs.
- The project lacks collaboration with FCEV OEMs. Aside from limitations resulting from lack of available data, it is unclear why CcH_2 storage was not considered in the packaging and mounting design options for HDV applications, given the known smaller dimensions that affect the volumetric requirement. Since carbon fiber is the dominant cost factor, it would be worth knowing the CcH_2 total baseline cost for carbon and its incremental reduction.
- The project could provide more clarity overall. Some of the charts are unclear, and descriptions of the work should be more detailed. The model should focus on smaller-scale production, as that is the more near-term case.

Recommendations for additions/deletions to project scope:

- The project team should develop a list of opportunities for DOE and researchers to consider for further reduction in hydrogen tank system costs. The project team could also determine the material cost target by conducting a reverse cost estimation of various material-based systems. In addition, the project team should consider determining the potential cost savings for other project efforts in the DOE portfolio.
- Two- and three-tank systems should be considered for the 700 bar Type IV systems, taking into account the stored hydrogen and balance-of-plant (BOP) configurations of the three commercial LDVs today (Toyota, Honda, and Hyundai). A one-tank system does not seem practical, considering LDV packaging restrictions. Therefore, the cost estimates may be too optimistic.
- The project should increase collaboration with FCEV OEMs to incorporate the industry perspective on storage system component choices, costs, and general packaging strategies. At this point, metrics such as dollars per kilowatt-hour, kilowatt-hours per liter, and kilowatt-hours per kilogram are not universally useful. These metrics are not very helpful in comparing FCEVs to battery electric vehicles since the BOPs are very different and the actual values for such metrics depend on the fuel cell efficiency in the system. The familiar, and more useful, units of measure should be dollars per kilogram, kilograms of hydrogen per liter, and kilograms of hydrogen per kg system.
- The project should include BOP data, though it appears to be on its way soon.
- No modifications to the project scope are recommended.

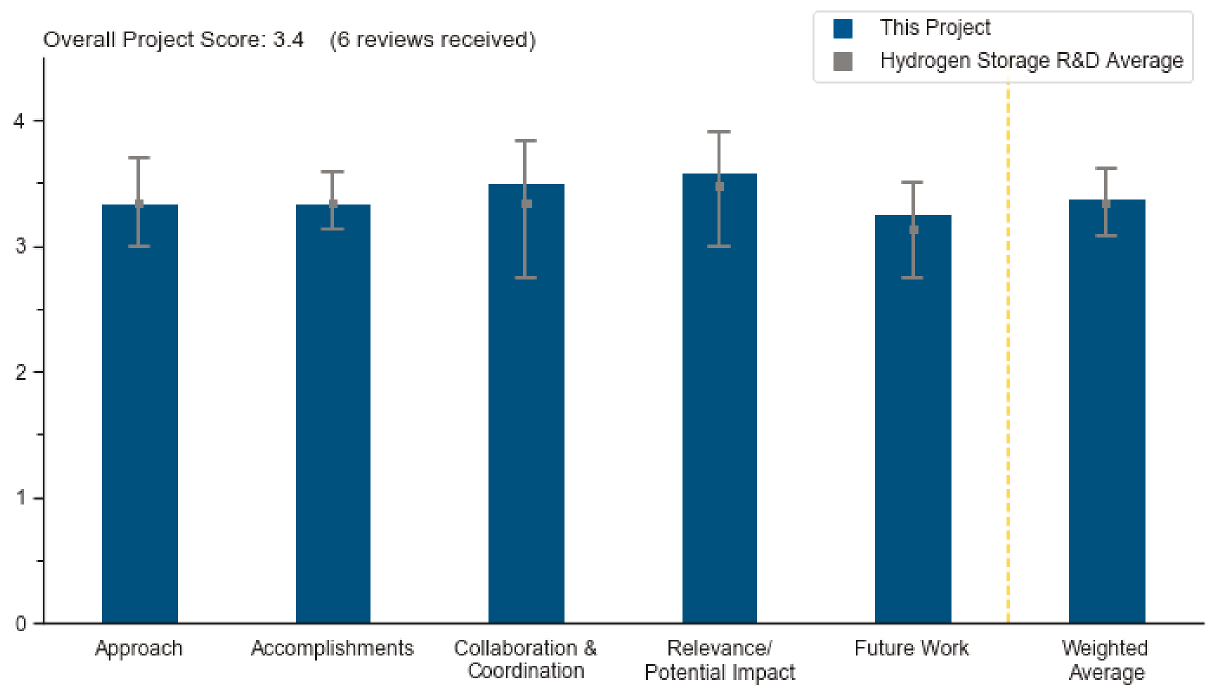
Project #ST-127: Hydrogen Materials–Advanced Research Consortium (HyMARC): A Consortium for Advancing Hydrogen Storage Materials

Mark Allendorf, Sandia National Laboratories, and Tom Gennett, National Renewable Energy Laboratory

Brief Summary of Project

Critical scientific roadblocks must be overcome to accelerate materials discovery for vehicular hydrogen storage. The project objective is to accelerate discovery of breakthrough storage materials by providing capabilities and foundational understanding. Capabilities will include computational models and databases, new characterization tools and methods, and customizable synthetic platforms. Foundational understanding is needed for phenomena governing the thermodynamics and kinetics-limiting development of solid-state hydrogen storage materials.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is comprehensive, broadly based, and multi-faceted. It comprises an impressive array of material synthesis, advanced diagnostics and characterization, multiscale theory and modeling, and innovative processing methods to address critical issue barriers that affect our fundamental understanding of hydrogen sorption processes and reactions in hydrogen storage materials. The approach adopted in the Phase II efforts builds directly upon the foundation established in Phase I, and it is well focused on the critical issues that limit the performance in candidate storage media. The consolidation of the HyMARC and Hydrogen Characterization and Optimization Research Efforts (HySCORE) consortia has facilitated the development of a more coherent and rational approach that avoids unnecessary duplication and overlap. The consortium is also provided with excellent technical collaboration and support for related "seedling" projects, thereby augmenting and extending the ability of those projects to achieve their technical goals.

The scope of the overall approach has been extended even further in this reporting period by the incorporation of a new technical effort on hydrogen carrier materials.

- Using a multipronged attack is meritorious, and lines of research and engineering are addressed at barriers; though many or most projects are at the front end of the development process, so it may not be clear to outsiders where the connection is to those barriers, but the connection is there. The adsorbents, absorbents, and hydrides are more or less the mainstream and of course must be included. Carriers are a nice addition to the approach both for their potential use in vehicles and, more likely, for moving hydrogen (for example, as highlighted in the plenary talks). The overall project portfolio is well designed, as can be seen by the many barriers addressed and the quality of the individual projects for attacking those barriers. Most of the projects are feasible; a few are high-risk but also high-reward, and a portion of that kind of work is good management.
- The Annual Merit Review (AMR) project presentation clearly aligned the focus area objectives with the U.S. Department of Energy (DOE) hydrogen storage system targets. The matrix of focus area tasks versus DOE targets was very effective in communicating the approach and responsible teams. A suggestion would be for the project team to attempt to quantify the system-level improvements if the focus areas are successful. This sensitivity assessment could help in prioritizing the many identified focus areas. For example, in the past, Jeff Long provided estimates of possible storage density improvement with several hydrogen molecules binding to a single open metal site. The Phase II approach and structure appear to be better than those of Phase I since the tasks are aligned to specific material storage technologies with supporting focus areas.
- The Phase II extension has brought storage on board for four additional years. HyMARC is covering the vast space in modeling and characterization at multi-length scales. High-risk–high-reward opportunities are core parts of the task. It was nice to see that tasks were added for seedling support and for the Data Hub. Separating advanced characterization into a new task is also a very good strategy. Having focus areas for the sorbent and metal hydride materials makes a lot of sense and is a wonderful management tool. The focus areas are mapped onto DOE targets and also mapped with the multi-laboratory teams focused on the topic. This should continue for the new and/or future focus areas. Face-to-face meetings twice per year with some focus on the seedlings is a great plan for keeping tasks organized. The structure of focus areas specifically for advanced characterization (and perhaps for computational materials) should be made clearer. On the one hand, these serve to develop new tools and computational approaches. On the other hand, these are tools expected to undergo utilization by other (e.g., sorbent and metal hydride) focus areas. It would be wonderful to separate the topics and tasks related to tool development from those related to tool utilization by other (e.g., sorbent and metal hydride) focus areas. This would provide a clearer, better-defined understanding of the importance and role for each of these.
- The high-level overview approach that was presented is along the same vector as last year and builds on the Phase I work. A new addition is the hydrogen carrier work related to the H2@Scale activity. The individual projects under HyMARC that are working on the new hydrogen carrier work are at present focused on new concepts and materials for bulk storage and transport. The high-level overview of the HyMARC approach to the carrier work includes developing metrics and targets via a technoeconomic analysis. A recommendation would be that, before the individual projects go down the research and development (R&D) path too far on developing new concepts and materials, HyMARC leadership should move quickly and with urgency to develop the technoeconomic analysis model(s), such that HyMARC leadership can ensure that the ongoing R&D efforts have the greatest potential for success and the current R&D efforts are not spent on concepts that cannot meet the metrics.
- The new approach in dividing tasks between 1 and 6 is rational. Because Phase II has a shorter duration of operation, it is unclear if the approach will produce the desired results. It is a good start for Phase II.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Solid progress was made in all core R&D areas. An impressive publication record based on Phase I work is evident. Especially impactful results were obtained in Phase I on the importance of the following elements:

  - Hydride surface chemistry on sorption reactions; joint theory and experimental work on hydrogenation and dehydrogenation reactions in $Mg(BH_4)$ and Li_3N, including $Mg(BH_4)_2$ phase diagram determination and reduction of activation energy by nanoscaling and additive incorporation
  - The application of sophisticated in situ or in operando diagnostic tools to explore material and surface properties at relevant pressure and temperature regimes.

  Likewise, important foundational work was conducted on improving binding energy and storage capacities in metal–organic frameworks (MOFs). The technical effort on hydrogen carriers is just under way. A well-formulated plan has been developed to employ HyMARC expertise to make progress in this important technical area. A general comment is that a more keenly focused effort on the critical problem of slow hydrogen sorption kinetics in metal hydrides is needed. This will require the formulation of a more coherent and coordinated strategy.
- The project has clear goals and is making progress toward them. The project's previous work has been extensive and has made a number of advances in understanding fundamentals, developing new, important techniques, and building up and using the theoretical underpinnings. The proof of two hydrogen per center is a big step forward (though there is still much to do to make it commercially viable). This is likewise for the development of a 21 kJ MOF. The reduction of the $Mg(BH4)_2$ desorption temperature is also a move forward. The advances in measurement via high-temperature and high-pressure pressure–composition isotherm (PCT) and high-pressure and high-temperature thermal property measurement are both excellent for understanding the scientific and engineering applications of the materials being developed. The project team is meeting milestones. It would have been preferable to see more actual numeric progress against goals for this big a project (in reference to Phase I), but these things take time.
- The AMR project presentation provided an excellent summary of the Phase I accomplishments that "moved the bar" toward DOE targets. The HyMARC team also had an impressive number of publications and patents. The progress seemed to be appropriate for the Phase I effort. The items that "moved the bar" were clear, but the quantification of how much the storage system bar moved was uncertain. The HyMARC team should attempt to evaluate progress based on system-level improvements or potential enhancement to the system, since a certain material-level enhancement may not have a significant impact on the system.
- Much of the discussion on accomplishments was directed toward what HyMARC accomplished in Phase I, and most of that was covered in the 2018 AMR presentation. There was little discernable high-level discussion of what HyMARC has accomplished since entering Phase II. From the individual project presentations, plenty of progress has been made in Phase II; it would be useful to have seen a cogent summary of highlights of collective progress, as has been done in the past, and less of a discussion of Phase I progress. To assess progress of HyMARC's foundational research aimed at filling in the "knowledge gaps" to enable R&D to accelerate the discovery of new materials or modifications of existing ones, it would be useful to have a clear and measurable graphical summary slide that addresses how HyMARC work is "moving the needle." For example, in the work on understanding how to address the kinetics barriers of hydrogen release or reuptake, it would be very helpful to present a plot of how HyMARC's various approaches (nanoscaling, nanoconfinement, etc.) have resulted in rate enhancements. It should not be difficult to extract maximum and average rates of hydrogen release from the instances in which HyMARC research has shown gains, and compare these improvements in kinetics against the onboard hydrogen-release-rate target. John Vajo has done some of this tabulation for the systems that interest him, and it is very useful and illuminating as a measure of how effective the "electrolyte" approach can be, relative to the target. This should be done for other areas as well, such as HyMARC's approach to understanding how to alter thermodynamics of release or rehydrogenation, and how the resulting work has enhanced the thermodynamics with respect to the idealized thermodynamics "window" for onboard storage and regeneration. These sorts of summaries would help greatly in the translation of HyMARC's foundational research approach into demonstrable progress. HyMARC has done a nice job of working with the seedlings to help them gain access to various HyMARC capabilities, accelerating their progress. Clearly HyMARC leadership has developed this culture of assistance among the individual HyMARC projects, and it is applauded.
- The group is making progress and has many publications to show for it. In the reviewer-only slides, it would have been nice to see a list of publications.
- The project has not had enough time to produce significant progress. The tasks and plans are in place. The leads are engaged with the team members.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- Extensive collaborations are vital elements of the consortium. The reviewer strongly supports the consolidation of the HyMARC and HySCORE activities. The effective management of such a large and multifaceted effort can be challenging, especially with regard to avoiding unnecessary duplication and overlap of technical activities. Although that clearly remains an issue, the principal investigators (PIs) are making good progress to ensure that focus areas are clearly established, well-developed lines of communication among the different groups are in place, and technical synergies are exploited. A serious challenge will be the acknowledgement of when projects and tasks should be brought to an end, allowing resources to be focused on more fruitful pathways. Excellent support of seedling activities is evident; collaborations with the HyMARC core team have effectively reinforced the seedling efforts.
- The extent of collaborations and coordination continues at the high level set during prior years. Internal collaborations and coordination among the HyMARC partners appear to remain strong, and collaborations with the DOE Office of Basic Energy Sciences facilities at Lawrence Berkeley National Laboratory's Advanced Light Source facility appear to be working reasonably well. Collaborations with the seedlings appear to be solid, as judged by the seedling presentations and the individual HyMARC partner presentations. Overall, the level of collaboration is commensurate with the scale and scope of the individual projects and is commendable. With the new activity in hydrogen carriers, HyMARC leadership needs to get out in front of the R&D activities with a well-developed set of metrics to coordinate these efforts to provide the largest impact.
- The project is pretty much an inherently high-collaboration program, but it also pulls in many outside groups. The use of seedlings and the support they get speaks to the coordination. The team seems to have a good approach for coordinating work, as well as spreading advancements and understanding through the many groups in the team.
- The project has a significant level of collaboration among the national laboratories. The presentation slides showed well-coordinated roles and responsibilities for the various national laboratory teams. A possible improvement to the collaboration is the consideration of industry or other resources to ensure the approaches being recommended have the potential for commercialization in the future.
- The HyMARC program integrates multiple institutions. The support for four seedlings is also a good addition to the portfolio.
- The Phase II seedlings include the University of Michigan, Liox Power, Inc., and the University of Hawaii. It seems like collaborative partners are chosen based on their past familiarity with the PIs. The project team has missed opportunities in the form of a more level playing field, the inclusion of a broader community and underrepresented groups, an open approach to seeking seedlings, and decision-making based on the potential for increasing the broader impact of HyMARC and establishing future U.S. leadership. This can be improved.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- HyMARC remains the centerpiece of DOE's hydrogen storage program and is expanding its work into hydrogen carriers in support of the H2@Scale initiative. Despite years of excellent work across decades of R&D worldwide, including significant DOE-funded efforts in the United States, no single material has yet to be able to fulfill the stringent requirements for onboard vehicular storage. HyMARC's approach to this problem is to take a step back and fill in the knowledge gaps that address critical barriers to success. Among those the consortium is addressing are understanding how solid-state complex metal hydrides develop into complicated multiphasic materials as hydrogen release proceeds. Gaining an understanding as to how the various interphases affect mass transport, the diffusion of reacting species, etc., and how these features influence reaction pathways and kinetics is critical to being able to ascertain whether there are routes to modification of materials or entirely new materials that can overcome these key barriers that have confounded prior hydrogen storage researchers. It is a hard—very hard—problem HyMARC is addressing, and the team is making progress. HyMARC has brought most of the right tools and capabilities, human and otherwise, to bear on the problem. The approach is potent: integration of experiments with computational modeling, coupled with state-of-the-art characterization capabilities, while maintaining a focus on the key barriers. This approach provides great potential to make a significant impact on the search for solutions to this vexing materials problem that has such a significant potential upside for cost-effective onboard storage.

- The HyMARC consortium is the centerpiece of the DOE Office of Energy Efficiency and Renewable Energy hydrogen storage activity, and as such, it is a critical element of the DOE Hydrogen and Fuel Cells Program (the Program). DOE's decision to create this consortium is sensible and commendable. Moreover, the consolidation of the HyMARC and HySCORE activities has resulted in reduced confusion, duplication, and complexity. The consortium is providing a foundation for understanding the complex processes operative during hydrogen sorption reactions in solid-state and liquid media. That understanding is crucial to guiding the development of improved materials that can meet DOE storage targets. The consortium provides a much-needed framework for making rational decisions concerning new materials development.
- The project has relevance for the Program in the area of materials-based hydrogen storage, although the impact is difficult to quantify since the ultimate influence on system-level attributes is uncertain. The project should consider using this highly capable team to evaluate the storage system benefits if this research is successful.
- A major, coordinated effort is the only way that a solution other than compressed gas is likely to be found. The addition of "seedling" studies and higher-risk, low-investment options is a good adjunct to the main-line, longer-term approaches. The emphasis on fundamental understanding is key, as the past decade has probably exhausted the options based on current understanding. Using theory to help guide experiments and using experiments to ground theory is obviously an excellent approach.
- The project supports the broad task related to sorbent and hydride materials. The most relevant problems have been identified. Without an effort as large and coordinated as the HyMARC program, progress on these topics would be substantially slower.
- Phase II is new, and the available data is not ready for answering this question or providing suggestions for improvements.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future work includes the development of a data hub, machine learning, and the expansion of hydrogen carriers as a focus area. These are all very good directions for the portfolio to move. The team should continue to develop areas with DOE targets in mind and also provide a clear picture of which groups will work on each task under these new areas.
- The future work on hydrides and sorbents builds directly upon the work conducted in Phase I. Plans are also in place for exploring new and novel hydrogen carrier approaches. With the introduction of new reaction chambers, the impact of the in situ and in operando diagnostics could be significant. Continued efforts are proposed to create a robust and streamlined management structure capable of effectively coordinating the large number of consortium activities. This will be essential to ensure that the R&D priorities are established and implemented in the most objective and rational way. There is a need for a well-formulated strategy keenly focused on significantly improving hydrogen sorption rates in complex metal hydrides.
- The future work for this project associated with Phase II has the right direction for improving the understanding of materials-based hydrogen storage. The concerns for future work are that the list of focus areas is extensive and the prioritization of these tasks is not understood.
- Each area and management has an appropriate set of goals for the year.
- The proposed future work description was adequate but somewhat uninspiring, given the urgency to fill the knowledge gaps. As this is an overview presentation, a roll-up of the highlights of the individual HyMARC project plans would have helped to place the ensuing individual presentations in context of the bigger picture. The future plan includes an evaluation of progress toward the "applied" focus areas, presuming that to mean quantifying the HyMARC-derived improvements in thermodynamics, kinetics, etc. This is a topic that should be addressed and updated in each AMR. Otherwise, it is difficult for the community to gauge

the progress being made in a quantitative manner. The future work in the hydrogen carriers area is to determine the state of the art. Ideally, this would have occurred prior to starting the experimental work that is already ongoing. Factoring in the much-needed technoeconomic analysis of carriers, along with an analysis of the state of the art, will provide a firm foundation for the selection of promising approaches.

Project strengths:

- This is a comprehensive and well-organized technical effort designed to provide DOE with foundational understanding concerning the kinetics and thermodynamics of hydrogen sorption reactions in existing and emerging hydrogen storage materials. The consortium team has expertise in all areas relevant to achieving R&D objectives, including multiscale theory and modeling, novel synthetic methods, and sophisticated material diagnostics. The consolidation of the HyMARC and HySCORE efforts has broadened the scope of the effort and has provided a more streamlined and manageable way to address R&D imperatives with limited overlap and duplication. The addition of the new hydrogen carrier effort addresses an important DOE need and will undoubtedly emerge as a critical element of the overall technical effort.
- The team that has been put together in general has a strength of capabilities and experience. They have developed or are developing access to new and state-of-the-art characterization tools and techniques, including in situ techniques, either through collaborations with appropriate DOE user facilities or through acquisition. A challenge for managing such a consortium is to keep a tight focus on the project's key problems, with a willingness to make changes as required. HyMARC leadership is doing an admirable job of this.
- The project's overall strength is the team's recognition of strengths and weaknesses revealed by the Phase I effort. Repeating such a path will not deliver results. The new definition of tasks is a good starting point to focus on areas of success and try to develop momentum for year 2. At this point, the team is making an effort by thinking through the issues and changing some of the previous issues with coordination that led to inefficiencies that are now getting addressed. It is a promising start by a very accomplished team.
- The strength of this project is the highly capable national laboratory researchers who have extensive history in developing and analyzing hydrogen storage materials. The project team appears to have made notable progress with Phase I and has constructed a good structure and focus for Phase II.
- The strength of the project is in the skill set assembled by the team members. The ability to pursue sorbents, hydrides, and hydrogen carriers with the most advanced computational and experimental tools is impressive.
- The project's strengths include its scale, facilities, people, and seedlings in addition to the main-line program. There are multiple ways to "win," such as in vehicles, transportation, stationary applications, etc.

Project weaknesses:

- The team leaders had to develop organizational structures and organizational tools to make effective progress out of the multidimensional task list. The leaders are well under way to doing this. Several suggestions have been made on the computational and advanced characterization focus areas (namely, that tasks related to tool development be separately and explicitly considered relative to tasks related to tool utilization). These, along with other fine tunings to the overall organization and management structure, will help. However, by and large, the vision and leadership shows through the structures developed as of now.
- There are two weaknesses that are more about the caution needed to manage the current effort to deliver the impact for DOE's investment in this team.
    - The first project weakness is in some of the assumptions about the future of hydrogen storage and the lack of connection to the marketplace. It seems highly internally focused and not connected to the marketplace where any commercial success in this domain will require a good deal of help from HyMARC. One example of internal focus is a turn toward effort in H2@Scale. An effort on sorbents is definitely important, but it is also reflective of the shifts in the Fuel Cells Technologies Office. Since separate funding opportunity announcements on H2@Scale and proposals will be getting reviewed, this can be viewed as an effort by the team to divert resources away from some of the strength of HyMARC in Phase I and anticipate potential areas where funded research can grow. It is understood that this is a strategic decision that will help the team. It is sincerely hoped that they will use the resources to help the community. Also, in coming years, the project needs to

be justified by demonstrating strong connections to the new efforts starting because of H2@Scale activities and their ability to leverage HyMARC to show a return on investment.
    - The project's second weakness has to do with the lack of spread of leadership to a broader number of people. The verticals are well defined, but the team had the chance to engage new task leads in Phase II and share the load of managing multidisciplinary teams while supporting a more inclusive organization structure for HyMARC. There is tremendous talent in the team, and spreading the load by adding co-leads to the team with different backgrounds, perspectives, and institutional affiliations for different tasks will be highly desirable. This will increase ownership for success to a broader group and train new leaders for the future endeavors. Another approach might be to define leads for cross-cuts. In some sense, theory and computation, data hub (as seen in task six), and characterization are actually cross-cuts and touch all other tasks. Under the current structure, it is hard to find the second and third level of leads for managing the connections between teams with the same degree of quality assurance and coordination. The PIs are encouraged to think more about potential ways of strengthening the matrix in which the current tasks exist and reflect on improving the flow of information, quality, knowledge management, and tracking of progress to build a "dynamic and agile" team, as proposed by the PIs.
- Sluggish sorption kinetics remains the dominant problem in the hydride systems. A stronger emphasis on this important issue is needed. A well-formulated strategy or pathway should be developed to address this important problem. It is hoped that by the 2020 AMR, a definitive statement concerning the principal "bottleneck" that limits sorption kinetics in borohydrides can be articulated. Actual data are needed; it is not sufficient simply to state (as seen on slides 23 and 24) that "[systems with] … reasonable kinetics" will be demonstrated. It is readily apparent that improved access to nuclear magnetic resonance (NMR) capabilities is needed. The importance of NMR as a diagnostic tool for this research cannot be overstated. Although impressive NMR capabilities exist at participating HyMARC organizations, the access to those capabilities seems to be limited. If those restrictions cannot be removed or reduced, then other sources for NMR work should be explored. The use of nanostructures and nanoscale engineering for enhancing hydrogen sorption reactions are important R&D topics in HyMARC and are being addressed by numerous organizations in the consortium. These organizations include, for example, Sandia National Laboratories (borohydride activation reduction, nanointerface engineering, nanoscale defects in sorbents); National Renewable Energy Laboratory (atomic layer deposition on nanoparticles, nanoscaling to improve magnesium hydride thermodynamics and kinetics, plasmonic nanostructures); Lawrence Berkeley National Laboratory (nanocomposites, nanoencapsulation, functionalized nanoribbons); and Lawrence Livermore National Laboratory (theory and multiphase modeling). It is not evident that these numerous yet related activities are being coordinated and managed in a way that ensures proper collaboration and unwanted duplication.
- After several years of pursuing development of the foundational research concepts to address the key knowledge gaps that are barriers to practical materials development for the applications at hand, the HyMARC management should be able to better communicate, in a quantitative way, the extent to which this general approach is having an impact. A potential weakness lies in the H2@Scale hydrogen carrier work that is moving forward without the benefit of metrics to provide rationale for system selection. A potential weakness is in the hydrogen carrier work and prompts a question for the HyMARC leadership team of whether HyMARC has the right set of capabilities and staff with catalysis and/or electrochemical expertise to effectively drive such a program forward with all the organizations involved.
- The project's weakness is that, although the fundamental research is interesting, there is no evidence that the Phase I results have produced any improvements in the storage system attributes. Another weakness is that the project does not include any prioritization of focus areas, and the research seems to be driven more by the preference of the researchers than the impact of improving hydrogen storage system attributes.
- While not a manifest weakness now, there is the potential for the current coordination to fray if it is not actively managed. Also, while the focus on fundamentals is needed, it is possible to lose sight of the eventual goal of application; again, this is not a problem now, but the project leads must be vigilant to always ask, if things go reasonably well, whether this can add value to the hydrogen economy.

Recommendations for additions/deletions to project scope:

- The project team should attempt to conduct simulations of their research on the potential impact to the hydrogen storage system. The HyMARC team should consider using technoeconomic analysis and factors with their hydrogen storage research direction, similar to their planned work with the carriers. The project has several activities still investigating $Mg(BH4)_2$, although this material has been studied for a significant amount of time without a clear understanding of the rate limitation. Therefore, the project team may need to consider another representative material for their fundamental research investigation. Additional information about the HyMARC team involvement with the seedling projects may be useful in future reviews.
- A potential addition to the HyMARC management plan, if it is not already in hand, would be a risk mitigation plan for actions that may be out of the hands of HyMARC. Specifically, it is unclear what the impact would be on the R&D plan moving forward if access to ALS or the Spallation Neutron Source falls through or is significantly delayed—or whether there is a "plan B.'"
- There must be increased emphasis on understanding barriers to sorption kinetics in complex metal hydrides; actual rates must be established. There must also be improved access to NMR capabilities and improved coordination of multiple R&D activities devoted to nanostructures and nanoscale engineering.
- The project team should maintain scope and possibly consider a slight shift of funds to increase the theory group size (with quality postdocs, not new PIs), as that group seems to serve all and may be overworked—or at least might be very able to increase overall program progress quickly with a bit more funding.
- The project's tasks are new and need sufficient time before such recommendations are warranted.

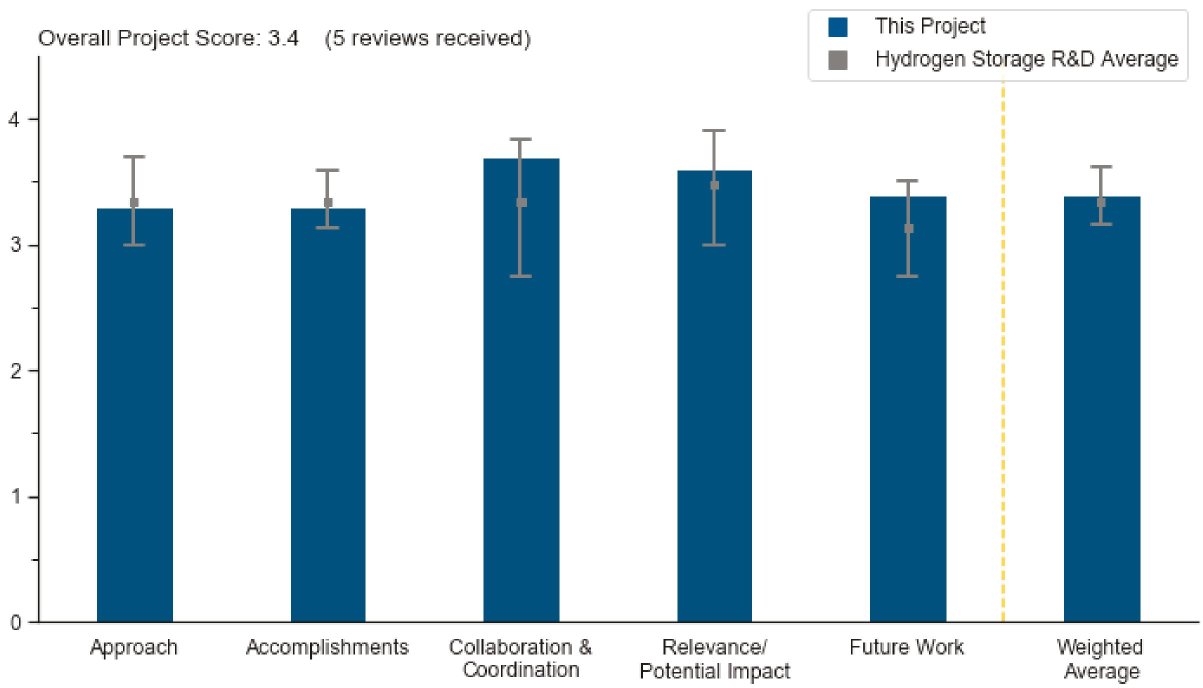
Project #ST-128: Hydrogen Materials–Advanced Research Consortium (HyMARC): Sandia National Laboratories Technical Activities

Mark Allendorf, Sandia National Laboratories

Brief Summary of Project

This project addresses a lack of knowledge about hydrogen physisorption and chemisorption. Researchers will develop foundational understanding of phenomena governing the thermodynamics and kinetics of hydrogen release and uptake in all classes of hydrogen storage materials. Sandia National Laboratories (SNL) will (1) provide data required to develop and validate thermodynamic models of sorbents and metal hydrides, (2) identify the structure, composition, and reactivity of gas–surface and solid–solid hydride surfaces contributing to rate-limiting desorption and uptake, (3) synthesize metal hydrides and sorbents in a variety of formats and develop in situ techniques for their characterization, and (4) apply multiscale codes to discover new materials and new mechanisms of storing hydrogen.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach adopted by the SNL HyMARC team is systematic, rational, and well formulated. A robust combination of theoretical, modeling, and experimental work is being employed to address issues that are critical to our understanding of phase energetics and kinetics of hydrogen sorption reactions in complex hydrides and sorbent systems. However, a keener focus on understanding the rate-limiting step(s) in dehydrogenation and hydrogenation of metal borohydrides is needed. Extensive collaborations are in place and are reinforcing and expanding the scope and depth of the SNL-led effort. The SNL team is also providing valuable support to associated seedling activities.
- The Phase II effort divides the tasks into three areas: sorbents, metal hydrides, and hydrogen carriers. The project has a good balance between theory and experiments. Density functional theory (DFT), DFT-derived

potentials for molecular dynamics, and calculations of thermodynamics have progressed well. It is not clear how much kinetics work started in Phase I; the multiscale approach presented will be pursued in Phase II.

- The SNL technical effort has provided many outcomes related to sorbent materials and metal hydrides. One area in which this group has excelled is in the development of new advanced instrumentation for measuring hydrogen on surfaces and with X-ray absorption spectroscopy (XAS).
- The presentation did not explicitly contain an overarching "approach" slide, so one must read between the lines a bit.
  - The SNL approach continues to be directed at providing the so-called foundational underpinnings that address the barriers in kinetics, thermodynamics, etc. for complex metal hydrides that are critical to making progress toward the targets. The experimental focus remains on understanding how nanoscaling may affect the kinetics and thermodynamics of complex metal hydrides. Two other areas of investigation appear to be getting some attention: the area of sorbent packing to improve the volumetric capacity of sorbents and a new area of hydrogen carriers to support the H2@Scale program. Overall, the approach appears to span a wide range of rather disconnected efforts for the size of the budget; one must wonder if the team members are spread a bit too thin to maintain this breadth of approaches and still keep their eye on the real barrier to success: kinetics.
  - The SNL team has collaborated to develop new low-energy ion scattering techniques to track the rates of hydrogen transport at surfaces and in the near surface. This appears to be a good approach that will hopefully help validate the computational modeling results that are intended to address the influence of buried interphases on the thermodynamics and kinetics of hydrogen release from magnesium borohydride ($Mg(BH_4)_2$). Another approach the team is working with is to understand how to influence the kinetics of dehydrogenation and rehydrogenation with additives or catalysts. The team uses TiF_3 as the precursor to put Ti onto MgB_2, and of course, there is no surprise that this results in MgF_2 being formed. Thus this approach is a little flawed; the team should rather look at other approaches wherein the Ti is placed on the surface without forming other Mg species that might confound the project studies and the ability to coordinate results with the parallel computational studies being performed at Lawrence Livermore National Laboratory (Woods et al.).
  - In the area of trying to further understand nanoscaling effects, the team has prepared a compound in which $Mg(BH_4)_2$ is complexed to the bipyridine (bipy) functionality of a metal–organic framework (MOF). It was not discussed how continued study of this system relates to the condensed phase studies of bulk or nanoscaled $Mg(BH_4)_2$, so the approach was not well explained. Perhaps what the project might focus on is how this is relevant to what Severa and Jensen et al. are doing with another donor ligand–$Mg(BH_4)_2$ system, THFx–$Mg(BH_4)_2$. Maybe there is some synergy to be gained there.
  - To approach the modeling of multiphasic materials relevant to the dehydrogenation and rehydrogenation in $Mg(BH_4)_2$, the team is using a suite of molecular dynamics and DFT techniques to gain information about the interaction potentials between reactants and intermediates such as the arachno-, nido-, and closo-boranes. This appears to be a good approach that has good potential to lend validation and feedback to the HyMARC theory effort.
  - In a rather disconnected approach from the bulk of their work, the project team is working on improving the volumetric capacity of sorbents by exploring the preparation of MOFs in monolith form via sol–gel techniques. While they are being successful, one must ask whether the system chosen is the "right one." It is unclear why they do not focus their effort on MOF-5 or one of the promising systems that Siegel et al. have identified from their machine-learning project. It is also unclear whether this task is a distraction from their work on the kinetics and thermodynamics of complex metal hydrides.
  - In yet another topic, that of hydrogen carriers, their approach is to explore dehydrogenation of diols as liquid organic hydrogen carriers (LOHCs). No rationale was given as to the choice of the carriers selected for research, nor was there a discussion of what the best catalytic routes might be for dehydrogenation (there are hundreds of papers in the literature on glycerol dehydrogenation alone). And lastly, it is unclear whether this approach has considered the technoeconomic analysis out of Argonne National Laboratory that indicates that two-way LOHCs are at an economic disadvantage relative to one-way systems. Another facet of this approach was to explore eutectics of $Mg(BH_4)_2$ as hydrogen carriers. No rationale for this approach was given, nor a discussion of how this could work in practice.
- The project team is attacking many different aspects of the barriers to many paths to success at a variety of levels. Use of materials techniques as well as theory and engineering to advance the performance of

systems should yield a better overall project. The project is part of a larger effort as well, so the team can easily avail themselves of other techniques and insights.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Solid progress has been made in numerous areas of this broadly based research activity. Notably, the development of an improved understanding of how oxides and hydroxides can influence sorption reaction barriers in $NaAlH_4$ (a Phase I effort) is especially intriguing and could be potentially important for other complex hydride systems; determining whether those effects extend to other systems is strongly recommended. Establishment of a molecular dynamics modeling framework capable of assisting development of hydrogen transport models is an important development. It will be interesting to see if the approach used to predict behavior in model systems (e.g., Pd, MgH_2/Mg) can also be extended to more complex reactants. The combination of experiments and theory to develop a phase diagram for bulk $Mg(BH_4)_2$ will undoubtedly pay dividends for understanding the thermodynamic properties and the evolution of reaction products in this important candidate storage system. It will be especially informative and valuable to understand how the phase diagram changes with decreasing magnesium hydride particle size. Likewise, results on force-field modeling of borohydride species created during hydrogen desorption may affect understanding of the thermodynamic properties and, to a lesser extent, kinetic behavior of hydrogen reactions in boron-based materials. Clearly, an important research direction is to develop a better understanding of how additives and catalysts might affect reaction rates in complex metal hydrides. Initial results are promising, but a more seriously focused and systematic research effort is needed. In addition to the work on metal hydrides, the SNL team has made important advances in understanding how novel nanoengineering methods can be brought to bear to alter sorption reaction rates and, possibly, thermodynamics in metal hydrides and MOFs.
- The project team is making good progress toward deliverables and toward surmounting barriers, too. The project has developed kinetic and phase diagram information on key materials, methods to understand molecular- and atomic-level states and changes in state, and science and engineering models, and the team has applied them. Especially appreciated was the blend of science and engineering looking at the encapsulated LiN system, which had lower fundamental capacity but better system capacity owing to a much-reduced heat-transfer system requirement.
- One of the most significant results of this project has been to examine the role of oxygen at the surface of $NaAlH_4$, to reveal that the Al-O-H phases that form change during desorption, and that this may play a role in the desorption pathway and kinetics. This was done by combining simulations with X-ray photoelectron spectroscopy (XPS) experimental data. This is the type of finding that requires a larger group and concerted effort. The research group has shown that the UiO-67 MOF monolith results in an uptake of high volumes of both CH_4 and hydrogen (relative to the powders). These results point to surface-limiting reactions occurring in the powders and not in the monolith. Another major accomplishment is the work shown on slide 15, which really illustrates the advances in moving toward nanoscale hydrides. Because of thermal management of the host structure, volumetric and gravimetric capacity is higher in the nanoscale Li_3N (even with the presence of the "inactive" host structure). Unlike the UiO-67 MOF monolith, consolidated MgH_2 acts as a diffusion barrier to hydrogen. Therefore, forming a fully dense surface layer of it could be problematic (from a mass transport perspective). The capacity drop is likely due to dense MgH_2 formation in the melted sample. MgH_2 is a very slow hydrogen diffuser (like native oxides, it provides an oxygen diffusion barrier in metals). For this reason, a porous layer would work better than a fully dense layer. It could be melted with additive or with gas elution to give porous nanoconfined $Mg(BH_4)_2$ borohydride.
- The phase diagram effort is commendable. Some differences between the previous year's and this year's presentation were noted for the phase diagram of $Mg(BH_4)_2$, but no explanation was provided on the changes. The same is true for the explanation on the role of the oxide layer in sodium alanate. The explanation changed somewhat between 2018 and 2019 in subtle but noticeable ways. The project's new work on eutectics is promising, although much effort in the past on this topic needs to be considered in order not to repeat the effort made under the DOE Metal Hydride Center of Excellence without a strong justification for repeating such efforts. More details were needed on additives and whether any theoretical effort was used for the choice. Overall, there is a strong effort and some gaps in explanation due to limited

scope of the review. The team should consider a more succinct way to connect the summary and conclusions to the data presented and identify the ones covered in the backup slides.

- Overall, the team is making progress, but on a rather diverse set of tasks. It must be asked whether the project would be more productive focusing a bit. It is also difficult to assess progress on the "foundational" approach, as there is a dearth of quantitative statements as to how far the team has "moved the needle" toward a given target. One instance in which the team has provided quantitative data toward progress is on the nanoscaling of hydrogenated lithium nitride; while positive results were described for nanoscaling, it was not made clear how what they have learned would be predicted to influence other complex metal hydride materials. The team continues to make incremental progress on integrating the modeling and experimental efforts directed at understanding what underlies the apparent kinetics issues associated with the multiphasic nature of the dehydrogenation/rehydrogenation of magnesium borohydride/magnesium boride. Where the project has shown nice progress is in developing the combination of low-energy ion scattering, XPS, and gas phase analysis to track hydrogen transport at and near the surface. It will be of interest to see how the team is able to give validation and feedback to the modeling effort in the future such that more rapid progress can be made toward understanding the kinetics barriers in $Mg(BH_4)_2$. The SNL team has made some progress on exploring eutectics and dehydrogenation of polyols for the H2@Scale effort, the preparation of monolithic MOFs for improving volumetric density of hydrogen sorption in MOFs, and molecularly supported $Mg(BH_4)_2$ on a bipy-functionalized MOF. These efforts lacked a firm rationale, and it seems that, while the team members were making progress here, they would perhaps be better served by focusing on the tasks surrounding the integration of theory and experiment on the $Mg(BH_4)_2$ system.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- Extensive collaborations with other HyMARC core team members and seedling projects are evident. The availability of the SNL high-pressure hydrogenation and characterization system and the sharing of high-pressure expertise with other consortium researchers have been vital to project success. The consolidation of the HyMARC and HySCORE activities has merged a variety of related projects, and the SNL effort overlaps much of that work. Although it may go without saying, frequent communication and interaction among researchers involved in those related activities is critical and strongly recommended.
- Collaboration is an area where the SNL team excels. They have brought unique SNL capabilities to bear on a number of seedling projects, and their capability in performing high-pressure hydrogen experiments is surely oversubscribed by external collaborators.
- The project has good interaction with four seedling projects that include a number of joint publications. Additionally, international collaborations with Aarhus University have provided a publication on the closo-borates.
- There is extensive, appropriate, and helpful collaboration with a dozen outside groups, many of which are the best in the business. There are clear examples of these collaborations accelerating progress toward goals.
- The list of collaborators is significant. The collaborative effort is opportunistic and not strategic. A better alignment of needs and a leveraging of complementary capabilities in different national and international institutions need to be clearly outlined. Assigning a lead for collaboration and outreach can improve the focus.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The work accomplished so far points to new directions and suggests that the project will have far-reaching impacts. For example, redefining the role of nanoporous host structures as actively participating in thermal management will open the doors to optimization of new porous materials and hydride combinations that outperform currently studied ones. The study of monolithic MOFs shows that a particular barrier in hydrogen uptake that exists for the powders is ameliorated with compaction. This reframes thinking around the notion that high surface area is necessary for more hydrogen uptake. Such high-density microstructures are not as effective when utilizing metal hydrides (e.g., $Mg(BH_4)_2$, which is melt-infiltrated into graphene aerogels), potentially because the entire monolith could form MgH_2 (which is a slow diffuser of hydrogen). Taken together, these studies point to the ability to tune kinetics by controlling microstructure and open the door to many more possibilities for designing optimal hydrogen storage materials.
- Three major areas are addressed: understanding, materials, and measurement capability improvement. This makes the project highly relevant in theory. The actual work in these areas is all essential to progress in solid-phase hydrogen storage, so this is a highly relevant project.
- The SNL contributions are critical to the success of the HyMARC consortium. The project is well aligned with DOE Hydrogen and Fuel Cells Program goals, and the potential impact of progress toward achieving Office of Energy Efficiency and Renewable Energy goals is significant. SNL's strong support of seedling activities is enabling and accelerating progress on those projects.
- The team has made some very important contributions. The overall talent and innovation were definitely noteworthy in Phase I. In Phase II, although some changes were made for somewhat unknown reasons, the team seems to be making progress toward the goals.
- There is very high relevance and potential impact of SNL and its collaborations in integrating the experimental and modeling efforts in understanding the underlying multiphasic issues of the hydrogenation and dehydrogenation of $Mg(BH_4)_2$. Given that they are also exploring several other rather unrelated areas, perhaps the impact of their efforts would be greater if there were fewer distractions, e.g., fewer tasks outside of the main tasks surrounding understanding bulk and/or nanoscaled $Mg(BH_4)_2$. Perhaps more of an "all hands on deck" focus on the main tasks would benefit the overall impact of the effort.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future works are each logical extensions of the prior year's accomplishments. A new feature in the proposed future work (not reported in prior years) is the study of catalytic materials for hydrogen generation from alcohols and polyols. This should be a fruitful direction for future work.
- The project's proposed future work in all areas is appropriate, both technically and relative to funding level.
- The proposed future work is a straightforward extension of the 2018/2019 Phase I and II efforts. Although investigations are proposed that relate to improving understanding of hydrogen sorption, reaction sorbents, metal hydrides, and carriers, as well as support of seedling activities, some additional detail would have been useful. For example, the effort to probe structural defects on hydrogen storage properties in MOFs assumes that structural defects actually affect the storage properties. Some justification would have been helpful. Also, as pointed out in the 2018 review, it is important to understand whether the conclusion derived from the oxide work on $NaAlH_4$ ("surface hydroxides serve as low barrier sites for H-H combination and hydrogen release") is extendable to other complex metal hydrides. This is an important research issue. Likewise, a more focused effort on understanding and overcoming kinetics barriers is needed. This will require the development of a clear and rational research strategy.
- The proposed future work on activation of B-B and B-H bonds is appropriate; more focus on experimentally verifying the modeling efforts is in order. There needs to be a subsequent quantifiable measure of progress in how the understanding being gained results in improved kinetics; the capacity is nice, but if the release rates are not beginning to approach the rates required to meet practical application, then the capacity is less important. SNL has historic data on hydrogen release from bulk, nanoscale, etc., as

well as $Mg(BH_4)_2$, and is gaining more data from the present work. In the future, it would help immeasurably to measure progress of the SNL and HyMARC efforts to have a compilation of (possibly maximal) release rates, benchmarked with respect to the required release rates from the technical target.

- The proposed future work is on the safer side. For example, powder compaction and tweaks of MOFs for sorbents will not change the current trajectory in any significant ways. The team needs to take more risk. In Phase I, the responsibility of achieving the DOE targets was assigned to the seedling, while the majority of resources were spent elsewhere. It is understandable since capabilities were developed. In Phase II, the team needs to take more responsibility for changing the trajectory through setting their own goals and stepping up to help seedlings achieve targets.
- The continued work on sorbents, while good, may be a distraction to their main efforts in complex metal hydrides. It is unclear whether the work on organic carriers is the best use of SNL's expertise.

Project strengths:

- This is a comprehensive project being conducted by a highly capable and dedicated R&D team. The project is addressing important issues relevant to our understanding of hydrogen sorption processes in both metal hydrides and sorbents. The work is forming a solid foundation for development of improved materials. The project is well managed, and extensive and fruitful collaborations are augmenting the core activity. The SNL team should be commended for the extensive support being provided to seedling projects.
- The strengths of the project are its demonstrated accomplishments. The discovery of the higher volumetric capacity for UiO-67 (by approximately 55%) is a result of the ingenuity of the project team members. This result opens the door to many more discoveries. Likewise, the notion that the nanoporous framework structures play a role beyond simply maintaining the nanostructure of the hydride is a key discovery that has the potential to open many more avenues of research pursuit.
- The project's strength is in the capability of the team, and some of the significant progress made in Phase I is in developing a strong base for theory and measurements. Synthesis efforts are still somewhat weak, but seedling projects are beginning to make progress. The team coordinated well with collaborators and seedling teams.
- The team is very good, the facilities are superb, and the collaboration is excellent and effective; the project is making good progress.
- There is good integration of modeling and experiments. Expert capabilities in high-pressure hydrogen experiments can be seen.

Project weaknesses:

- A clearly defined pathway to addressing the critical problem of sluggish kinetics in complex metal hydrides is needed. Various approaches (e.g., nanoscaling, additives) are being used, but a more coherent and well-formulated strategy for generating reaction rate data would be helpful. It is hoped that a definitive statement concerning the identity of the rate-limiting step(s) in the $Mg(BH_4)_2$ reaction system can be made in the 2020 Annual Merit Review (AMR). Although not a weakness per se, as pointed out in the 2018 AMR, a more keenly focused effort is needed for determining whether the intriguing results and conclusions on the effects of oxides and hydroxides on $NaAlH_4$ hydrogen sorption can be extended to other systems (especially metal borohydrides).
- The weakness is mostly in the lack of a roadmap for achieving DOE targets and in taking more risk using the advancement made in Phase I. Overall, there are no major weaknesses in technical capabilities or execution.
- It is not certain that the liquid carrier work aligns with SNL strengths. There are perhaps too many task areas; it is possible that productivity and impact could be improved with greater focus on the modeling and experimental areas surrounding the key kinetics and thermodynamics issues of complex metal hydrides.

Recommendations for additions/deletions to project scope:

- This is not a recommendation but a general question or observation for the SNL team: it seems possible that the hydrogen carrier work being proposed by the SNL team dilutes the attention and emphasis needed for other important tasks. It may make sense to transfer that activity to another group in HyMARC (e.g., Pacific Northwest National Laboratory).

- There are no recommendations at this point. The only suggestion for the team is to look for work already reported in the literature and develop stronger rationale for going down the same path.
- LOHC work may not be the best fit to the SNL program.

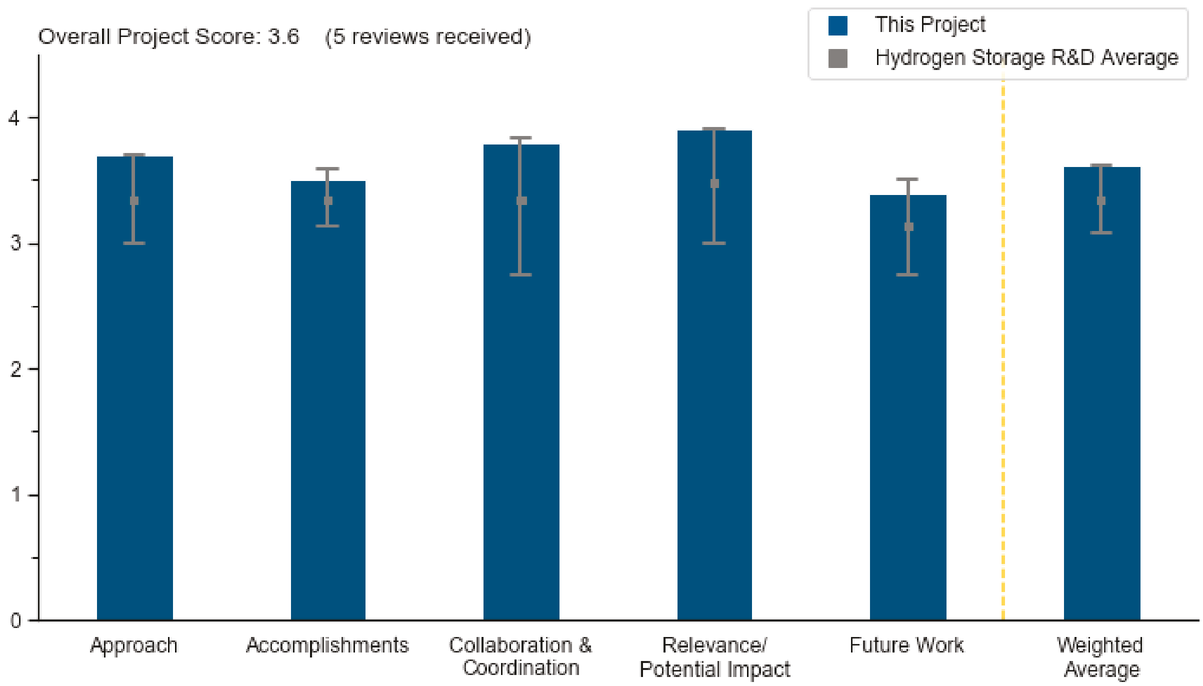
Project #ST-129: Hydrogen Materials–Advanced Research Consortium (HyMARC): Lawrence Livermore National Laboratory Technical Activities

Brandon Wood, Lawrence Livermore National Laboratory

Brief Summary of Project

The Hydrogen Materials–Advanced Research Consortium (HyMARC) is providing community tools and foundational understanding of phenomena governing thermodynamics and kinetics to enable development of solid-phase hydrogen storage materials. HyMARC team member Lawrence Livermore National Laboratory (LLNL) is conducting porous carbon synthesis; X-ray absorption/emission spectroscopy (XAS/XES); and multiscale modeling including density functional theory (DFT), ab initio molecular dynamics, phase-field mesoscale kinetic modeling, and kinetic and quantum Monte Carlo (QMC).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is comprehensive and addresses issues that are critical to the fundamental understanding of hydrogen sorption thermodynamics and kinetics in candidate hydrogen storage systems. The approach utilizes numerous theoretical and modeling methodologies and spans a broad range of relevant time and length scales. The approach is aligned with experimental work being conducted by other HyMARC investigators. Moreover, the project provides important and useful support for associated seedling projects.
- LLNL's approach is divided into two areas: tuning thermodynamics and kinetics. The approach is based on strong hypothesis-driven research. The use of nanoscaling to improve thermodynamics and kinetics, the adoption of an emphasis on the complexity of interfaces, and the use of eutectic as hydrogen carrier may produce important results.
- The team is making good progress on deliverables. The HyMARC theory group is guided by the needs of its partners but is also guided by synthesis work and X-ray measurement work. The team effectively assists

the rest of the consortium. The "Assess, Interpret, Model, Understand and Design" paradigm nicely sums up how the team adds value.

- The LLNL modeling approach remains firmly focused on developing an understanding of the complex energy landscape along the dehydrogenation/rehydrogenation pathways of magnesium borohydride using a wide variety of computational tools to address the multiple length scales involved. The modeling approach employed addresses the key features that influence the kinetics and thermodynamics of this material, nanoscaling and confinement being among those. The modeling effort toward understanding the reverse reactions resulting from magnesium diboride's direct use of additives and catalysts approaches the key issue of kinetics and is one of the main barriers that must be addressed for this class of materials. The modeling approach, which utilizes complex, state-of-the-art tools, is well communicated and well implemented, as usual. More thought should be given to the progress and relevance of the interaction between "additives" or catalysts and the boron nitride (BN) sheet structure. In the current model, investigators consider a naked titanium atom. This is likely unrealistic in practice; under hydrogen pressure, one would expect to find TiH_2 species, or even $TiH_{(2-x)}$ species. Therefore, the approach should be adjusted to better accommodate compounds more likely to be found under experimental conditions. LLNL also includes activity directed at modeling the electrocatalysis of hydrogen carriers. While the approach is good, this effort may be premature until more details as to the precise electrochemical system from the experimental effort are forthcoming.
- The standard test conditions comprise theory and advanced characterization. The investigators plan to improve current understanding of thermodynamics and kinetic limitations in storage materials and liquid hydrogen carriers. The project has developed a realistic plan to implement modeling and theory for solving problems identified in the hydrides (namely, borohydride regeneration, effects of nanoscaling and amorphization, and understanding catalytic and electrocatalytic additives). Validation work is under way for several portions of the computational work. This annual report discusses only briefly the advanced characterization work the team has accomplished. Since in situ kinetics is mentioned in slide 2, the topic should be better addressed throughout the presentation.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made significant inroads in understanding the role of alkali, alkaline earths, and 3D/4D transition metal dopants on MgB_2. This understanding of ionic versus covalent contribution to the surface is potentially significant for understanding borohydride regeneration. The enthalpy-versus-entropy compensation effect work related to examining the excess surface energy as a function of particle size is novel. There are few published reports that discuss enthalpy as a function of particle size in the nanoscale regime. These effects relate back to specific heat variation as a function of particle size (resulting from a change in optical phonon modes as a function of size). A 1954 report in the *Journal of the Royal Society Interface* examined these effects for titanium dioxide. Additionally, a 2016 report in the *International Journal of Thermophysics* reported on these effects on CuO, along with a loss in the Debye T^3 rule for nanoscale particles. Further work, which pushes computational frontiers on this topic, will serve the hydrogen storage community as well as the broader scientific community. It is unclear what is meant by "early results on Ti vs. Li agree with predictions" (slide 11). These results were not covered during the presentation.
- The LLNL modeling effort continues to make progress in assessing the effects of nanoscaling, mechanical stress from confinement, activation of the B-B sheets in MgB_2, and the Mg-B-H phase diagram. Aspects of the model are presented in such a way as to inform the experimentalist and suggest experimental approaches. This is highly valuable. The modeling effort is highly responsive to new experimental input and uses this input to refine the model. Overall, the team has made excellent progress in areas that support DOE metrics.
- The team is making excellent headway toward project milestones and has already made substantial progress toward many future milestones. Examples of the team's progress include the phase diagram for $Mg(BH_4)_2$, their understanding of the tuning limits of particle size and confinement, and their understanding of the impact of phase attributes on $Mg(BH_4)_2$ decomposition. Furthermore, the team has developed a brand new model for diffuse interface reactive systems. The project is currently undergoing

more interpretation, but in Phase II, more guidance is expected. Most importantly, the team interacts with experiment groups to advance in ways that neither theory nor experiment could accomplish alone.

- This research and development (R&D) activity is a vital component of the HyMARC consortium and is contributing significantly to its success. The ability to simulate and model processes at multiple time and length scales is a powerful and impressive component of the overall HyMARC activity. For example, in 2018 and 2019, the project addressed a wide range of important problems, including clustering and nucleation kinetics, developing and refining phase diagrams, predicting effects of metal dopants and other additives on bonding character, understanding metal boride decomposition pathways, assessing the role of nanoscaling on thermodynamics, and demonstrating how confinement stress can effectively destabilize hydrides and alter both thermodynamics and kinetics. The results obtained from these studies are significantly improving our understanding of the complex phenomena and processes operative during hydrogen sorption reactions in storage materials.
- The publications and presentations show that the team is wrapping up project results and making an impact on the progress of the HyMARC team. Phase diagram work is important, and though the experiment–theory feedback cycle is limited, it remains an important part of the focus. It remains to be seen whether the force field work can advance or benefit DOE targets. The discussion of metal dopants for MgB_2 decomposition began with some interesting hypotheses. The team needs to develop the theory further to extend predictive power to realistic clusters rather than restricting it to single-site dopants. The progress percentages noted are reasonable, but there are too many open threads on each. A careful recalibration of effort may be needed to achieve the Quarter 4 targets.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration with an experimental team is reasonable. The team is aware that progress on the models for higher-length scales will strengthen the team. The diffuse reactive interface nonlinear kinetics (DRINK) model seems somewhat disconnected from the team's efforts. At the very least, an experimental connection was not evident in the presented slides. The collaboration on symmetry-adapted perturbation theory (SAPT) potential is a good connection. The confinement stress work can be complemented by the experimental effort using coherent diffraction imaging to obtain better validation data.
- The project's interactions with seedlings are rich. These interactions include collaborations with the University of Hawaii and two National Renewable Energy Laboratory projects. New seedling interactions with Liox Power, Inc., and the California Institute of Technology have developed this year. Several other collaborations with the University of South Carolina, Tennessee State University, Georgia Institute of Technology, and Michigan State University are under way. Additionally, international collaborations are being developed.
- The LLNL modeling effort continues to be a model for collaboration among national laboratories, as well as among academic institutions. While investigators continue to make good progress on their own tasks, the LLNL effort has demonstrated that LLNL can work effectively with the seedling projects in a highly collaborative and supportive mode. The modeling effort collaborates extensively in the development of enhanced modeling tools to support the HyMARC effort. Overall, the LLNL modeling effort is a world-class effort.
- The principal investigator and the LLNL team are involved in extensive collaborations with other HyMARC core team members, other U.S. and foreign researchers, and seedling project investigators. The LLNL team is commended for their active engagement and cooperation with other members of the entire HyMARC consortium. Those collaborations are exceedingly valuable and are critical to the overall success of HyMARC.
- This group is likely the most collaborative group in HyMARC. The team has participated in many valuable collaborations both inside and outside the project. These collaborations are very beneficial to other groups and benefit this group in turn.

Question 4: Relevance/potential impact

This project was rated **3.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This is perhaps the most impactful of the HyMARC projects, as the LLNL effort addresses the key thermodynamics and kinetics issues surrounding the release of hydrogen from a complex metal hydride. The output from this modeling effort continues to help drive the experimental efforts, amplifying the impact of the modeling effort. The LLNL modeling effort collaborates extensively with other modeling efforts, has an excellent feedback system with experimentalists, and continues to have a high impact on progress within HyMARC.
- The work is a strong example of HyMARC's impressive progress toward technical maturity and leadership. The team has developed a new approach and hypothesis that can affect the results of the funded team and others engaged in similar research beyond the immediate team.
- The LLNL project directly supports the core mission of the HyMARC program. The research effort is focused sharply on the most relevant and consequential issues, and it is fully aligned with the overall research, development, and demonstration objectives of the Hydrogen and Fuel Cells Program.
- The project is relevant in and of itself through the results obtained, but the project also adds value to partner work via guidance of experimental theory or explanation of results. The project assists HyMARC in speeding progress toward goals and milestones that would be much slower by experiment alone.
- As prior work has shown, particularly work related to borohydride activation, computational and theoretical work provides a major impact. The annual report described little of the impact of advanced characterization (mentioned on slide 2).

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work continues to address important problems relevant to our understanding of the kinetics and thermodynamics of hydrogen sorption reactions. The team seeks to provide a more coherent pathway to overcoming barriers and problems. The proposed work is a reasonable and straightforward extension of the earlier studies, extending the results to more practical operating regimes. The refinement of phase diagrams for $Mg(BH_4)_2$ is important, especially with regard to changes in the phase diagram as particle size decreases.
- The team will apply their current approach to proposed future work. This is the correct decision, as their current approach is excellent. The application of more chemical intuition to the modeling of the additives could help to inform the experimentalists' approach to catalytic rehydrogenation/dehydrogenation of complex metal hydrides.
- Though the list of proposed work is not long, all items are excellent and important for realizing the strong Phase I effort. A good set of activities is under way in Phase II.
- The proposed future work is a logical extension of past accomplishments. The DRINK model will provide a method for understanding processes occurring during partial hydrogenation.
- The team outlines suitable goals in all areas. A more thorough description of the plans and the team's intended approach to handling the workload would be helpful.

Project strengths:

- A highly qualified and experienced team is conducting the project. Extensive and progress-enhancing collaboration is evident. This team is a critical component of the overall HyMARC effort. The project team has demonstrated the ability to move rapidly and effectively to address emerging problem areas. This has made the project's contributions even more valuable to the consortium because these contributions facilitate the creation of more fruitful R&D pathways for both the core HyMARC team and associated seedlings.

- The team is highly collaborative. The team provides and receives excellent feedback to and from the experimental efforts. The team is very responsive to current and changing needs. The project demonstrates a world-class modeling and simulation effort.
- This team is a strong and hard-working group that demonstrates excellent rapport with partners and external projects. The team is highly valuable to HyMARC.
- The project tackles some of the toughest computational problems that exist within the discipline. The plan to address kinetics and other nonequilibrium phenomena (including amorphization) is important.
- The strength is in the results. Therefore, the team worked hard to see the results published and ensure follow-up experiments are done. Some projects understandably originate from requests from the experimental side.

Project weaknesses:

- There are no meaningful problems.
- In Phase II, the main challenge will be to maintain the momentum. This will require effort since all of the tasks diverge in needs. As a result, the tasks generate more need for theory. Managing the proposed future tasks will be challenging, and the team may need to prioritize their effort and automate some of their workflows to expand the work to a broader set of materials. Also, the investigators are encouraged to develop more publications with a combined theoretical and experimental team in order to demonstrate the application of the modeling work and improve the overall impact.
- The only weakness of this project is the lack of results reported under a declared portion of its portfolio (in situ characterization). Since the computational and theoretical aspects of this portfolio are extremely strong, it is suggested that the team choose to either (1) address only in situ characterization in the context of using data of this type to validate computational or theoretical models/results or (2) remove in situ characterization from this project.
- A keener focus on understanding kinetic barriers and a strategy for overcoming slow kinetics in metal hydrides are needed. This applies to the entire HyMARC effort, not just the theory/modeling project. A more rational, comprehensive, and keenly focused strategy for elucidating kinetics mechanisms should be established. The kinetics problem is the “elephant in the room” for hydrogen storage in complex metal hydrides.

Recommendations for additions/deletions to project scope:

- This group is in strong demand from other parts of HyMARC and contributes in many ways. If funds are added or shifted in the future, it would be wise to consider the theory group as the recipient of more funds so the team can bring on more people (likely postdocs).
- To help future reviewers assess progress toward goals, investigators should set priorities and clearly explain how resources will be allocated.
- The application of more thought and chemical intuition to the additives modeling would result in more realistic outcomes and enhance progress in the experimental area.
- The in situ characterization section of this project is not matched well with the computational work or theory work. Either the in situ characterization should be removed, or its scope should be redefined within the standard test conditions.

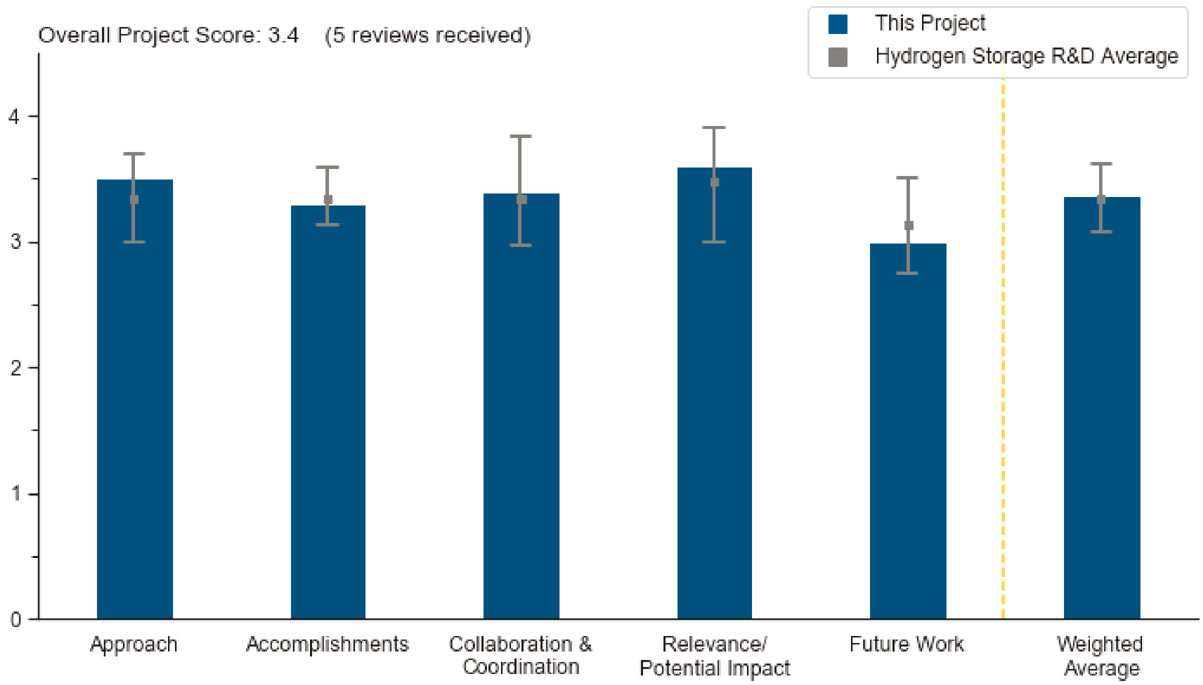
Project #ST-130: Hydrogen Materials–Advanced Research Consortium (HyMARC): Lawrence Berkeley National Laboratory Technical Activities

David Prendergast and Jeffrey Long, Lawrence Berkeley National Laboratory

Brief Summary of Project

The Hydrogen Materials–Advanced Research Consortium (HyMARC) is providing community tools and foundational understanding of phenomena governing thermodynamics and kinetics to enable development of solid-phase hydrogen storage materials. Lawrence Berkeley National Laboratory (LBNL) will (1) focus on light materials and synthesis strategies with fine control of nanoscale dimensions to meet weight and volume requirements, (2) design interfaces with chemical specificity for control of hydrogen storage/sorption and selective transport, (3) explore storage concepts, (4) develop in situ/in operando soft X-ray characterization capabilities in combination with first principles simulations to extract details of functional materials and interfaces, and (5) refine chemical synthesis strategies based on atomic- and molecular-scale insight from characterization and theory.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- There are two separate pieces to the LBNL effort, the Prendergast effort and the Long effort, and the two projects are scored together as one.
  - Prendergast's approach is to utilize the LBNL Advanced Light Source (ALS) capabilities to develop in situ characterization of reacting storage materials. Sheet-like nanocarbons are used as encapsulants to nanoscale complex metal hydrides or simple metal hydrides (e.g., MgH_2). Magnesium borohydride is nanoencapsulated in metal–organic framework (MOF) cavities. The approach integrates preparation of nanoencapsulated materials with the use of ALS and conventional capabilities to characterize hydrogen release and reuptake properties of the nanoencapsulated materials. This approach is a good one, given the number of encapsulated

systems that have shown enhanced kinetics or capacities. Additional research on well-characterized materials is needed, and this project seeks to provide this research. The approach that includes the addition of metal halides to destabilize sodium borohydride would seem to have been preempted by numerous studies of metal additives that appeared in the literature 10–15 years ago. Overall, Prendergast's approach deserves a score of 3.0.
  - Long's approach is to leverage the team's expertise in preparing MOFs with open metal sites that have previously been shown to adsorb hydrogen with enthalpies approaching what is thought to be the optimal range of 15–25 kJ/mole for practical applications. To achieve this, the team is designing strategies to incorporate metal ions with open coordination sites that should have a high propensity to bind H_2 and potentially multiple hydrogen molecules. Once synthesized, these candidates are characterized in the presence of variable and high-pressure hydrogen using infrared spectroscopy and neutron scattering techniques. This is a very cogent approach, and one that is well thought out and well communicated. Overall, if it could be scored independently, Long's approach deserves a score of 4.0.
- Four major approaches were implemented to meet several Hydrogen and Fuel Cells Program goals, including the improvement of sorbents and the modification of metal hydride compounds to improve properties, carriers, and characterization. The multiple approaches greatly increase the odds of success. The goals being addressed are well defined, and the approaches have merit.
- It is key that LBNL holds the in situ X-ray absorption spectroscopy (XAS) and infrared capabilities, as well as other ex situ characterization including X-ray photoelectron spectroscopy (XPS) and X-ray absorption near edge structure (XANES). The development of a flow reactor for liquid carriers is under way and will be useful to other projects.
- The approach follows the work in Phase I and involves new Phase II tasks 1–4. The team is strong in operando experiments and theory. The MOF binding and multiple hydrogen molecules per site are continued in Phase II. The in situ X-ray and ex situ X-ray work backed by density functional theory (DFT) calculations was well planned and executed. The host encapsulation work and reduced graphene oxide (rGO) work needs a pathway to ramp up or ramp down. Currently, the approach does not involve any clear link to targets or metrics. So, in principle, all of the effort could continue indefinitely. Although all aspects of the approach are important for the science of reversible hydrogen storage, setting priorities can help the project's overall impact on the progress toward meeting U.S. Department of Energy targets.
- The approach is broadly based, comprising three principal research thrusts: (1) development of sophisticated in situ/operando diagnostics for probing hydrogen sorption reactions at relevant temperature and pressures, (2) nanoscaling of complex hydrides to reduce hydrogen sorption temperatures and increase rates, and (3) synthesis of MOFs containing open metal sites to facilitate increased binding enthalpies and hydrogen capacities. In addition, work on new concepts for boron-based storage and reactors for hydrogen carrier research has been initiated. The approach complements other related work in the HyMARC consortium. However, the work on nanoscaling generally lacks direction, especially with regard to overcoming cycling problems. A clear delineation of future work is absent.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team has made good progress toward the goals that have been set. All members are addressing significant barriers, and if these are surmounted, the work could yield valuable approaches or materials. The in operando and at-pressure tools developed are impressive and should be very useful in determining the mechanisms at work in advanced materials. The 21 kJ/mol binding in MOFs is a big step forward. Also, the crossover ideas of using BN (famous from hydride work) as a potential sorbent and MOFs (famous sorbents) as modifiers for $MgBH_4$ shows out-of-the-box thinking that may translate to a breakthrough.
- The project has made contributions to rGO enapsulated hydrides (produced by S. Jeong at LBNL) and has shown that the nanostructure is preserved after rehydrogenation. The team has shown differences in surface and bulk structures in nanoencapsulated $Mg(BH_4)_2$ (within UiO-67), revealing chelation of the boron with the surrounding Ni(BBY). The suite of characterization tools enables this project to make substantial

contributions to the HyMARC program. Furthermore, the project is involved in development of flow reactors for hydrogen carrier research.

- The development of an in situ/operando diagnostic capability to probe structure and reaction products at relevant temperature and pressure regimes is an important accomplishment that should greatly benefit the HyMARC program. Use of nanoencapsulants for $Mg(BH_4)_2$ confinement has been shown to facilitate dehydrogenation at reduced temperatures. However, cycling efficiency is low, and plans for overcoming kinetics obstacles were not addressed. New results on the synthesis of an MOF containing open V^{2+} sites were presented. The new MOF has an H_2 adsorption energy of -21 kJ/mol, consistent with hydrogen binding at practical operating temperatures. Similarly, an MOF containing Cu(I) sites is also predicted to be in the optimal range. This is clearly an important advancement in the development of adsorbent systems that can meet DOE storage targets.
- The team made good progress on the tasks. The V^{2+} synthesized and experimental data made important contributions. However, the Phase II effort still needs to gather momentum. More results from the new reactor from Professor Gabor Somorjai's laboratory at LBNL will be interesting. Future plans need to integrate other laboratories to achieve widespread project success and increase the quality of the results.
- Separate comments on both principal investigators' work are below.
    - Regarding the Prendergast work, progress on the rGO encapsulated materials appears to be incremental. The work on magnesium borohydride in rGO was much the same as last year. There did not seem to be enough presentation time to discuss the in situ characterization of this material in detail, nor was there any apparent progress in understanding the cycling behavior/reversibility of this material and the implications for other systems. The nanoencapsulation of magnesium borohydride in an MOF was described, and investigators witnessed a very low-temperature evolution of hydrogen at around 120°C. There was little rationale given for this approach, nor was there a discussion of the quantity of magnesium borohydride that was enclosed within the cavities of the MOF that could then be translated into an effective gravimetric capacity. Furthermore, there has been, as yet, little characterization other than some XPS. Hopefully, infrared and nuclear magnetic resonance (NMR) characterization will be implemented in the future. The statement that the material releases "mostly H_2" is insufficient to gauge whether this is interesting. The Prendergast section of the project deserves a score of 2.5 for Accomplishments and Progress.
    - The Long portion of the project successfully synthesized the first V(II) MOF, and V(II) should have a propensity to bind H_2. The team cleverly characterized hydrogen sorption on the material by using infrared difference spectroscopy to identify the H_2 as well as deuterium (D_2) stretch of bound hydrogen on vanadium. This is another accomplishment and a logical stepping stone on the way to attempting to discover open metal framework sites that can bind more than two hydrogen molecules. The accomplishments were well communicated, and it was easy to determine the good progress made. The Long section of the project deserves a score of 3.5 for Accomplishments and Progress.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration and coordination with other institutions is very good for both projects, and the degree of collaboration is commensurate with the size and scope of the projects.
- The team has a wide group of collaborations with excellent groups that yield value to the project.
- The project has joint publications with other HyMARC laboratories. Since the team's contribution is characterization, this is not unexpected. In the future, it would be helpful for the team to publish advances in technique development.
- Beneficial collaborations with other HyMARC investigators in most project research areas are evident. The overall HyMARC program is benefitting significantly from advanced diagnostic capabilities at LBNL. However, it is not entirely clear whether the nanoengineering activities at LBNL are coordinated in a meaningful and direct way with other nanoscaling efforts within the consortium.

- The team is strong and has good connections inside LBNL. It is unclear that collaboration with others and seedlings is used to this project's advantage. More effort is required in the area of collaboration, especially considering that other laboratories' broad use of operando work will benefit the team.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Separate comments on both principal investigators' work are below.
    - Regarding the Prendergast work, nanoscaling to alter the thermodynamics and kinetics of the dehydrogenation/rehydrogenation in complex metal hydride materials has been shown by many others to be a promising pathway. This project's focus on using nanocarbon sheet-like materials is thus very relevant to this topical area. The potential impact of the work in nanoscaling is lessened by the incremental progress displayed in the presentation. The state-of-the-art characterization tools being developed using ALS capabilities is highly relevant to gaining detailed understanding of certain structural and chemical aspects of these complicated reacting systems, especially the opportunity to access X-ray spectroscopies from light elements that are of course of interest in these complex metal hydride materials. The development of operando techniques to examine these reacting materials under dynamic hydrogen conditions is very relevant to the needs of the hydrogen storage community, and the continued development of these techniques and tools can have a large impact on the area. However, it is likely that the achievable temperatures and pressures in their sample environments may ultimately limit the potential impact of these tools. If this work could be scored separately, it would receive a 3.0.
    - Regarding the Long work, developing materials that can sorb significant quantities of hydrogen at something closer to ambient temperature is a "Holy Grail" of sorbent research. Long and his group have made substantial progress in prior years, and this year is no different. The relevance of their approach to gaining adsorption enthalpies in the range of 15–25 kJ/mol is very high; if the group is successful in ferreting out MOFs that can bind multiple hydrogen molecules with the appropriate adsorption enthalpy, the potential impact on the knowledge base in hydrogen storage would be significant. There still needs to be a candid presentation on how close this approach can come to DOE targets. There is no argument that this is great science, but the practical implications need to be described in detail. If this work could be scored separately, it would receive a 4.0.
- The project is an important element of the overall HyMARC activity. The advanced characterization activities and MOF synthesis work are especially innovative and noteworthy. For the most part, the research effort is well aligned with DOE research, development, and demonstration objectives and is focused on issues that have important potential impact on the advancement of progress toward DOE targets.
- The work performed has an excellent chance of making an impact on many important unknowns in host materials design and understanding of measurements (task 4). In contrast, the theory effort seems to have slowed down somewhat. The team needs to continue some of the excellent contributions made in Phase I to ensure best practices are shared with and adopted by the community in general.
- Several major DOE objectives are well aligned with this work. This is highly relevant work.
- The relevance of the project remains high.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The plans for future work are in line with past accomplishments and will add competencies to the HyMARC portfolio. For example, the development of measurement tools for entropy and enthalpy of adsorption will aid ST-129 in performing computationally derived enthalpy as a function of hydride particle size.
- The proposed future work is logical and promises to deliver good results. The priority assigned to the various subtasks proposed was not clear from the presentation. A more deliberate effort to engage outside

collaborations to increase the output of the team can help the team, which is already doing an excellent job in terms of strong science, synthesis, and innovation on characterization techniques.

- The future work is well designed, and clear goals are outlined. The team considers many pathways to improve chances of success on one of the many paths.
- The proposed future work in the sorbent research area is clearly stated and follows directly from the earlier work. In contrast, future work in the areas of advanced characterization, nanoencapsulation, hydrogen carriers, and boron-based storage material areas is neither presented nor discussed. This lack of discussion makes it impossible to ascertain the direction of future research in those areas.
- The Prendergast effort did not present a slide on future direction, so it is difficult to assess what directions that work will emphasize in the future. The combined future work would benefit from including an analysis of potential practical outcomes. The scientific merit of this work is abundantly apparent; however, the practical aspects require some discussion. The Prendergast section of the project deserves a score of 2.0 for Proposed Future Work. The Long effort supplied a cogent, logical path forward toward the goal of obtaining higher isosteric heats of adsorption. The Long section of the project deserves a score of 3.5.

Project strengths:

- A well-qualified team with expertise in all relevant areas is conducting work on this project. The advanced characterization and diagnostic instrumentation is world-class and provides a powerful and unique capability to the HyMARC program. The MOF research is especially innovative. Excellent progress is being made on a difficult research challenge that has a high payoff.
- LBNL provides high-performance computational tools and state-of-the-art characterization tools that take advantage of the unique capabilities of the ALS. The synthetic capabilities in open metal sites in framework materials and the characterization capabilities for hydrogen sorption under hydrogen with variable temperature capability are world-class.
- The project has many strong components that are highly exemplary. The in situ and ex situ measurements are very well executed. The synthesis of new candidates and new ideas on the table is promising. The theoretical effort has strong links to the needs of the community for MOF and host–guest materials design. It is too early to fully judge the progress of the remainder of the work.
- The strength of ST-130 is its use of both in situ and ex situ characterization techniques to address some of the most unique hydride materials (i.e., rGO encapsulated borohydrides).
- The principal investigators have strong backgrounds in their areas, great facilities, and clever approaches.

Project weaknesses:

Although it is not a weakness per se, the rGO wraps may not have good durability in containing material that alters size and requires many cycles. It will be important to check early in testing to be sure the wraps do last hundreds of cycles.

- The team needs to better integrate its effort with the other laboratories. The theory team should improve its impact by providing the wider community with data for screening on MOF and multiple binding site possibilities. It is not evident that the team engages in discussion with the University of Michigan seedling project. There seems to be a large gap between the thousands of MOFs but limited understanding of their synthesis or deeper chemical physics, and the LBNL team is trying to understand the subtle shifts in binding frequency and dependence in the new functionals studied. HyMARC investigates both aspects of MOFs, and LBNL has an excellent track record in synthesis; the project team should provide more leadership to the rest of HyMARC in identifying targets and discussing the suitability of candidates. Greater engagement by the LBNL team to provide leadership would assist HyMARC and strengthen the whole effort in certain domains.
- A number of nanoencapsulation methods are being employed to alter kinetics and perhaps thermodynamics while ensuring that the metal hydride particle size is maintained. Although some progress has been made, significant obstacles remain (e.g., a gravimetric penalty imposed by the encapsulant, poor sorption cycling, and sluggish kinetics). There seems to be no recognition of these problems, and unfortunately, the presentation does not describe future work that might address those issues. Likewise, the overall encapsulation effort seems to be largely decoupled from other nanostructuring work in HyMARC. Coordination among the related activities with other HyMARC investigators was not evident. The work on

porous BN is not compelling. In the original paper by Zhang, the adsorption binding energy for hydrogen in p-BN is very low (~65 meV/H_2). The binding energy was increased by lithium doping, but it still remained too low for practical applications. The present work does not provide a useful path forward.

- The Prendergast section of the presented materials suffers in focus and in apparent progress made. It is not clear whether this is in fact the case or whether the presentation was not constructed in a way to highlight the essential approaches and accomplishments that tie directly to HyMARC goals. The LBNL computational modeling effort was not described, and one must ask how this might be affecting experimental progress.

Recommendations for additions/deletions to project scope:

- It is too early to recommend deletions to the project scope. The scope is appropriate, and progress is reasonable for Phase II.
- It would be useful to conduct continuing evaluation of the durability of the rGO encapsulation (i.e., ensuring there is no change in rGO or in the MgBH compound composition and segregation). If the encapsulation approach fails to last, then modification of rGO or perhaps other encapsulants are needed.
- A much more compelling delineation of future work in the areas of nanoencapsulation, hydrogen carriers, and boron-based storage is needed. Future work should focus on critical issues and technical barriers. The team should eliminate the work on p-BN or present a much stronger case as to why the work should be continued.

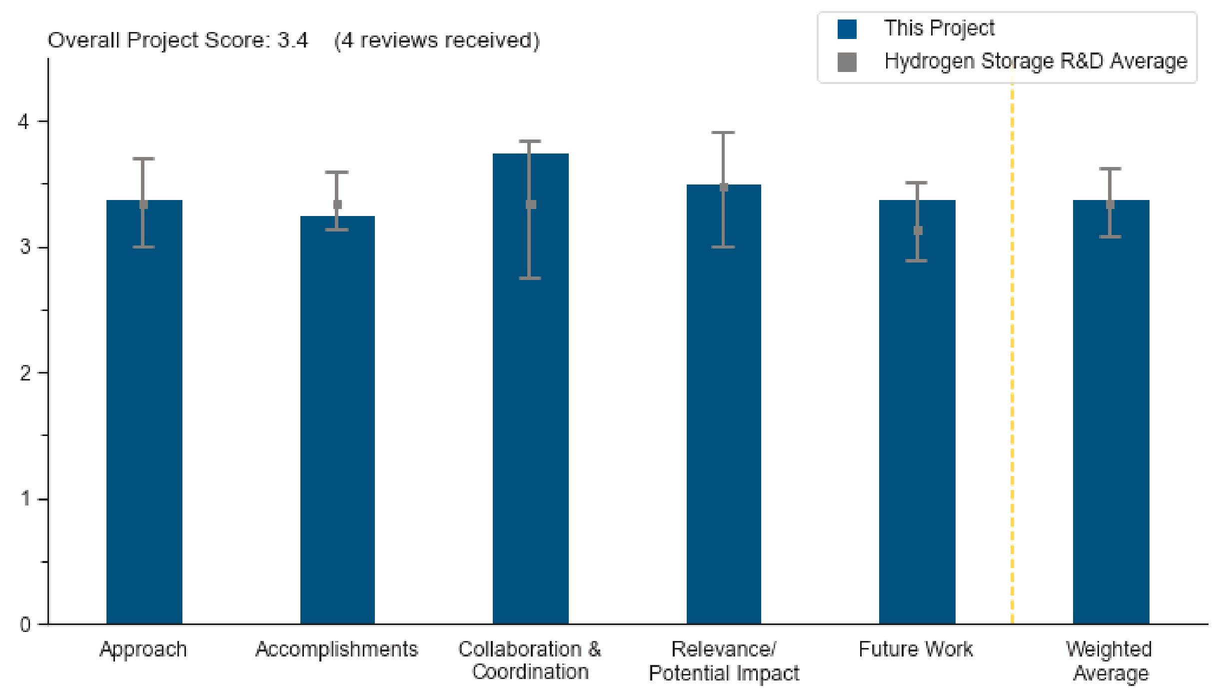
Project #ST-131: Hydrogen Materials–Advanced Research Consortium (HyMARC): National Renewable Energy Laboratory Technical Activities

Thomas Gennett, National Renewable Energy Laboratory

Brief Summary of Project

This project represents a collaboration between national laboratories to investigate the properties of promising new hydrogen storage materials and works in coordination with the Hydrogen Materials–Advanced Research Consortium (HyMARC) core team. The National Renewable Energy Laboratory (NREL) leads the collaboration, which includes Lawrence Berkeley National Laboratory (LBNL), Pacific Northwest National Laboratory (PNNL), and the National Institute of Standards and Technology (NIST). The objectives include the following: (1) develop new characterization capabilities such as nuclear magnetic resonance (NMR) spectroscopy, diffuse reflectance Fourier-transform infrared spectroscopy (DRIFTS), calorimetry, diffraction, and scattering, and (2) validate performance claims and theories critical to the design of new hydrogen storage materials.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach comprises tasks on advanced characterization and validation measurements, activation of B--B and B-H bonds in borohydrides using organic compound additives, and exploration of concepts employing adsorbents as hydrogen carriers. In addition, NREL provides characterization support and validation for HyMARC seedling projects and coordinates advanced characterization work at SLAC National Accelerator Laboratory. Although the characterization work is well focused on important problems and barriers, the materials effort seems disjointed and lacks a compelling strategy for addressing critical issues and obstacles.
    - The overall approach of the NREL project generally complements other related efforts in HyMARC. In addition, the project provides useful and important support for seedling projects. A

couple of research and development (R&D) topics that were not on a path to meet U.S. Department of Energy (DOE) goals were eliminated from the R&D portfolio in 2018–2019. This was a prudent decision that allowed the team to focus on more relevant problems.

- This is a multipronged approach with many chances to add value to DOE's program portfolio. All work is well aligned with goals. The project has clear goals. The emphasis on defining best techniques helps not only HyMARC but hydrogen storage work worldwide. Some of these are aimed at transport not onboard, which is helpful as well.
- This Standard Test Condition (STC) provides detailed thermodynamic measurement, including isosteric heat (Qst) data. These are valuable measurements for reliability in Van't Hoff measurements. This is especially important at high loading.
- The NREL approach slide contains 19 tasks to be dealt with in the near- to mid-term. This seems excessive, and in the absence of a corresponding clear rationale for each approach, it appears more like a shopping list than a well-thought-out plan to address the key barriers to "enabling twice the energy density for onboard storage." For many of these approaches, there was no high-level justification or rationale for the approach, and so it was difficult to assess the real potential of each item in the list to map onto a HyMARC thrust area, leading to progress toward DOE goals.
    - Here are examples of instances where a clear justification would help. The Task 2c approach did not set apart how NREL was going to distinguish the approach and potential outcomes from the effort of Severa et al. in exploring tetrahydrofuran (THF) as a donor ligand in the magnesium boride–borohydride system. Other examples lie in the hydrogen-carrier-focused activities. In the absence of DOE targets for hydrogen carriers, NREL could and should describe the potential for improving the quantity of hydrogen to be transported versus, for example, methylcyclohexane as a model benchmark for two-way carriers. The NREL approach for the porous liquids did come close to this by describing the potential benefits but did not address some type of analysis for each approach proposed (sorbents, BH_4/ionic liquids, etc.) that could prioritize the various efforts. This is true not just for the NREL effort in hydrogen carriers but within the associated HyMARC projects in general. In the absence of technical targets, an improved approach would factor in such prioritization.
    - An exception to this deficiency in developing a rationale for proposed work is in the work of Parilla, Hurst, et al. in describing the approach to solving the difficulty and errors in extraction of isosteric heats from adsorption data. The approach here is well defined, the relevance and impact were made abundantly clear, and progress was demonstrated.
    - Another exception was the clear rationale and justification given for the approach to the preliminary investigation of the plasmonic heating/hot electron project for obtaining "on demand" hydrogen release from magnesium borohydride.
    - If the latter two examples were not the exceptions, the NREL approach would receive a 3.5 or a 4.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Good progress was made in most project areas. Most notably, a better understanding of isosteric heat measurements was developed using a variable pressure-composition-temperature isotherm (PCT) apparatus. This reduces the possibilities for confusion, bias, and misinterpretation of adsorption results. A novel method for activating B-H/B-B bonds in MgB_2/$Mg(BH_4)_2$ using THF incorporation via vapor phase transport facilitated better control of THF concentration, thereby providing means to understand the role that the organic additive plays in enhancing hydrogen sorption reactions in the Mg-B-H system. New work on the use of adsorbents as hydrogen carriers ("porous liquids") is being explored as a means to deliver hydrogen-containing molecules in a more efficient and higher-capacity format. Advanced diagnostic capabilities at SLAC are now part of the core HyMARC effort. Although no results were reported, these capabilities will undoubtedly provide the consortium with a more robust and powerful suite of diagnostics for all aspects of the experimental effort. The NREL effort also provided beneficial support for multiple seedling projects. In general, the HyMARC program should be commended for its continued support of and contributions to seedling projects. The collaborations have been effective in accelerating progress on those projects.

- In addition to thermodynamic measurements, the group is working on understanding THF adduct in $Mg(BH_4)_2$. THF is introduced to $Mg(BH_4)_2$ by gaseous route. This is done to limit the amount of THF that is adsorbed. The vapor pressure of THF was controlled to ensure that it was bound in the structure (and not in excess). The results indicated that THF adducts alter the desorption pathway for hydrogen.
    - Additionally, unique work on liquid carriers is taking place within this project. The liquid phase is a "porous liquid" whereby porous nanoparticles are dispersed in a solvent. This work seems to be quite early. However, the potential for a different type of liquid carrier is promising here.
    - One of the major innovations in this portfolio is the release of hydrogen by on-demand heating of plasmonic nanoparticles. This work enables the use of a lower power source for hydrogen release. This is similar to ideas published on hydrogen release using microwave irradiation back in 2009 (see https://www.mri.psu.edu/sites/default/files/file_attach/212%29.pdf).
- The accomplishments of the work by Parilla, Hurst, et al. are top-notch. Their exacting work enables the adsorption community to extract isosteric heat information from data and to communicate results in this area more effectively and accurately, further enabling an "apples-to-apples" comparison of literature results.
    - The very preliminary results from the plasmonic "on-demand" release of hydrogen from magnesium borohydride is intriguing. The community awaits further characterization and quantification of how much hydrogen can be extracted per light pulse per gram of material and other details such as purity of hydrogen, etc. Also of interest is the additional characterization of the material. It is uncertain whether any chemistry occurs upon the deposition of TiN onto the borohydride and, if so, how that would influence the plasmonic response. It is intriguing, and it will be interesting to see more progress in this area.
    - In the area of developing new hydrogen carriers, NREL has made good progress in the synthesis of a few systems. However, it is not known how these systems stack up against other proposed two-way carriers in regard to energy efficiency, capacity, reversibility, etc.
- The project is making good progress in line with the plan. The research team developed cryo-PCT-based isosteric heat measurements, which will help develop better sorbents. At the same time, the team developed a technique to avoid temperature term bias and thus improper results. At the opposite end of the spectrum, the team developed a high-temperature PCT for accurate measurements in high-temperature systems.
    - The project improved the MgB system with precise amounts of THF to lower desorption temperature. Though more progress will be needed, this is still a new avenue to pursue. The project showed that low-energy light can be used to release hydrogen from the MgB system via the TiN layer.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- Solid collaborations with HyMARC core and seedling projects and external investigators are evident. The project is providing HyMARC with excellent support and expertise in advanced characterization, test protocols, and validation. The principal investigator (PI) serves as a co-leader of the recently consolidated consortium. This will help to ensure the coordination and management of the technical efforts in such a broadly based and multifaceted activity.
- Many collaborations are ongoing with NIST, SLAC, LBNL, PNNL, Sandia National Laboratories, and Lawrence Livermore National Laboratory team members. Additionally, collaborative projects are ongoing with Colorado School of Mines, University of Hawai‘i, and University of Geneva (Hans Hagemann and Angelina Gigante).
- There is significant collaboration inside and outside of the HyMARC group. There are collaborations with high-grade researchers—and in ways that help the project.
- In the work on the use of THF as a donor ligand to activate bonds in the Mg-B-H system, it was not clear if NREL was collaborating and/or communicating with the University of Hawai‘i or the PNNL groups. NREL has been active in supporting the needs of the seedling projects with NREL characterization capabilities. It appears the degree of collaboration outside of HyMARC is commensurate with the level of funding.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is going after some of the most innovative ideas in materials development. That means there is potential for high-risk–high-reward research. Currently, the porous liquids and on-demand hydrogen are developments unique to the HyMARC program led by this group. Additionally, the detailed thermodynamic measurement work is of high value and general interest to the hydrogen storage community.
- The project is an important component of the overall HyMARC activity. The project directly supports the goals of the Hydrogen and Fuel Cells Program. The advanced characterization capabilities and expertise at NREL provide DOE with a vital resource. The consolidation of the Hydrogen Storage Characterization Optimization Research Effort (HySCORE) and HyMARC programs has created a more sensible and natural "home" for the NREL materials efforts. However, additional work still needs to be done to more firmly establish the relevance and importance of the materials activities.
- There is a heavy emphasis on developing measurements and techniques to ensure the rest of HyMARC and, by extension, researchers worldwide obtain precise and dependable data. This is critical in an efficient march toward the DOE goals. Also, the project is completing highly relevant work in the new carriers area that will matter in the transport of hydrogen.
- The relevance and impact of the work by Parilla, Hurst, et al. are high, as the work has elucidated where errors can arise in the characterization of certain aspects of gas sorption on solids, and has addressed improvements and prescribed improvements in techniques and sorption instrumentation to mitigate these errors. The work is really first-rate.
    - In the new area of hydrogen carrier work, the proposed future work includes developing an analysis of what the thermodynamics "window" needs to be for effective hydrogen carriers. The current work would have likely been more impactful with some sense of prioritization had the researchers done this task first and then considered candidate systems. Absent some set of metrics, it is difficult to assess whether the systems the team has chosen will be relevant.
    - NREL's impact in the area of using THF as a donor ligand to alter the kinetics of hydrogen uptake/release in the Mg-B-H system is difficult to assess without a cogent discussion as to how NREL is starting where the University of Hawaiʻi left off or how the preliminary results contrast and/or amplify the results of Severa and PNNL.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- NREL's role in providing improved methodologies and validation of sorption measurements of promising adsorbents is clearly a high-priority item for the hydrogen storage community.
    - The future work on hydrogen carriers will now benefit from the inclusion of a preliminary thermodynamics analysis of carrier properties, coupled with the LBNL and Argonne National Laboratory technoeconomic analyses, which are apparently ongoing. NREL's future work in carriers may benefit from applying these analyses before getting too far down the road on carrier synthesis and characterization.
    - There was not a mention of what the future plans are for this intriguing plasmonic-induced release of hydrogen from magnesium borohydride. It is to be hoped that a thorough characterization of the materials and the products can lead to more interesting results in this area.
- The future work capitalizes on earlier results with further optimization and introduction of new characterization techniques. These are all useful directions. At this stage in the HyMARC portfolio for this project (at the start of Year 2 of 5), it may be too conservative of a plan (i.e., to optimize and characterize the novel materials developed in Year 1 or earlier years). Because the team is less than halfway through its five-year grant period, additional exploration of innovative materials concepts could be more suitable (particularly given the innovative ideas put forth so far). Support for seedlings is also planned for the future. This is also good.

- The future work is a logical extension of the prior studies. It is concerning that the second bullet in slide 23 (future work) describes further developments of polyetheretherketone (PEEK) materials. However, apart from a statement that a no-go decision was made on compaction, PEEK materials were not mentioned in the presentation. It is not clear why the metal–catechol modified materials are being explored or what the impact would be if successful. Also, a more compelling argument for the inclusion of the plasmonic hydrogen release activity would be helpful. Although it is an intriguing result, the impact and value to the HyMARC activity, or where or how the plasmonic hydrogen release activity fits in, are not especially clear.
- There are suitable and broad future work plans with gates.

Project strengths:

- Thus far, the merger of the HyMARC and HySCORE efforts appears to be successful—kudos to both teams for making a relatively seamless transition to a less complex and confusing organizational structure. The NREL team brings important expertise and experimental capabilities to the HyMARC core team and seedling efforts. Incorporation of SLAC into the overall effort should provide access to additional sophisticated diagnostics.
- The NREL work of Parilla, Hurst, et al. on sorption methodologies and validation is world-class.
- Truly, this project stood out among most of the others for the innovative concepts in materials development.
- The project strengths include facilities, people, and alignment with laboratory strengths. The project activities are excellent.

Project weaknesses:

- It is not clear where the work on PEEK materials is heading. Apart from a no-go decision regarding compaction, PEEK materials were not highlighted in the presentation. However, the PEEK work is included in the Future Work slide. Clarification and justification for continuing that effort are needed. Although the results on the new plasmonic hydrogen release activity are interesting, a more compelling justification regarding the potential impact of that work and how it fits into the overall HyMARC mission should be provided.
    - Overall, the materials work seems to represent several largely fragmented and uncoordinated activities. The PI is urged to work closely with other members of the HyMARC team to create a unifying framework for the materials efforts to ensure that they are truly relevant to the overall mission of the consortium.
- The future work could be more ambitious on the materials development side of things (at this stage). Much of the future work presented in slide 23 is optimization and validation.
- The use of photonic material as onboard with a flow system is fraught with difficulty. It may not be worth the effort, and the team should at least consult the Hydrogen Storage Engineering Center of Excellence results in this area before trying. The project should continue to work on the material.
- It is unclear where the THF/Mg-B-H system is heading, and this effort could use better justification to strengthen the case for continued research.

Recommendations for additions/deletions to project scope:

- Without a more compelling justification for continuing the work, a no-go decision on PEEK materials is recommended. It is unclear whether the NMR capabilities at NREL are available for more extensive support of the HyMARC activities. It is apparent that the overall HyMARC effort is in serious need of additional NMR support. Perhaps NREL could provide that support.
- The project team should consider a reasonable design for a dehydrogenation unit using the photonic material at a station or other use point so that the material is a carrier.

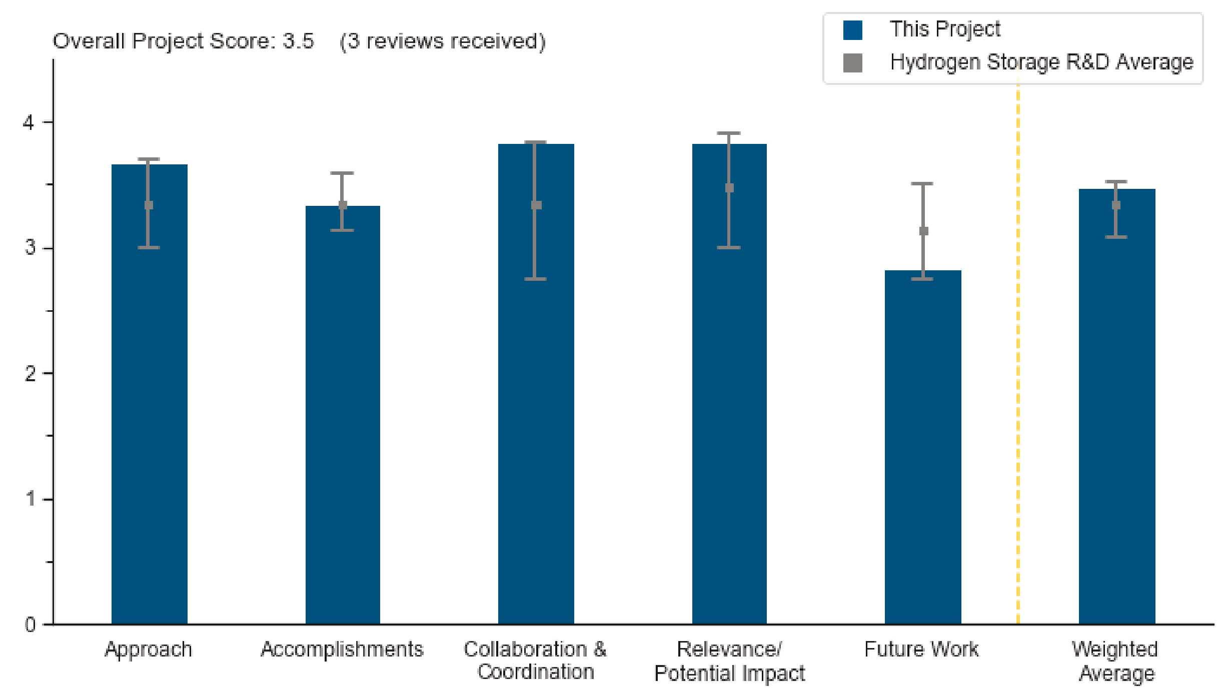
Project #ST-132: Hydrogen Materials–Advanced Research Consortium (HyMARC): Pacific Northwest National Laboratory Technical Activities

Tom Autrey, Pacific Northwest National Laboratory

Brief Summary of Project

This project is part of a collaboration between national laboratories to develop new characterization capabilities to investigate the properties of promising new hydrogen storage materials. The project works in coordination with the Hydrogen Materials–Advanced Research Consortium (HyMARC) core team. Pacific Northwest National Laboratory (PNNL) will focus on nuclear magnetic resonance (NMR) spectroscopy and calorimetry to complement parallel efforts at other national laboratories. The project will also work toward validating claims and theories critical to the design of new hydrogen storage materials that show promise.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is broadly based and comprehensive, and it addresses issues that are important and relevant to U.S. Department of Energy objectives. PNNL serves as the focal point for the emerging effort on hydrogen carriers. The principal investigator (PI) and collaborators have formulated a solid research plan devoted to development of novel concepts and materials. This will undoubtedly be a critical research and development (R&D) area for HyMARC in the future. The approach on complex hydrides focuses the role of organic additives on sorption reactions in the Mg-B-H system. The effort augments the work at the University of Hawaiʻi and elsewhere in HyMARC. The PNNL team brings valuable synthetic chemistry and mechanistic understanding to this potentially important research topic. Advanced synthesis characterization capabilities (e.g., high-pressure reactors and high-pressure in situ NMR) are being used effectively to measure thermodynamic properties, rates, and cycling efficiency and to identify/characterize intermediates in all experimental elements of the project. In addition, the approach includes extensive support for seedling projects. (Seedling support is a hallmark of HyMARC; PNNL and the entire HyMARC team are commended for supporting and reinforcing the seedling activities in such a valuable way.)

- The PNNL approach utilizes a demonstrated close coupling of computational modeling with experiment. PNNL's approach is a chemical sciences approach, which is highly complementary to the general materials science approach of the overall HyMARC effort. PNNL brings to bear its capabilities, expertise, and deep knowledge of chemically reacting systems to provide chemical intuition and insight into the breadth of topics involved in storage of hydrogen in complex metal hydride compounds. PNNL also brings its world-class NMR capabilities to bear on HyMARC problems.
- The general theme here is to pose a good question and then to use the team or find expertise and partnerships to find the answer. This team is extremely efficient at conducting this process. This has led the team to extremely useful findings in the borohydrides. The team is poised to make new discoveries in the liquid carriers.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- PNNL's computational modeling of the energy landscape of the multiplicity of possible chemical reaction networks interconnecting magnesium borohydride with one of the intermediate products, decaborane, has provided new insights into the most likely pathways, and then suggests experimental approaches to validate potential pathways via spectroscopic techniques. These are important contributions to understanding the initial steps in dehydrogenation of magnesium borohydride and also understanding where the thermodynamic "traps" lie.
  - Using experiments supported by the laboratory's capability in solid-state NMR, PNNL has found that the presence of MgH_2 influence leads to the lower-temperature, lower-pressure regeneration of magnesium borohydride from magnesium triborane. This piece of experimental work contributes important additional experimental evidence to support a piece of the puzzle regarding the energy landscape of the Mg-B-H system in the early stages of dehydrogenation or, conversely, the late stages of regeneration of dehydrogenated material. This presumably allows for the "benchmarking" of the PNNL computational modeling effort that is ongoing in parallel. In parallel, PNNL is performing a detailed "postmortem" of the reaction products from the regeneration of magnesium triborane to look for minor products that arise during reaction. This is anticipated to again provide additional support to the development of more detailed understanding of the energy landscape that drives the chemical reaction pathways in the rehydrogenation of light polyboranes, as well as the early stages of dehydrogenation.
  - PNNL is conducting collaborative work with the Severa et al. group at the University of Hawai‘i on how the influence of a donor ligand such as tetrahydrofuran (THF) can alter reaction pathways. This work is providing insight into the role of THF. How the ratio of THF:$Mg(BH_4)_2$ influences the recyclability has been explored in some detail using the combination of X-ray powder diffraction (XRD) and variable-temperature, high-field NMR.
  - In the area of hydrogen carriers, an H2@Scale activity, PNNL has taken on a leadership role. A technoeconomic analysis (TEA) activity has been initiated with Lawrence Berkeley National Laboratory (LBNL) and Argonne National Laboratory (ANL) that will, in the future, focus any R&D effort that may be required. This activity needs to be accelerated, as there are many nascent experimental activities under way across HyMARC, and it is not clear that these independent activities are prioritized or justified against technological needs or with regard to technological potential. ANL has shown in a preliminary analysis that "one-way" carriers may be more economically viable than "two-way" carriers; PNNL appears focused on one-way carriers, which may be the right niche to distinguish HyMARC's approach in this area from the many others that are cropping up. PNNL, LBNL, and ANL need to get out in front of this—quickly.
  - PNNL's activities on one-way carriers appear intriguing, as the use of electrochemical approaches to regenerate carriers and to release hydrogen at pressure (electrochemical compression) appears intriguing; but these activities must, in the near future, be backed up by detailed TEA of the round-trip costs and efficiencies from "well" to city gate. While little of this electrochemistry is new, the

utilization of non-hydrogen pathways and electrochemical compression of the hydrogen released and the integration of these processes may be novel.

    - In PNNL's work on the computational modeling of hydrogen sorbed in metal containing open framework materials, it was not clear if this was being done in collaboration with the LBNL effort (J. Long). While the work is of high quality and topical, it appeared to be a bit of an outlier in PNNL's overall approach in supporting HyMARC activities. The reviewer-only slides provide additional information on the collaboration with LBNL using PNNL's high-pressure Magic Angle Spinning (MAS) NMR capability and also looking at hydrogen diffusion in open framework materials using pulsed field gradient (PFG) techniques. More details of the extent of the collaboration will likely emerge as this activity matures, and perhaps it will include this tie to the computational modeling effort at PNNL and how it fits in with what M. Head-Gordon is doing with J. Long at LBNL.
- Solid progress was made in all project areas. The PNNL team is off to a great start on hydrogen carrier development. The team members have proposed a range of novel concepts and approaches, and they are working in close collaboration with other HyMARC investigators to develop those ideas further and to identify critical materials needs and challenges. The PI is working closely with other collaborators to understand the role of organic additives on Mg-B-H sorption reaction kinetics and cycling efficiency. This is currently one of the more promising approaches to improving reaction kinetics, and the PNNL team is providing vital chemistry expertise and experimental resources to the effort. In related work, both theoretical/modeling and experimental work (mainly in situ NMR) are being used to understand reaction pathways and ways to activate B-B and B-H bonds. A candid assessment of remaining challenges and barriers serves as a useful means to motivate the technical activities.
- The research group is very good at locating partners and establishing collaborations for characterization. An effective example of this is using NMR to understand what is occurring in borohydrides. It was discovered that the B-B bond activation rate is limiting for re-hydrogenation. Coupled with thermodynamic modeling and solution NMR, these studies have provided researchers with the ability to tackle borohydride re-activation and reaction pathways.
    - The borohydrides are just one example. Another is the use of chemical hydrides (hydrogen carriers) such as formic acid. Earlier work done on formic acid showed that catalysts such as Pd (see Krame, Levy, and Warshawsky, 1994) and iron (see Laurenczy, *Science* 2011) are extremely important to the formate/bicarbonate cycle and to H_2/CO_2 production. This work instead utilizes electrocatalytic regeneration. Little is discussed related to the catalysts that were effective (slide 18).

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The group is very good at locating partners and establishing collaborations for characterization. The team has developed international partnerships with the Korea Institute of Science and Technology, the Association for Iron & Steel Technology, and the Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research (HZG). The interaction with seedlings (the University of Hawai‘i) on borohydride regeneration is one of the high-profile outcomes of seedling support. Other interactions with seedlings seem to be under way in the form of thermodynamic modeling and NMR characterization.
- Extensive and valuable collaborations with HyMARC core and seedling activities and with external R&D institutions are evident. Those collaborations are extending the scope of the investigations and accelerating progress. The technical effort is well managed and coordinated.
- A forte of PNNL's efforts in support of HyMARC is their demonstrated participation in collaboration, both within HyMARC and with external global scientific collaborations. The quality of several of the collaborations is confirmed by the number of joint publications that have arisen.

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project is an important component of the overall HyMARC activity. The project is focused on issues that are directly aligned with the goals and objectives of the DOE Hydrogen and Fuel Cells Program. The inclusion of PNNL in the consolidated HyMARC effort brings valuable chemistry synthesis expertise, mechanistic understanding, and advanced diagnostics capabilities to the consortium.
- The PNNL effort in computational modeling of the early stages of magnesium borohydride dehydrogenation (or the reverse reactions) is highly complementary to the theory effort at Lawrence Livermore National Laboratory (Wood et al.). These parallel activities have potential to gain insights more rapidly into the underlying chemical and physical barriers that limit the kinetics of hydrogen release and reversibility in the Mg-B-H system.
- The project set has already made a major impact on understanding borohydrides and is poised to lead in liquid hydrogen carriers work. So long as the team has the ability to attract and assemble the best expertise (worldwide) on the topics it pursues, it will continue to make great impacts.
- PNNL's expertise in chemistry and reaction mechanisms, collaborations, and experimental capabilities have a significant impact across many HyMARC activities and are accelerating progress.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- Liquid hydrogen carriers is a new component of the portfolio. It is a relatively new area and has the ability to encompass work in the hydrides (with adduct formation) to formic acid. The researchers have the relevant tools necessary to tackle these problems. Characterizing the amorphous phases formed by XRD or PDF (Pair Wise Distribution Function) could be added as a logical next step.
- The proposed future work flows logically from the prior research efforts. The work on the Mg-B-H system remains focused on developing understanding of the effect of side reactions, byproducts, additives, etc. on the reaction pathways that relate to hydrogen release and reversibility and kinetics limitations in this material. The future work should include some urgency in developing a detailed TEA to help guide HyMARC experimental activities in hydrogen carriers to enable prioritization and down-selection criteria. Ideally, this would have occurred prior to starting an experimental program, so now the team must catch up quickly.
- Unfortunately, the future work is not summarized in a single slide. Although some future plans are incorporated into the narrative in a few selected slides, it is difficult to extract that information for the entire project. It is probably safe to assume that slide 21 (Remaining Challenges and Barriers) provides the motivation for future work, but what will actually be done to address those obstacles remains uncertain in most cases. It would be helpful to include a Future Work summary slide that succinctly states the future work in a compelling way.

Project strengths:

- The research group has assembled a unique toolset for pursuing advanced materials. The tools include solid-state and solution NMR and thermodynamic modeling and experimental data. The scientific output has resulted in numerous publications in 2018 and 2019 alone. The group is collaborating with those from around the world who can bring insights to the problems under study. It is a wonderful idea to categorize the liquid hydrogen carriers more broadly (as in, to include adducted borohydrides) and to pursue them with the same tools as other liquid carriers (i.e., formic acid). This section of the portfolio appears to have risen out of the ammonia work done in 2004–2010—but is now extended to more promising liquid carriers.
- The PNNL team is experienced and highly qualified. The team brings valuable synthetic chemistry expertise and mechanistic understanding as well as advanced and novel characterization capabilities to HyMARC. The team has demonstrated the ability to adapt quickly and shift to new R&D problems and opportunities. This is contributing to the overall value and importance of the PNNL effort to HyMARC.

The PNNL team has assumed the leadership role in HyMARC for hydrogen carrier work. The involvement of experienced chemists at PNNL in that technology area will undoubtedly pay big dividends for HyMARC.

- The PNNL effort provides a good deal of chemical expertise, intuition, and state-of-the-art NMR characterization capabilities for gaining a detailed understanding of the critical bond-breaking and bond-making pathways, where potential kinetics barriers may exist, and where thermodynamics traps may lie in the very complicated Mg-B-H system. These are important strengths of the project and, coupled with PNNL's ability to coordinate and integrate the laboratory team's efforts and results with those of others within HyMARC, amplify the project impact.

Project weaknesses:

- The activities themselves have few weaknesses. The project reporting has many.
    - For example, on slide 9, it is impossible to read the x-axis for the data presented in the graph on the right-hand side of the page.
    - Slide 14 mentions TEA without any definition. Within this context (of adding liquids to borohydrides and also using these liquids directly as hydrogen carriers), TEA could represent triethylamine. It was not until the review presentation that TEA was defined as technoeconomic analysis. Since an entire slide title (slide 14) is about TEA (with the take-home message related to TEA), it would have made sense to spell this out earlier.
    - There is little time in the review to provide background and context to the studies; however, it would have been useful to mention earlier work done (since 1994 by Krame, Levy, and Warshawsky and since 2011 by Gabor Laurenczy) on the liquid hydrogen carriers under study in this project.
- A more complete and compelling presentation of future work in all PNNL project areas is needed. Also, there is a general comment for HyMARC (not a PNNL project weakness, per se): As pointed out in other HyMARC team reviews, slow kinetics remains the most critical obstacle to adoption of high-capacity complex metal hydrides for practical hydrogen storage applications. Although multiple research efforts (both theory and experimental) are being devoted to the problem, there is no clear strategy that rationally and objectively addresses the critical issues. PNNL is strongly urged to work closely with the rest of the HyMARC team to develop a coherent and rational pathway to addressing this critical challenge.

Recommendations for additions/deletions to project scope:

- It is apparent that the overall HyMARC experimental effort is limited by the lack of NMR instrumentation. Although PNNL's NMR capabilities are powerful and are advertised as important support resources for the HyMARC program, it seems that those capabilities are not readily available in a dedicated and timely way for HyMARC work. The PNNL NMR system(s) also support other major programs, so HyMARC work may be getting lower priority. Perhaps the PNNL project team and DOE Hydrogen and Fuel Cells Program could exert pressure on PNNL management to make these valuable resources more readily accessible to HyMARC. Clearly this is a thorny political issue, but nonetheless, it is crucial to find a way to free more NMR time, either at PNNL or elsewhere, to support HyMARC.
- It is recommended that PNNL, in its leadership role in the hydrogen carrier HyMARC effort, accelerate the TEA activity to provide guidance to the experimental efforts that are arising. Targets or down-select criteria must be determined quickly so that experimental efforts are not wasted on carrier concepts that cannot lead to the desired outcomes.

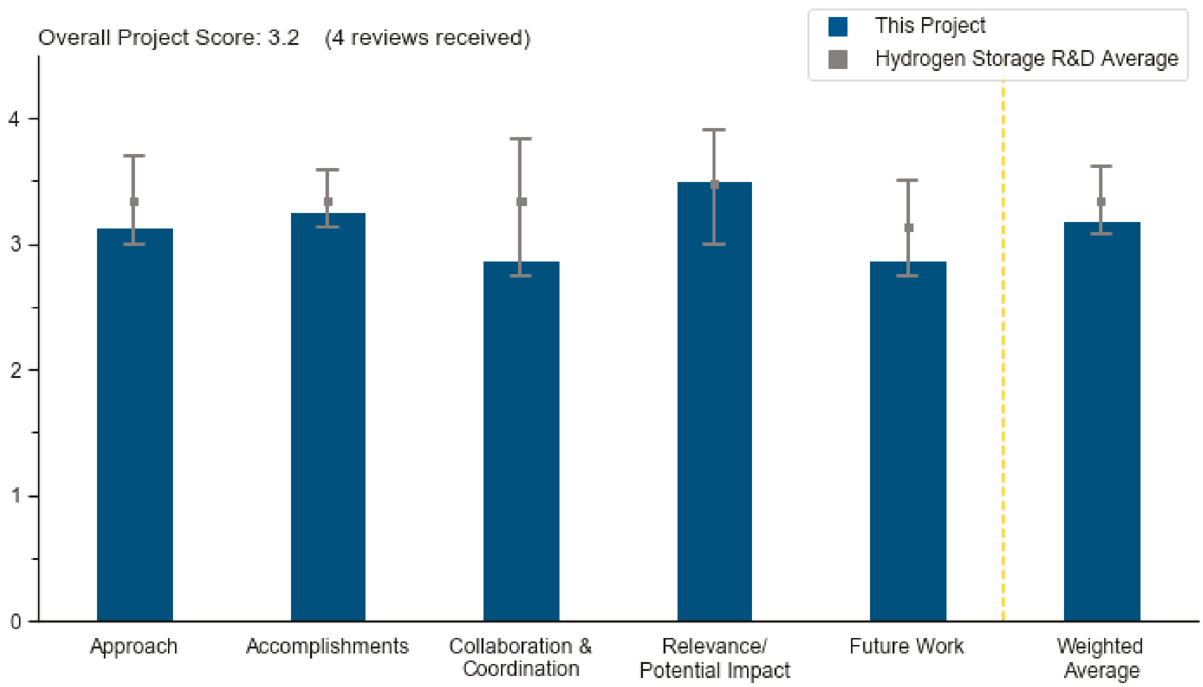
Project #ST-137: Hydrogen Materials–Advanced Research Consortium (HyMARC) Seedling: Electrolyte-Assisted Hydrogen Storage Reactions

Simon Jones, Liox Power

Brief Summary of Project

The project will address kinetics of multiphase hydrogen storage reactions that are severely limited. The project seeks to overcome kinetic barriers of hydrogen storage candidates with high capacities (and appropriate thermodynamics) for polymer electrolyte membrane fuel cell use that otherwise contain multiple solid phases that must nucleate, grow, and be consumed during cycling. The reaction rate and transport of solid-state reactions are limited by relatively small solid–solid interfacial surface area. The project will instead use electrolyte-assisted hydrogen storage reactions that facilitate transport and enable the reaction to occur over the full surface area that is exposed to the electrolyte. Salt and borohydride electrolytes, which are the most stable for this application, will be used to promote solubilization and diffusion of species relevant to hydrogen storage release and uptake. The work will improve understanding of hydrogen physisorption and chemisorption.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach for this project is novel and could provide use for previously problematic materials. The approach does well to consider the full material density, which will provide a more honest performance of the material. Investigating combinations that can operate at a lower pressure, allowing the project to bring the testing in-house instead of relying on other laboratories, will probably save cost and increase throughput.
- The project takes a unique approach to overcoming kinetic barriers in hydrides through the addition of molten salts. This approach is analogous to additions of tetrahydrofuran (THF). However, THF forms adducts with hydrides that are not easily reversed. The use of molten salts could avoid this problem.

Additionally, fewer organic solvents are available that are compatible with the hydrides relative to the selection of molten salts.

- The approach attempts to address the key barrier to the storage of hydrogen using complex metal hydrides, i.e., the kinetics of release and rehydrogenation of spent material. In previous results from this project, the effect of solvents was shown to overcome, in part, intra-particle and particle surface diffusion limitations of reacting species in multiphasic, solid-state materials such as in the Mg-B-H system. To follow on, the team's approach will involve trying to optimize (i.e., minimize) the amount of solvent required to mitigate, to the extent possible, the weight penalty of adding solvent to the material. Additionally, the team proposes to screen additional materials that exhibit kinetics limitations and have hydrogen contents of >4 wt.%. In its published work, the team has demonstrated that the presence of a solvent/electrolyte in a model system (MgH_2/Sn) improves the hydrogen release rate by 25 times. This result is impressive but perhaps one to two orders of magnitude short of the rates required for onboard storage applications using a more realistic higher-capacity material. More work on higher-capacity materials is warranted, and so this approach continues to be of interest. The approach for exploring molten low-temperature eutectics as solvents is well thought out and is backed up with careful considerations of the prevailing thermodynamics constraints to select potential candidates for additional study. In a third approach, the team proposes to evaluate electrochemical reactions to supplement or supersede thermochemical approaches to hydrogen release from complex metal hydrides. This approach needs better definition as to what is intended; for example, the team does not explicitly define a source for the electrochemical driving force. A detailed schematic of the process and an energy balance is needed to describe this opportunity to supersede onboard, closed system thermochemical approaches to hydrogen release.
- The approach is novel and untried; it decouples the evolution of hydrogen from the formation of byproduct while greatly increasing the area available for reaction in both generating and receiving moieties. Of course, this approach will lower the mass percent by adding electrolyte but will have a minor impact on volumetric storage, so it could be useful for transport of hydrogen. Expanding the search to other systems of materials will help the chance of success. On the negative side, the team has yet to prove its conceptual model is correct. Until the researchers determine whether the liquid phase is merely a solvent increasing mass transport or an electrolyte facilitating ion transport, they cannot readily pick the right solvent and salts. Likewise, for the electrically assisted desorption, the team needs to verify whether it is indeed oxidizing BH_4 species and, thus, every hydrogen requires an electron, or if it is in some way catalyzing the production of hydrogen with less than one electron per BH_4.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team has completed a careful assessment of several materials against logical, well-justified criteria. Using literature thermodynamics data for hydrogen release and regeneration along with best estimates of kinetics from literature studies, the team has prioritized a number of candidates for further study. These materials have enough "head room" to add small quantities of low melting eutectics as solvent and still result in useful capacities. Armed with this list, the team is moving forward to assess these down-selected candidates in the presence and absence of added solvent. The quality of this work is demonstrated by a recent peer-reviewed publication of preliminary project results in the *Journal of Physical Chemistry C*. The team has made progress in performing additional studies on the hydrogenation of magnesium diboride, including MgB_2 with additives, or catalysts. The work has shown that, in the presence of a ternary iodide eutectic, MgB_2 with additives may be rehydrogenated to mixtures of magnesium borohydride and dodecaborane at reduced pressure of 700 bar versus 1.0 kbar in the absence of additives. Experiments are in progress to examine more carefully whether the quantity of the problematic thermodynamic trap, dodecaborane, can be minimized at lower temperatures and pressures. The team has fabricated and tested, in a proof-of-principle experiment, an electrochemical cell for the electrolysis of Li/K borohydride eutectic to produce hydrogen and some diborane from the electrochemical oxidation of borohydride. More details of how this approach to the onboard generation of hydrogen will have an impact on the overall onboard, closed system energy balance are hoped to be forthcoming.
- The assessment of electrolyte-assisted systems with 4 wt.% capacity appears to be very thorough and well done. Much consideration has gone into the analysis, providing a strong understanding of the systems. The

work related to reducing the pressure required for hydrogenation reactions is encouraging, especially since the principal investigator will be able to perform the testing in his own laboratory, thereby increasing throughput. The electrochemical work is interesting. Further work is required to understand the advantages of this storage method over conventional batteries.

- The researchers are making good progress. They have found, based on rational screening criteria, that several known systems could work well in this method. The team is following the test plan on lowering pressure and temperature in MgB system cycling. Furthermore, the team has developed apparatus for current testing.
- The research has shown nice results reporting rehydrogenation of MgB_2 in molten salts. The kinetics are still sluggish because the rehydrogenation takes 50 hours. Still, this points to promising rehydrogenation schemes that overcome diffusion limitations for ions.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration with Sandia National Laboratories (SNL) on the application of SNL's high-pressure hydrogen capabilities to the rehydrogenation of magnesium diboride has been effective and crucial to the team's success to date. Overall, the level of collaboration is commensurate with the budget and scope of the project.
- The collaboration between partners seems adequate, but there was not much collaboration outside the project.
- The project is a collaboration between California Institute of Technology, HRL Laboratories, LLC,, and Liox Power, Inc., with one Hydrogen Materials—Advanced Research Consortium (HyMARC) collaborator (Vitalie Stavila of SNL). The work would benefit from the characterization and computational tools available at other HyMARC partners.
- The team's collaboration with other HyMARC members could be improved. Though it is understood that this is a niche application for hydrogen storage, the utilization of HyMARC capabilities is highly encouraged.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project has led to new ways of thinking about mass transfer diffusion limitation mitigation in systems with complex reactions (e.g., the Mg-B-H system). The use of low melting eutectics as solvents has led to significant increases in dehydrogenation and rehydrogenation reaction rates. This effort has led to progress against the difficult problems represented by the sluggish kinetics of hydrogen release and reuptake in the Mg-B-H system—perhaps more progress than any other project in the HyMARC sphere of internal projects and seedlings.
- This project is doing great work toward developing an understanding of the hydrogenation and dehydrogenation processes that are both severely limited on their own, as well as with electrolytes added to assist the reactions. If the reactions can be performed at considerably lower pressures and maintain their overall capacity, there could be significant impacts on storage space.
- Previously discarded systems can be taken and made viable by lowering pressure and temperature requirements and increasing kinetics. The project is well aligned with current Hydrogen and Fuel Cells Program goals.
- The use of molten salts to aid in ionic kinetics is a novel idea. Molten salts provide a wide parameter space for lowering the pressure and temperature for MgB_2 recharge.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The proposed future work is encouraging, especially the improvements to MgB_2 uptake and the electrolyte-to-active-material ratio. The practical application of such a system is of great interest and will allow for the system tradeoffs to be identified. A practical application will also allow for a better range of material applications to be identified and test the suitability for vehicular applications.
- The team's future work follows logically from its preliminary work in Phase 1 and the subsequent period. The team continues to focus on the key problems that are inherent to employing additional mass to a material system while maximizing the benefits from the weight penalty of added solvent. In the project's future work on electrochemically driven hydrogen evolution from metal hydrides, it is suggested that the team provide a clear picture of how this will work in the vehicle system framework.
- The proposed future work is consistent with the outcomes.
- If the model is correct, the plan is viable. However, it is difficult to assess the validity of the model based on the data presented.

Project strengths:

- This project has a novel approach with the potential to change many aspects of the hydrogen charging and discharging process. The project team includes strong investigators with notable records of accomplishment. Since there are several chemical systems to pursue, there are many ways for the team to succeed.
- The team is excellent. The approach to developing low melting eutectics as solvents is well thought out. The team has developed well-considered selection criteria to determine which materials can best take advantage of the inclusion of a solvent to enhance the kinetics of hydrogen release/reuptake and have potentially practical applications.
- The project is very thorough. A great deal of attention has been paid to the details of this work, allowing for a strong understanding to be developed. Good progress has been made that enables future work, especially the reduced pressure operation of the reactions.
- Theoretically, the use of molten salts should work. These studies provide a wide parameter space (i.e., the molten salt and hydride system vary).

Project weaknesses:

- The project seems to have focused more on the assessment of materials rather than the empirical assessment of the materials, making the results look a little thin. It is important to understand which systems have the potential to work. Weeding out systems that are unlikely to work will hopefully speed experimental progress. The electrochemically driven system needs more justification; its advantages over other electrochemical systems are unclear. The plan to study materials at a practical level may be premature, as the performance at large quantities may not be understood sufficiently to make an accurate assessment.
- The team's commercial partner seems to be rather uninvolved. The team has not shown that the liquid is acting as an electrolyte. If the electrolytically assisted desorption works by BH_4 oxidation, then every electron made in the fuel cell will need to run through the storage system. This makes sense only if the voltage drop extracted is very small. Even if the investigators are correct, there are many parameters to consider, such as secondary (chemical) effects of electrolyte, possible catalysts, choice of base system, etc. Choosing the correct parameters is potentially a complex puzzle.
- The project lacks theory to guide the selection of additives (slide 11). Likewise, other factors should be considered. For example, the capillary forces between the particles that drive ionic motion (slide 2) could be important.
- The strategy of the electrolysis of metal hydrides to supersede thermochemically driven hydrogen release is unclear.

Recommendations for additions/deletions to project scope:

- First and foremost, the team should study the system in operando and verify the presence of the correct ions at the right concentration to be consistent with $Mg(BH_4)_2$ creation or desorption according to the project model. If the model is confirmed, the team should proceed. Otherwise, the team should regroup to determine the best solvent and salt if the liquid is a solvent, not an electrolyte. If this work has already been completed and was not presented, then there is no need to repeat it. The team should determine how many hydrogen molecules are produced per coulomb in the electrically assisted desorption of hydrogen. Unless there is far more than one hydrogen molecule for every two electrons, then the voltage should be measured or estimated. If there is found to be one electron per hydrogen molecule, as implied, and if the voltage is more than, say, 10% of the voltage in a single fuel cell plate, then the parasitic load is too high to be practical, and the electrically assisted work should be dropped. If the voltage drop is minimal or many hydrogen molecules are released with one electron, then the work should be continued. The team may consider removing material in various levels of hydrogenation and characterizing the particles to look for inhibiting layers or changes in morphology or other factors that might be stopping or greatly slowing uptake.
- A study of electrochemically driven hydrogen cycling compared to other electrochemical devices, such as batteries, should be done to identify the advantages (or disadvantages) of such a system. The team should focus especially on gravimetric efficiency and overall system efficiency when paired to a fuel cell. A practical study should be deferred until a better understanding has been gained and a more appropriate system demonstration has been performed.

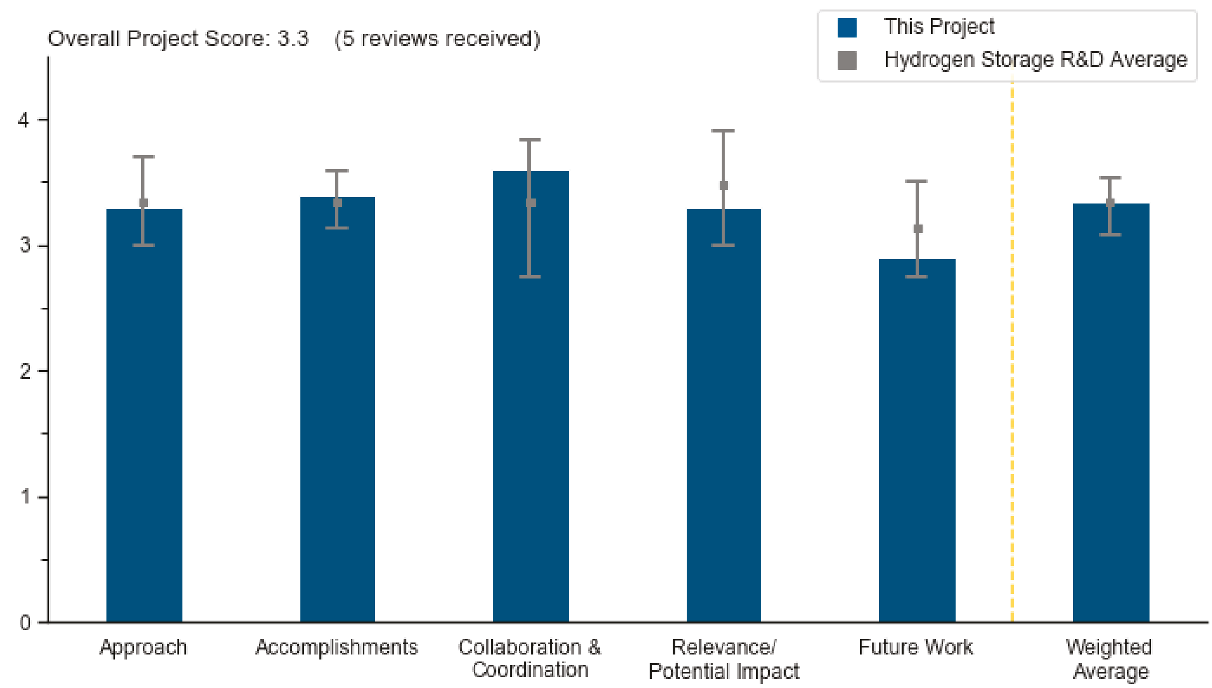
Project #ST-143: Hydrogen Materials–Advanced Research Consortium (HyMARC) Seedling: Atomic Layer Deposition Synthesis of Novel Nanostructured Metal Borohydrides

Steven Christensen, National Renewable Energy Laboratory

Brief Summary of Project

Metal borohydrides (MBHs) such as $Mg(BH_4)_2$ possess high hydrogen storage capacity but insufficient charging/discharging rates and cyclability for U.S. Department of Energy targets. The project seeks to improve cycling/reversibility by increasing cycle life and to improve charging/discharging rates/kinetics. The project will achieve its objectives by incorporating a durable nanostructured phase and chemical additives that enhance reaction rates. The project team will use atomic layer deposition (ALD) to give the MBH a hard permeable coating to retain the nanostructured MBH phase for cyclability, as well as to catalyze the MBH using a thin layer of additives that enhance rates. The project addresses barriers associated with durability/operability, charging/discharging rates, and the lack of understanding of hydrogen chemisorption.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an exciting approach: encapsulating metal hydrides within permeable oxide layers for the purpose of protecting the air-sensitive hydrides. Given the results of recent X-ray photoelectron spectroscopy (XPS) data regarding the structure of the surface of $NaAlH_4$ during dehydrogenation, Al-O-H phases are predicted to play a more significant role in the desorption process. It begs the question whether the alumina protective layers are also aiding in the surface rearrangement (by seeding Al-O regions) to aid in desorption.
- This seedling takes a different approach to nanoconfinement of complex metal hydrides, which is thought to enhance the kinetics of hydrogen release and/or alter the thermodynamics of multiphasic interactions in

the reacting material(s). The use of ALD to coat a complex metal hydride with an inert or possibly catalytic confining coating to enhance release and/or reversibility is an intriguing approach. Given that this is a seedling with limited funding and hence limited time, the scope of the approach is appropriate.

- The project approach is very strong and provides a solid foundation for investigating the coatings of MBHs. The use of ALD to coat the particles is clever, as is the methodology for understanding the mechanism for charging and discharging of the materials.
- The approach is interesting and innovative. It focuses on improving hydrogen sorption kinetics and cycling efficiency in nanostructured $Mg(BH_4)_2$ by using thin coatings formed by ALD to prevent particle agglomeration and serve as catalytic agents to enhance hydrogen sorption reaction rates and improve reversibility. ALD is a well-established technique for depositing thin films and coatings with single-atomic-layer precision. $Mg(BH_4)_2$ nanoparticles are provided by Sandia National Laboratories (SNL) as part of the Hydrogen Materials–Advanced Research Consortium (HyMARC) activity. That being stated, recent results, although provocative and potentially important, raise many questions that require detailed investigations that were not provided in the presentation.
- The concept of stabilizing the base material and doping it with a coating is good. However, using ALD raises cost concerns. Perhaps the same results could be achieved using another, higher-throughput method. The team has identified important barriers, and its work addresses these barriers.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Progress was made and clearly demonstrated in that the team improved the rate by using alumina coating and achieved even better success using titanium nitride. The team obtained a fortuitously good discharge result using boron nitride; however, boron nitride does not cycle. In contrast, the TiN coating might cycle. In total, over a dozen coatings were tried. Evidence suggests a surface contact effect. The team should be congratulated for acting on a serendipitous impact of BN coating. The team seems to be on track and may be verging on serious headway on the kinetics barrier, at least.
- This project has made great strides, especially with the development of the BN coated particles with a very good discharge performance. The particles themselves appear to have a good-looking structure and to be what the project seeks. The ability to get clean hydrogen out of the material at temperatures below 230°C is encouraging. If the material can cycle well (given that the mechanism is understood and the right kind of additives are used), considerations will need to be made to ensure the material does not go above 230°C and release products other than hydrogen. The ability to somewhat control the rate of reaction with additives in the coating is encouraging, as the current kinetics are very aggressive for fuel cell applications.
- The project seems to have managed to produce a surprising, but as yet unexplained, result: the rapid release (at 120°C) of hydrogen from nanoscaled magnesium borohydride upon which a BN or TiN coating has been applied using ALD techniques. This surprisingly facile release at a surprisingly low temperature of around 120°C is remarkable for a magnesium borohydride sample. It is heartening that this result has arisen from a fairly new seedling project. To explain this observation, significant questions must be addressed with experiments and characterization. Greater characterization of the nature of this material is important; however, the fact remains that a reasonable quantity of hydrogen is rapidly released by this material at a low temperature. Regardless of whether the process is reversible, the results have technological applications other than onboard vehicular storage.
- Nitride and oxide coatings have demonstrated enhanced desorption kinetics. The TiN/$Mg(BH_4)_2$ system shows good cyclability (slide 10). The BN with $Mg(BH_4)_2$ does not show as much cyclability.
- Modest progress was achieved using only an Al_2O_3 oxide coating on the nano-$Mg(BH_4)_2$. Compared to uncoated material, thicker oxide coatings produced improved H_2 desorption (approximately four times higher). However, when the team decided to forego the oxide layer and deposit a boron nitride “additive layer” directly onto the nanoparticles, a remarkable result was obtained. Heating of the nano-$Mg(BH_4)_2$ coated with a BN ALD layer to approximately 110°C produced extraordinarily rapid evolution of hydrogen. This was followed by evolution of other gas phase species (i.e., NH_3, H_2O, B_2H_6, and N_2) at higher temperatures. However, subsequent attempts at sorption cycling were not successful. This rapid dehydrogenation in the presence of the nitride coating is certainly provocative, but it raises numerous

questions. For example, it may be the case that the chemically aggressive precursor gases used to form the BN coating modify the composition of the nano-$Mg(BH_4)_2$ in some way that leads to a new species having a much higher dehydrogenation rate. It is certainly conceivable that in the presence of a highly reactive precursor gas, the very small (i.e., 50 nm diameter) $Mg(BH_4)_2$ particles could be consumed and converted to a different entity with entirely different hydrogen sorption rates. If that is not the case, the role of the thin BN overcoating in facilitating such rapid dehydrogenation from $Mg(BH_4)_2$ is unclear. If $Mg(BH_4)_2$ is indeed present, it is unclear why cycling was unsuccessful. Also, when a thin TiN layer is deposited on the nanoparticles prior to BN deposition, less H_2 is evolved, but the dehydrogenation temperature is still low. Similar questions need to be addressed in that case as well. In addition to the $Mg(BH_4)_2$ results, initial experiments using nano-Mg coated with BN and TiN also showed enhanced desorption rates. Overall, these are certainly intriguing results, but considerably more work must be done to elucidate the mechanisms, confirm the identity of the reactants, understand why cycling is limited, and validate the conclusions. In general, these issues were not discussed in the presentation.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- Valuable collaborations with the HyMARC core team (on nanoparticle synthesis and material characterization), H2 Technology Consulting (on pressure–composition isotherm), and the Colorado School of Mines (on material characterization) have enabled the progress achieved thus far. Expertise and resources from cooperating organizations will undoubtedly be valuable in understanding results from the present experiments and in planning and conducting future work.
- There are a number of collaborations established with other researchers. These collaborations include the Colorado School of Mines, HyMARC partners at SNL, National Renewable Energy Laboratory (NREL), SLAC National Accelerator Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, and industry partner Forge Nano.
- The active collaborations with which the project is involved have been effective in the achievement of a remarkable result. The collaboration with HyMARC to obtain nanoscaled magnesium borohydride has been key to getting the project off the ground quickly. There should be some urgency in the team's future collaborations, and the team should focus on gaining spectroscopic information concerning the nature of the encapsulated material. The degree of collaboration appears commensurate with the scale of the project.
- The team has great collaborations with other partners and institutions. It makes great use of HyMARC resources, as well as those of outside organizations.
- The project demonstrates excellent collaboration, with real work being done by many players.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- While the project sought to explore another pathway to nanoencapsulation of magnesium borohydride, which was anticipated to be a complementary approach to either using porous material scaffolds or nanoscale graphene or related sheets, the project appears to have stumbled upon more interesting results. The rate of hydrogen release and the low temperature at which the release occurs suggests that this material is potentially interesting for applications in which reversibility is not a requirement. This material could thus have an outsized impact on solid-state storage for a variety of defense and national security applications, among others.
- The use of ceramic coatings as protective layers for hydrides is important. The reported data hints at the potential of these ceramic coatings to aid in desorption or uptake. If the coatings play a role in desorption or uptake of hydrogen, then it is crucial to determine this role using advanced characterization and careful design of experiments on coating/hydride pairs.

- This project aligns very well with the goals of HyMARC and DOE. The potential to develop a great storage material that challenges the current state of the art is very exciting and could have profound impacts on the hydrogen storage space.
- The desired impact, better kinetics and reversibility of $Mg(BH_4)_2$, would be game-changing. However, the cost of application remains a question. This project is aligned with DOE goals for storage.
- The project addresses problems that are central to the potential use of complex metal hydrides in practical hydrogen storage systems. Consequently, the project generally supports DOE research, development, and demonstration objectives. However, the provocative results raise numerous questions that must be addressed before the conclusions can be validated and the relevance and impact of the project can be firmly established.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The proposed future work for the project will help identify the mechanism for charging and discharging of the coated materials and will help optimize the performance of the materials themselves. The future studies planned for the materials are on the right track to develop and increase understanding of related processes.
- The proposed future work is consistent with prior experimental results.
- Determining the mechanism is a key goal, which is excellent.
- The exploration of additives to achieve cycling is planned for next year.
- The team's proposed future work involves meeting one of the go/no-go decision points related to recyclability and determining the ALD-driven mechanism. It may be advisable, given the amount of funding, to prioritize the efforts and focus more on gaining information on the nature of the "encapsulated" material that gives rise to the rather remarkable hydrogen release rates at low temperatures. As the ALD process may give rise to doing chemistry between the substrate magnesium borohydride and the ALD reagent hydrazine, there needs to be some thorough spectroscopic characterization (infrared and nuclear magnetic resonance [NMR]) and elemental analysis to better define the nature of the material. This is likely of greater import than attempting to improve upon cyclability at this point in time.
- The recent results raise numerous questions and concerns that the NREL team should address (e.g., the composition of the nano-$Mg(BH_4)_2$ particles after BN exposure, the composition and microstructure after H_2 evolution, the failure to cycle). Although the NREL team is likely aware of these questions, none of the critical issues that should be addressed to support and confirm the conclusions are presented. The proposed future work in slide 15 is abbreviated and very general. Given the intriguing nature of the results, particularly the H_2 evolution rate, a more complete outline of proposed future work is needed.

Project strengths:

- This project has developed a very high-performance material that has encouraging potential for storage applications. Even if the material is not cyclable, if the cost is low enough, this material could push the state of the art. Furthermore, the project is structured very well. The group has an excellent and methodical approach to developing the materials and understanding how the materials work. The ongoing work has great potential to yield very fruitful results.
- The team members have obtained a surprising result, and the strength of the project now lies in this result. The onus is now on the team to explain the underlying chemistries responsible for this result. The decision to bring in an expert, Karl Gross, to validate the hydrogen release data is a strong choice.
- The strength of this project is in the potential for coatings to interact with hydrogen uptake and desorption rather than simply facilitate protection from oxidation. This aspect of the work deserves even more attention.
- This is an innovative project conducted by a well-qualified team. The results to date are intriguing and should stimulate interesting future work.
- The project concept is interesting. The team members have a good partnership and have obtained interesting early results.

Project weaknesses:

- The only project weakness is the investigators' choice to show the data on slides 9 and 10 prior to a verbal explanation by the presenter. There is beauty and elegance to representing many parameters on a single chart. However, these parameters require explanation. A slide explaining how these data should be read would have been useful. Such a slide is essential for reviewers who plan to read through the slides before the presentation date. It was only possible to understand and read these charts after being walked through the first one on slide 9.
- Given the observation of extremely rapid H_2 evolution from the BN-coated nano-$Mg(BH_4)_2$ particles at comparatively low temperatures, a variety of critical, detailed questions must be answered to elucidate the mechanism and support and validate the conclusions. These questions concern the possible reactions of precursor gases with the particles, changes in microstructure after evolution of gas phase products, reasons why the BN actually affects the H_2 evolution rate, and low cycling efficiency (among others). Special consideration must be given to understanding the composition and microstructure of the metal hydride nanoparticle after hydrogen liberation. None of these issues were addressed in the presentation. A candid examination of the results and a much more detailed plan for future research are needed.
- The application of a coating on the particles may make it difficult to understand exactly what is happening with the particles during cycling. Studies will have to be carefully designed to identify what is happening to the particles after discharge and charge when they are cycled to truly understand what the mechanism is and whether there is any way to improve the cycling of the material.
- Given that this is a seedling at a national laboratory, and the funding does not go very far, a potential weakness is the potential lack of funding to perform the needed characterization studies in detail. These studies are necessary for understanding how the ALD process has so significantly altered the chemistry of magnesium borohydride.
- It is necessary to better understand the commercial viability of the approach or alternate methods that might reasonably work if the project is to be technically successful. While battery particles are ALD coated, they are generally larger as well. It would be useful to perform a rough engineering calculation of the number of ALD machines needed to generate millions of tons of 10–50 nm particles.

Recommendations for additions/deletions to project scope:

- Spectroscopic characterization of the ALD-derived materials is recommended. Boron and nitrogen NMR is also recommended. Infrared spectroscopy will be useful in examining alterations in the B-H, N-H, and N-N bonding. The project should conduct elemental analysis of B, N, Cl, Ti, etc. It is recommended that a systematic series of ALD experiments be performed to explore what, if any, effect the order of addition has on the produced material's hydrogen release. Such experiments might entail comparing the currently practiced addition of hydrazine before BCl_3 with the addition of BCl_3 before hydrazine. Given the distinct possibility of a chemical reaction between hydrazine and magnesium borohydride, perhaps hydrazine should be deposited alone on magnesium borohydride. In the absence of magnesium borohydride, the ALD reactions may be performed on an inert substrate. Recyclability should be deprioritized until more is understood about the nature of the material that has been produced.
- If the material can be cycled to meet the targets, the mechanisms can be identified, and the material composition after ALD and cycling can be identified, it may be interesting to optimize the ALD coating thickness to reduce gravimetric and volumetric losses. However, this step is only recommended once a strong understanding of the material and its performance is developed.
- Investigators should perform a rough estimate of the cost to produce one million tons per year of ALD-coated particles of the size, thickness, and composition the team is using. At the very least, the amount of coating material needed per kilogram of particles should be determined.

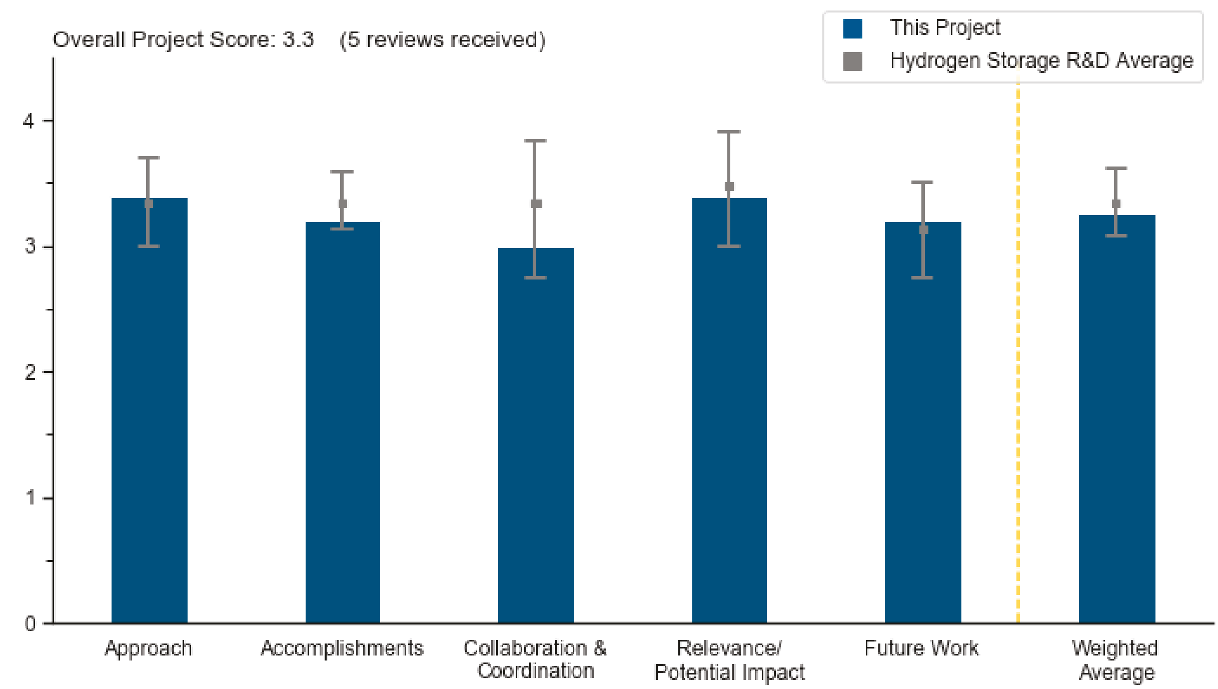
Project #ST-144: Hydrogen Materials–Advanced Research Consortium (HyMARC) Seedling: Optimized Hydrogen Adsorbents via Machine Learning and Crystal Engineering

Don Siegel, University of Michigan

Brief Summary of Project

Screening of approximately 500,000 metal–organic frameworks (MOFs) revealed that essentially no compounds exceed 40 g/L usable capacity. New MOFs are needed to break through the volumetric ceiling. The project aims to develop purpose-built MOFs with high volumetric capacity, overcoming volumetric limitations associated with physisorptive hydrogen storage at both the materials and systems levels in MOFs. The project will apply machine-learning techniques to identify, design, and demonstrate high-capacity MOFs that demonstrate usable volumetric capacities exceeding 50 H_2 g/L (single-crystal/pressure swing) with no compromise to gravimetric capacity, kinetic performance, or reversibility. The project will also address packing inefficiencies, which can result in significant volumetric penalties in adsorptive hydrogen storage systems. Packing density will be increased at least 30% via crystal engineering, specifically control of MOF crystal morphology and crystallite size distribution. The project addresses barriers associated with volumetric density and gravimetric density.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project addresses two important aspects of the sorption of hydrogen on high-surface-area MOFs. The project approach is twofold. One task attempts to apply machine learning to screen, in silico, the many hundreds of thousands of MOF structure types, most of them not as yet synthesized, in the search for MOFs that can exceed what has been currently identified in the laboratory and hopefully exceed the technical targets for onboard storage. The second task is to explore crystal engineering approaches to significantly improve the packing density of microcrystalline MOFs, resulting in improved volumetric capacity for hydrogen storage without decreasing the gravimetric capacity. The team has a very powerful approach to address the first task. This approach involves applying machine-learning computational tools to screen for high-capacity MOFs. This is a highly aggressive approach that is designed to utilize the high speed of computation. Machine learning is preferable to the very slow, mostly one-at-a-time attempted laboratory synthesis of all possible MOFs, currently a near-impossible task. The research has involved exploring the research team's previously developed database of nearly half a million MOF structures and applying a wide variety of machine-learning algorithms to explore the interconnectivity of a number of the key physical parameters that are likely involved in hydrogen sorption on the internal surfaces and volumes of the individual MOF structures. Such parameters include cavity diameter, pore diameter, surface area, density, pore volume, and void fraction. The team then ranked the algorithm's ability versus its own ability to predict the sorption properties of known benchmark MOFs. The "best" algorithm was then applied to the large database of structure types, and the gravimetric and volumetric capacities were computed for this huge set of MOFs, many of which are known but most of which are unknown (synthetically). This is truly an impressive feat. The attempted synthesis of a very small subset of structure types that appeared to have substantially higher performance than the benchmarks and the targets was then undertaken. The challenge to the approach then comes up against the need to rapidly attempt the synthesis of all of the promising "hits." The second approach aims to achieve higher volumetric capacities for sorbent materials. To this end, the project explores crystal engineering approaches to alter the shapes of the synthesized microcrystals to more symmetrical crystal shapes that have higher propensity to pack in dense three-dimensional arrays or alter the size distribution of microcrystallites to achieve higher overall packing densities. Both approaches, if successful, can enhance the overall volumetric capacity of a sorbent. This is also a very valid and focused approach to exploring the possibility of achieving enhanced volumetric storage capacity.

- The use of theoretical and other automated techniques is a valid and helpful approach to save time and resources relative to experiment only. The improved crystallite performance and improved packing are appropriate methods for achieving the goals. The use of machine learning on inputs to predict capacity and then reversing the model (using desired capacity to set the target zone of properties that will meet project goals) is an excellent idea. In the best case, this approach will be helpful, and in the worst case, this approach will confirm that we know most of what there is to know about what makes a good MOF. The risk in the approach is that there is no way to determine whether the selected MOF can actually be made, or will perform correctly. The hope, of course, is that the creation of the MOF will be successful and that it will perform as expected. Project barriers are clearly defined, and the project work is aimed toward surmounting them.
- The approach is focused on addressing the limitations of hydrogen storage volumetric capacity in MOFs. The strategy is reasonable and innovative; it involves control of MOF morphology and crystal size distribution to increase packing density and the use of machine learning techniques to identify candidate systems. Notably, the use of machine learning is a powerful and effective approach to extend predictive capabilities developed in prior work. The parameter space accessed in this study is huge. It provides researchers with a valuable baseline for initiating and benchmarking future work. However, the transition from identification of candidate MOFs using high-throughput machine learning screening to successful synthesis of the most attractive candidates remains problematic.
- The approach to the work is very thorough and does a great job of processing a very large amount of a data to separate out potentially interesting materials. The analytical methodology used is sound but could be improved by adding considerations for "synthesizability" that could improve the quality of the experimental results.
- This work focuses on computational and machine-learning approaches to selection of MOFs for maximum hydrogen uptake. As part of that objective, the work strives to close the gap between single-crystalline performance and powder performance (slide 5). A 500,000-item dataset was composed and analyzed for storage. Both pressure and temperature (together) and singular pressure were used as variables in assessing the MOFs.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team has made remarkable progress on the machine-learning approach to search for candidate MOFs that may have volumetric capacities that exceed the current benchmarks. The project has extended this year's approach to include temperature and pressure swing operation. The team has also performed further validation of the potential high-performing MOF structure types via more rigorous Grand Canonical Monte Carlo (GCMC) computational modeling. The outcome of this year's computational screening uncovered a large number of possible MOF candidates. The approach runs into the problem of then having to synthesize these structure types, many of them not previously synthesized, in the laboratory. The team chose to examine the top 10 candidates and attempt to synthesize them. The synthesis of the candidates is a laborious process that requires experimentation with many different conditions, solvents, and other parameters. Furthermore, many synthesis approaches may result in materials that are unstable or metastable upon removal of the solvent used in synthesis. This has been the case to this point, as two candidates resulted in apparent collapse of their porous structures upon solvent removal. More work needs to be done, but the team's effort is a very good one that will require patience. The crystal engineering effort shows promise. The team has demonstrated that control of the particle size distribution can lead to enhanced packing densities. The team's early efforts to control the morphology of microcrystalline habit shows promise, as the team has identified an additive that alters the morphology of MOF-5 crystallites to a variety of high-symmetry habits.
- A great deal of progress has been made in this work. The identification of MOFs that meet or surpass the targets is encouraging and will make experimental verification much simpler, as the number of materials is on the order of tens rather than hundreds. Though the results of the experimental work are encouraging, the work could be modified to include experimentation with different activation methods in an attempt to maximize measurable surface area. The results of the packing density work are very encouraging, especially with regard to the MOFs that have been synthesized with a higher packing density than previously seen.
- The team is making progress toward project milestones. The maximum error in prediction relative to GCMC calculation is about 1% and 5g/L and is less than one-third of that for most values, so the methods are consistent. Two of the high-capacity predicted MOFs were synthesized; however, neither had the properties desired. The project demonstrated that size control of particles can achieve enhanced system-level performance, which extended the range over which system performance is at particle performance levels. This is the main way in which measurable progress has been made toward DOE goals. To be clear, the theoretical side has made good progress in building tools, but the team has not had enough time to use them to find a winning MOF.
- The ability to predict the hydrogen storage properties for hundreds of thousands of MOF candidate materials is quite an accomplishment. Unfortunately, the "silver bullet" has not been found. Moreover, efforts to synthesize the best candidates from the machine-learning study have been largely unsuccessful. It is really quite amazing that MOF-5, among the first adsorbent systems studied, remains as one of the most promising candidates. The inability to synthesize a candidate that meets DOE targets notwithstanding, good progress was obtained in this seedling project. Methods for controlling MOF crystal morphology crystallite size distributions were developed. The machine-learning methods were optimized and validated to the extent that MOF compounds and associated adsorption properties could be predicted with confidence. All milestones through Quarter 7 of the project have been met.
- Most MOFs found using the machine-learning methods in this work are hypothetical. Therefore, variables related to processability should be used to optimize for yield in future computational work of this type.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- The collaborators and the degree of collaboration exhibited by this project are appropriate to the size and scope of the effort. The team has utilized outside collaborators in key areas. Namely, the team has used systems models developed by the Hydrogen Storage Engineering Center of Excellence (HSECoE) to provide guidance to its approach and, as needed, has collaborated with Ford Motor Company and University of Michigan faculty in materials synthesis and characterization efforts.
- Valuable collaborations within the University of Michigan and with the Ford Motor Company and HSECoE have accelerated project progress. The project is well managed and coordinated.
- The collaboration with other groups is good but could be strengthened by reaching out to other groups within and without HyMARC that have experience synthesizing MOFs. Such groups could provide feedback to maximize the value of the experimental testing.
- The team's collaboration between partners seems good and received some help from the HSECoE. However, there has not been much external collaboration so far.
- There were few collaborations outside of the University of Michigan and Ford Motor Company. Savannah River National Laboratory is listed as an unfunded collaborator.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is highly relevant in the search to break the "volumetric ceiling," a significant challenge in enhancing the volumetric capacities of sorbent systems. Success in this area will have a dramatic impact on achieving sorption materials that can meet or exceed the hydrogen capacity targets, which are significant barriers to practical application of sorption materials in engineered systems.
- Machine learning is a very useful technique for examining hydrogen sorbent materials. This work is extremely relevant to the field. However, it would be useful to quantify a "processability parameter" to decide on MOFs for inclusion.
- A system-level dense storage by adsorption would certainly be very useful. The general area (sorbents) has the best odds of success of the various methods outside physical containment, so progress in the area is relevant and aligned with DOE goals and targets.
- The work being done has the potential for great impact on cryogenic hydrogen storage materials. However, unless high uptake is shown at more useful (near-ambient) temperatures, the applications of this work will be limited to niche applications.
- The project is well aligned with DOE research, development, and demonstration objectives. This is a unique project in the Hydrogen and Fuel Cells Program (the Program) portfolio. The ability to computationally identify and benchmark thousands of MOFs for their potential as hydrogen storage candidates is valuable and has a positive impact on our understanding of hydrogen storage materials and development approaches. However, the fact remains that a superior candidate based upon the extensive machine-learning work has not yet been synthesized and tested.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed future work will help push the state of the art even further. The development of a high-capacity MOF would be a significant breakthrough. If performance is impressive enough to warrant further work, an increase in MOF tap density will be important for demonstrating the material's behavior in larger systems.
- Future work is tightly focused on achieving substantial improvements in volumetric capacity without sacrificing gravimetric capacity. The team's future work aims to break through the "volumetric capacity

ceiling" and remove the volumetric barrier in order to meet the technical targets for capacity in hydrogen sorbent materials.

- The project is scheduled to end December 31, 2020. The future work will focus on meeting the second go/no-go milestone: (a) identify an MOF with 10% increase over the current state of the art or (b) increase packing density by 15%. Ongoing synthesis work to produce a promising candidate selected from the results of the machine learning study is proposed. This synthesis work should be a research and development imperative for the remainder of the project.
- Given the team has two independent wings, the future work should include both milestone objectives (engineering and MOF selection). Both objectives are advantageous to this project and other related projects. However, since the decision to limit future work to one objective was approved, it is acceptable to focus on only one objective.
- The future work focuses on the second go/no-go milestone. The work will either focus on an MOF with a single-crystal volumetric capacity greater than 38 g/L usable capacity at 77 K or focus on a 15% increase in tap density through crystal engineering methods for a specific MOF compared to its non-optimized powder. It is unclear why there is an "or" statement (rather than an "and" statement). It is possible for the team of researchers to focus on both future work objectives.

Project strengths:

- This academic project is guided by industry. Though the project is led by theory, its results are experimentally confirmed. The project treats both engineering and material properties, giving it two ways to succeed and yield value. The team is excellent. The presentation was very well organized, easy to follow, and well constructed for the purpose of evaluating the work by Program Annual Merit Review metrics.
- The University of Michigan team is highly qualified and capable. This is an innovative project that provides DOE with an opportunity to explore a vast parameter space that has been too large and cumbersome to access experimentally. The project provides baseline and benchmarking data that is valuable to researchers investigating adsorbent systems for hydrogen storage.
- The project uses an aggressive approach backed by a knowledgeable, effective team. The approach of using machine-learning algorithms to enable high-speed screening of hundreds of thousands of compounds as sorption candidates contains many daunting challenges. This team is highly effective at addressing those challenges both in a computational sense and in an experimental sense. The team recognizes the need for accurate benchmarking of the computational results.
- The project has a very thorough and well-defined methodology that allows for fast identification of potentially high-performing materials. The ability to synthesize MOFs with a higher packing density than previously measured is a great step forward. The clever testing methods for packing density are commendable.
- Machine learning is an extremely valuable tool. Applying it to assessing MOFs for hydrogen capacity at pressure and temperature together and also only pressure swings is a good objective.

Project weaknesses:

- Synthesis of a few of the top 10 candidates represents a large potential bottleneck to future progress for this team. While the team appears to be very good at the synthesis of framework materials, perhaps the project could use some additional expert assistance or collaboration with the rather large-scope synthesis landscapes that may be required to successfully synthesize a few of the top 10 candidates that the machine learning approach identified. While this additional assistance is undoubtedly beyond the ability of the project to fund, the scope of the project suggests that this seedling needs its own seedling.
- Overall, it seems that the translation from a promising candidate identified from the high-throughput screening and machine-learning work into a real material synthesized in the laboratory has been largely unsuccessful. This is the most noteworthy project deficiency. It was unclear from the presentation why the synthesis of two promising candidate materials (MOF-31 and TMOF) failed to produce materials with significantly higher Brunauer–Emmett–Teller (BET) surface areas. It is also unclear whether any promising candidates with high surface area have been synthesized in this project. Perhaps additional synthesis collaborators should be brought into the project for the remainder of the activity.

- It would be beneficial to conduct an analysis of likely success rates from machine-learning prediction to experimental confirmation, based on predictions for MOFs with existing data (both good and bad MOFs).
- The experimental activation of the MOFs could potentially be improved by trying different methods to avoid pore clogging or collapse. There could also be a way to identify MOFs that are easier to synthesize than others to improve the quality of experimental results.
- Many of the highest-capacity MOFs (slide 26) were hypothetical.

Recommendations for additions/deletions to project scope:

- An investigation into an additional parameter that could identify how easily an MOF could be synthesized may be a worthwhile undertaking to improve the experimental results and increase throughput. This could potentially reduce the bottleneck of reviewing potential MOFs before synthesis.
- It would be useful to collaborate with experimentalists to determine processability of the hypothetical set of MOFs or to work within the confines of a series of MOFs that have been processed already.
- The project should be extended either to further examine machine-learning predictions of MOF stability or to determine the likelihood of possible synthesis for MOFs that pass the high-capacity screen. If likelihood of possible synthesis is determined, researchers can screen out MOFs with a lower likelihood.
- Additional attention to the attempted synthesis of the best candidates identified by the machine-learning approach is required. To thoroughly and successfully survey the usual synthetic parameters, the team may require additional staffing and funding.

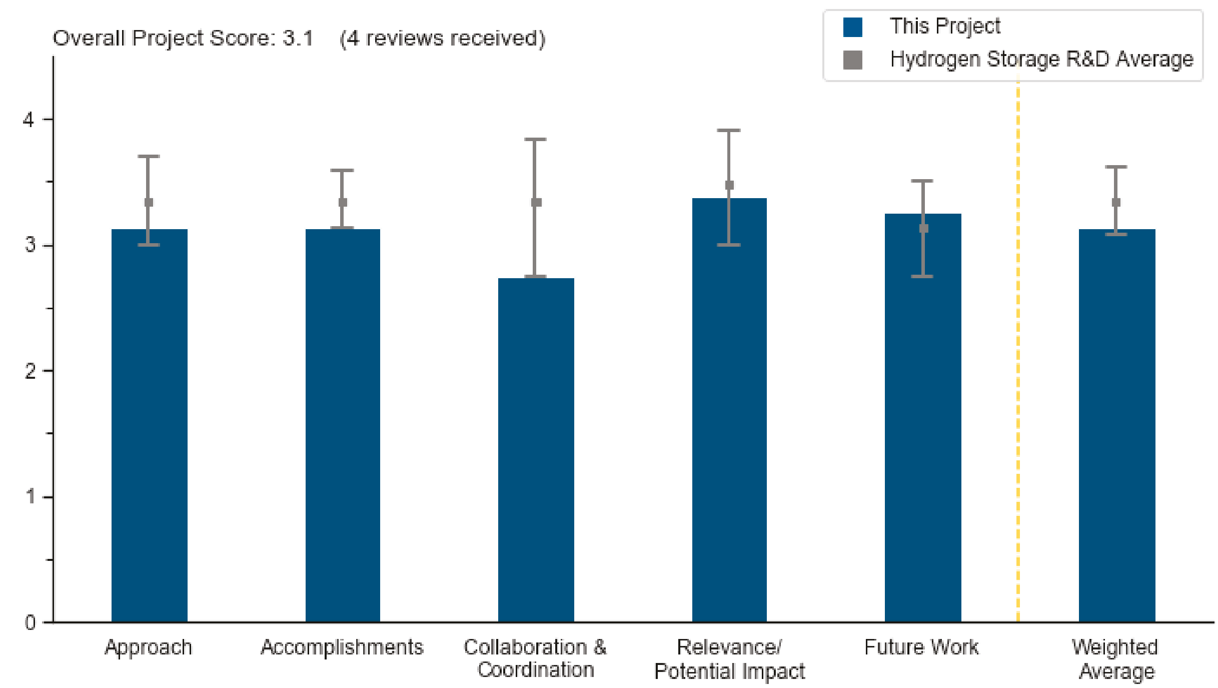
Project #ST-146: Precursor Processing Development for Low-Cost, High-Strength Carbon Fiber for Composite Overwrapped Pressure Vessel Applications

Matthew Weisenberger, University of Kentucky

Brief Summary of Project

This project aims to use low-cost carbon fiber precursor and develop a processing technology that can produce carbon fiber for hydrogen storage applications with tensile properties comparable to the current state-of-the-art at the U.S. Department of Energy target cost of $12.60 per kilogram or less. Cost savings are expected from several innovations: (1) use of non-exclusive, low-cost, high-quality polyacrylonitrile (PAN) known as Tech-PAN polymer as precursor instead of a proprietary PAN polymer, (2) use of hollow carbon fibers that enable up to 35 times faster oxidization and carbonization than existing processes, and (3) water use reduction and solvent recovery using activated carbon. These process improvements in carbon fiber production have the greatest impact on product cost.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach focuses on four cost drivers to reduce the cost of T700S-equivalent fiber toward a target of $10.68/kg, which is below the U.S. Department of Energy goal of $12.60/kg. The demonstration using TechPAN appears to be validated in that carbon fibers were produced in the laboratory with over 10% exceeding T700S average tensile strength. Carbon fiber made using TechPAN is expected to result in 13.8% cost reduction, and as an open-source PAN, it offers a path forward toward commercialization and innovation. Better utilization of PAN using the hollow-fiber approach, eliminating the poor quality core, has some validation based on the literature and should result in net cost reduction. The faster oxidation rate of 35x seems unlikely, in that oxidation in a continuous fiber is unlikely to occur from the center, but for a thinner-wall fiber, it will still be faster than a solid fiber.

- The approach is strong. It is difficult to improve an approach that could reduce carbon fiber cost from $29.40/kg to $10.68/kg.
- The hollow-fiber approach is novel and could offer additional cost savings. It is not clear if all of the cost savings are being realized. For example, the fiber-mass-per-foot would be lower for the hollow fiber relative to the solid fiber, thereby providing more material for additional fiber length. It would also be prudent to discuss defect challenges that need to be overcome in increasing fiber strength and modulus. The presentation did discuss hollow-wall collapsing, which the project demonstrated did not happen, but it is unknown whether there are other issues that have been identified that need to be addressed as well.
- The project was able to produce hollow fibers. The presenter did not give an adequate response to how oxidation would be reduced from over an hour to 10 minutes. Assumptions were made that the process would occur faster because of stabilization occurring both from inside the hollow fiber and outside the fiber. There was no clear approach to reaching this goal. The economic analysis lacked important details. It showed percentage improvements that somehow got to $10.68/kg cost for carbon fiber. This was not supported in the presentation other than slide 6 indicating how one could get to $23.82/kg. No estimate was provided on how improved specific properties and increased oxidation would result in an additional $13.14 in savings. The solvent recovery using activated carbon should be a separate project, given the challenges of winding, oxidizing, and utilizing hollow fibers.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made strong progress to date. (1) Fiber was spun with the TechPAN, and initial properties showed the potential to meet or exceed T700S strength. (2) Hollow fiber was spun using a scalable approach; there may be some possibility of refining the approach by shaping the die, but for now, at least, hollow fiber has been spun. (3) Initial feasibility of solvent recovery has been demonstrated using activated carbon. (4) The oxidation rate should be evaluated soon to get a better estimate of kinetics via a small-fiber sample in thermal gravimetric analysis (TGA). The effect of wall thickness to fiber diameter as it relates to oxidation rate and morphology needs to be evaluated before scale-up. (5) The effect of using hollow fiber, and hence the expected reduced composite fiber volume, should be discussed with compressed gas system (CGS) tank manufacturers to forestall unexpected consequences, such as thicker shell-wall requirements.
- The project has clearly defined goals, and the presenter showed the approach and how the project was going to partly lower the cost. An area of improvement would be to demonstrate how the cost is going to be reduced even further. It would be beneficial to know if the research team has ideas about how they are going to move beyond the current savings they believe they can achieve. The first data sets for the fiber properties are okay. They do fall short of the T700S target, but they are pretty good. The one challenge the team will need to overcome for the pressure vessel fiber use is the low coefficient of variation (CV). The pressure vessels will design to the lower part of the CV, which will increase weight, volume, and cost. The strength goal is important, but the CV is just as important. The current data set has a lot of variation. It is unclear whether a calculation has been performed on the stress of the hollow cross section or whether it is based on the fiber diameter itself. How the strength was determined was not clear in the presentation.
- Fibers with strength similar to T700S were made and solvent recovery was successful, resulting in some cost reduction.
- The presentation lacked consistency. Slide 22 indicates that filaments of ~100 um were produced, with a pathway to reaching ~14 um to be determined. Slide 18 states that fiber of ~150 um was successfully spun. Slide 11 indicates that 76 um was achieved. If this is correct, then the project has already reached the year 2 go/no-go milestone. The project team has also claimed that the project met the $23.82/kg fiscal year (FY) 2019 go/no-go. Part of that was attributed to TechPAN, which is not part of the project development but a separate proprietary development of the University of Kentucky (UK). The project's progress seems limited on avoiding collapse of fibers during spinning and oxidation rate.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- The UK Center for Applied Energy Research is collaborating with Oak Ridge National Laboratory (ORNL) via funding under the Lightweight Materials Consortium (LightMAT) in carbonization. There was some discussion whereby UK could spin fiber from the other two programs. As the project proceeds toward validation of the cost-saving concepts, it is suggested that the project team engage in discussions with a CGS tank manufacturer to learn of any concerns or suggestions regarding handling characteristics or properties of a new fiber.
- It was clear on the collaboration efforts between ORNL and UK where they were contributing. It would be beneficial to have a tank manufacturer as part of the advisory team to provide relative design feedback required by the fibers, such as the CV.
- The collaboration with ORNL seems to be working well and providing good value to the project. There may be additional collaborations within the Hydrogen Materials Advanced Research Consortium (HyMARC) that could be leveraged for this project.
- The project's collaborators have no commercial interests. The role of ORNL was not clearly defined, other than scale-up. This reviewer is not familiar with the separate LightMAT objectives, so there may be an insufficient basis to rate this criterion.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project has the potential to significantly reduce the cost of high-strength carbon fiber for use in CGS tanks. The project begins with a basic cost model, which is useful for tracking progress regarding cost reduction in each of the four areas. The project has potential synergy with the other carbon fiber projects. If the hollow fiber concept meets expectations, it might be applied to the other precursors under development. The use of activated carbon to capture solvent also may be applied to other PAN precursors. Follow-up research will be required to understand any issues regarding the use of hollow fiber versus conventional fiber. Low-cost, high-strength carbon fiber is expected to have broad applications as a structural material.
- This project is extremely relevant and its potential impact would be advantageous to meeting DOE's targets and to the industry.
- It is well known that compressed hydrogen technology cannot meet all of the DOE targets, so a project focused on this technology could not be said to significantly advance toward the DOE project goals and objectives. However, this project does align with the Hydrogen and Fuel Cells Program objectives and has the potential to advance progress toward DOE goals. Of all of the projects, this is the most likely to have impact on the industry in the near term.
- The project aligns with system weight and cost objectives.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The project's milestones and go/no-go's are appropriate and at a high level, regarding meeting tensile strength targets of 4.9 GPa. Details regarding the experiments and approach to meeting these goals were not presented. Data tables and/or charts of the kinetics of oxidation, microstructure, and carbon fiber properties should be prepared as a function of fiber diameter and wall thickness to help establish a basis for future process optimization.
- The project team's proposed future work discusses more on fiber-spinning development and cost reduction processes, but the team needs to be focused on increasing the fiber strength and reducing the CV after reducing the fiber diameter. Cost reductions in the wastewater will be irrelevant if the fiber performance cannot be achieved.

- The project team provided the planned milestones for FY 2020 and barriers to be addressed. The team should not wait until the end of the project for cost evaluation; there should be a preliminary estimate for all cost factors by end of FY 2019.
- The project's remaining tasks are a logical continuation of the work done so far and will focus on all three critical barriers.

Project strengths:

- The project explores the following potential technologies, which individually provide value for meeting DOE goals. (1) TechPAN may serve as a low-cost, commercial, open-source model precursor for future fiber development work. (2) The concept of hollow-core fiber may transition to other fiber precursors; the effect of process conditions on morphology and properties needs deeper study and perhaps modeling. (3) The recovery of process solvent has the potential to save energy, water usage, and cost. (4) Micromechanics analysis of carbon fiber surface area to fiber cross-section should show benefit in stress transfer across the matrix and throughout the composite. Detailed analysis should be used to help establish optimized geometry.
- The project's strengths include a novel approach in making hollow carbon fibers. The work in cost reductions can benefit DOE's targets, and the goal to achieve strength parity with T700S is a good target.
- The project's strengths include the team's facilities and that it has achieved a measure of success in producing hollow fibers.
- The overall project methodology and approach are strong. There are clear milestones and a clear outline of the progression of the project. The results are clearly presented.

Project weaknesses:

- The project is focused on the fiber spinning, which is important, but there seems to be less discussion or emphasis on the approach to achieve the high performance of the hollow fiber. With a hollow-fiber design, the wall stress will be higher in tension, with a reduced cross-sectional area. A simple calculation comparing the solid-fiber strength average to the theoretical hollow-wall strength average should be considered to demonstrate what level of fiber quality will need to be achieved. Another item not addressed is the fiber wall buckling or collapsing on bending. The solid core, even without the additional strength proved in tensile, does keep the fiber wall from collapsing inward, thereby minimizing additional stresses.
- A majority of the expected fiber cost savings is based on a much higher oxidation rate of 35x. This higher rate includes an assumption that oxidation could occur from inside the core. It is unlikely oxygen can penetrate into the core unless fiber defects exist that allow for oxygen transport. Regardless, a shorter distance for diffusion, assuming a thinner wall, will allow for less time to oxidize the fiber. If an oxygen-carrier gas or liquid is included in the core during spinning, it may be possible to accelerate oxidation, but this would add to the complexity.
- There is a lack of clear direction to solving critical problems, at least as described in the presentation and question-and-answer segment. The project's other weaknesses include a reliance on a non-commercial grade of precursor, the lack of industrial participation, assumptions on oxidation rate and ability to achieve diameter and spinnability, and reliance on tensile properties. Although this is correctly focused on the gas storage application, something should have been mentioned about suitability of hollow fibers for other applications.
- The whole project hinges on the assumption in slide 10 that hollow fibers could be as strong as solid fibers because the core section does not significantly take on a tensile load. Some quantitative analysis would have been useful to show that this could be the case, although on slide 22, the principal investigators state this is beyond the scope of this project.

Recommendations for additions/deletions to project scope:

- Two additions to the scope could be recommended. One is analysis of critical assumption number three ("the sheath of the carbon fiber carries the majority of the force when in tension, and therefore hollow carbon fibers should provide the same tensile strength performance as conventional solid carbon fibers"). The second would be an analysis of the effect of using a hollow fiber in a composite pressure vessel. There are questions to be investigated, such as whether load transferred between carbon fiber layers is the same as with solid fibers, whether the fiber will remain a hollow cylinder or flatten out when under tension while wrapped around a cylinder, and whether it will flatten during winding. This could be an opportunity to collaborate with some of the modeling capabilities within HyMARC and so would not necessarily be an additional workload for the principal investigators.

- The project as proposed is on the right track. Future results may drive changes, but at this stage, it is too early. The project team should make sure that data collection allows for scientific understanding relating to the processing of hollow carbon fiber, particularly relating to kinetics and morphology as it relates to fiber diameter and wall thickness.
- The project team should delete the activated carbon for solvent-capture work and focus on the fiber challenges.

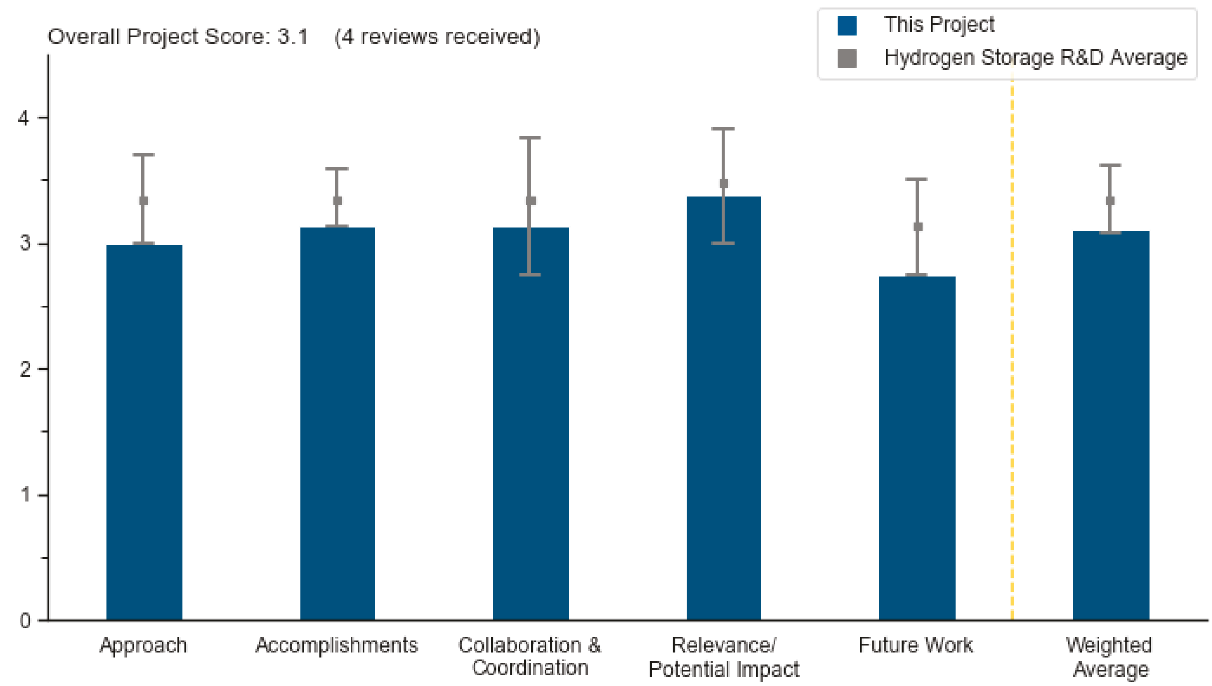
Project #ST-147: Developing a New Polyolefin Precursor for Low-Cost, High-Strength Carbon Fiber

Mike Chung, Pennsylvania State University

Brief Summary of Project

This project seeks to identify new potential low-cost alternatives to polyacrylonitrile (PAN) to be used as a precursor in the manufacture of high-strength carbon fiber. A systemic study will be conducted to identify several new hydrocarbon polymer precursors that can offer greater than 80% yield in a one-step carbonization process under nitrogen atmosphere. Use of a new class of polyethylene (PE)-co-pitch polymer precursors and boron-containing pitch precursors will also be investigated. The most promising precursors will be selected for further development and analysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach to producing low-weight carbon fiber precursors by looking at alternatives to PAN is well-thought-out and presented. It is clear that the cost will be reduced by using a less expensive precursor. However, it is not clear from the presentation how this project is tackling the system weight and volume and suitable hydrogen-binding energy barriers.
- The project's approach is a serious attempt to change how carbon fiber is manufactured, using a pure hydrocarbon polymer that is melt-processable and provides high carbon yield in one-step carbonization. One downside is that the presentation provided support for chemistry and some processing but little information on what was actually achieved versus metrics and milestones.
- The approach is high-risk and yet high-payoff. The polyolefin precursors are developmental at small scale; however, they do use commercial feedstocks, and the synthesis has a high yield. The precursor has the potential to have low cost and very high conversion yield to carbon fiber. The carbon fiber does not require

oxygen stabilization, which should also save cost. It would be beneficial to see a basic cost model developed for this approach as the technology matures.
- The approach to melt-spinnable PE fiber with C content is demonstrated as possible; however, the fiber quality is lacking significant defect-free surface and core in the fiber. As shown, the current approach in increasing the carbon content and stabilizing through cross-linking will be irrelevant if the fiber spinning quality cannot be met. There will be no advantage or improvements in fiber strength.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has done an excellent job of evaluating a number of approaches to achieving a precursor with high char yield that is spinnable into a fiber. The first fibers spun appear to have many defects and would have low tensile strength. The precursors could establish a new paradigm for carbon fiber; however, it will be very important to demonstrate the ability to achieve high strength. A basic cost model should be established at this point in the project.
- Polyolefin precursors have been melt-spun and carbonized, and good mass-loss characteristics have been observed. The project is well on its way to meeting the next set of milestones. There is some concern about the roughness seen in the scanning electron microscope (SEM) pictures on page 15, compared to that of T700 (see figure 7e in http://dx.doi.org/10.5714/CL.2016.18.018); there is also concern that, although the fiber may cost less, the fiber is going to be much weaker.
- A new class of polymer precursors has been developed, and another has shown high conversion yield. The presentation lacked information on economics and was not clear about what precursor will be down-selected and scaled up in the remaining fiscal year (FY) 2019 work. It appears that improvement in fiber morphology may be needed, as indicated in results from Oak Ridge National Laboratory (ORNL).
- Based on the current status of the project, the strength performance needed for DOE goals will not be met. The cost may be reduced, but it does not matter unless the fiber strength requirements are met.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- Based on the information here, the collaborations with ORNL and within The Pennsylvania State University seem to be working well and providing good value to the project. Results from the ORNL team are also presented. There may be additional collaborations within the Hydrogen Materials Advanced Research Consortium (HyMARC) that could be leveraged for this project.
- The project team is fortunate to have ORNL helping spin and convert fibers. There should be more interaction to help improve the fiber-spinning quality and fiber performance measurements after conversion.
- The project's collaborators include the Lightweight Materials Consortium (LightMAT), with ORNL to spin the fiber and convert to carbon. This level of collaboration should be sufficient to meet the project goals.
- It would be helpful to have a better understanding of how LightMAT's funding of ORNL supports work directly related to this project. There is no independent assessment or report seen from ORNL.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project could have a very significant impact if the ultimate carbon fiber has the required mechanical properties. The starting materials should have much lower cost than current PAN, and the simpler and faster processing into carbon fiber should be much cheaper. It will not be possible to fully explore and

optimize the best precursor and processing approach under this current project; rather, it is important to show the potential of the technology to produce high-strength carbon fiber.
- The goal of reducing the cost of carbon fiber is well within the relevance and potential impact to help DOE reduce pressure-vessel costs.
- If successful, the project could have significant technical achievement.
- It is well known that compressed hydrogen technology cannot meet all of the DOE targets, so a project focused on this technology could not be said to significantly advance toward the DOE project goals and objectives. However, this project does align with the Hydrogen and Fuel Cells Program's objectives and has the potential to advance progress toward DOE goals.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The proposed future work discusses continued work on the melt-spinning PE, with various x-link and B pitch materials. This may be appropriate for investigating the quality change in the fiber and the direction of adding the downstream process of the spinneret with heating and tensioning for better molecular alignment. However, the surface quality and fiber porosity need to be critically addressed, and it is hoped that this is the intention for the future work that is planned.
- The most critical step of developing and producing fiber from a new polyolefin precursor has been met. Future work needs to focus on producing better-quality carbon fiber with a baseline precursor and then perhaps modifying the precursor to make carbon fiber of even better quality. A basic cost model should be developed, and metrics should be captured during the remaining project.
- The future work is in line with the milestones and project goals. However, as in the approach, it is unclear how suitable hydrogen-binding energy is being addressed.
- The linkage of the milestone summary table to the few slides on summary of future work was unclear; it was hard to tell if this was remaining FY 2019 or FY 2020 work.

Project strengths:

- The project is well planned, and it is clear that the principal investigator is a leading expert in polymer chemistry. It is appreciated that, although there was a good deal of chemistry in this project, it was presented in a way that could be easily understood by a physicist. The systematic approach and analysis make the project valuable to DOE.
- The project's strengths include the development of new pitch precursors and a possible one-step carbonization process.
- The team did a thorough job of developing and evaluating a number of new polyolefins, which may provide high-strength carbon fiber as well as other important applications.
- The project's strength is the reduced costs of fiber spinning and precursor materials.

Project weaknesses:

- The project is laser-focused on the materials aspect, which is both a good and bad thing. Because of that, it is not always clear how the research is addressing the barriers seen on slide 2. For instance, it is clear that the cost is being addressed in a general way and high polymer surface area is addressed through the chemistry, but these are the only barriers that appear to be directly addressed. This is likely partially due to the scope of the project and the way the milestones are defined.
- While it is still early in the project, the initial fiber spun from the precursor was of poor quality. Further work needs to be done quickly to validate that high-quality fiber can be produced from this new class of precursors. A cost model needs to be developed, perhaps in collaboration with ORNL.
- There is no clear path described on how the project team will increase fiber quality to meet the strength requirements for the low-cost, high-strength fiber.
- There is a lack of standard project management reporting.

Recommendations for additions/deletions to project scope:

- The project has potential for high payoff; however, given the amount of effort required to develop and characterize the new precursors, the project is underfunded. More effort needs to be applied toward ORNL to spin high-quality fiber.
- Although this is definitely a materials research project, it would be interesting to see some estimation of the cost savings for using polyolefin precursors over traditional PAN. Otherwise, no change to the scope is recommended.
- The project team should focus on improving fiber quality.

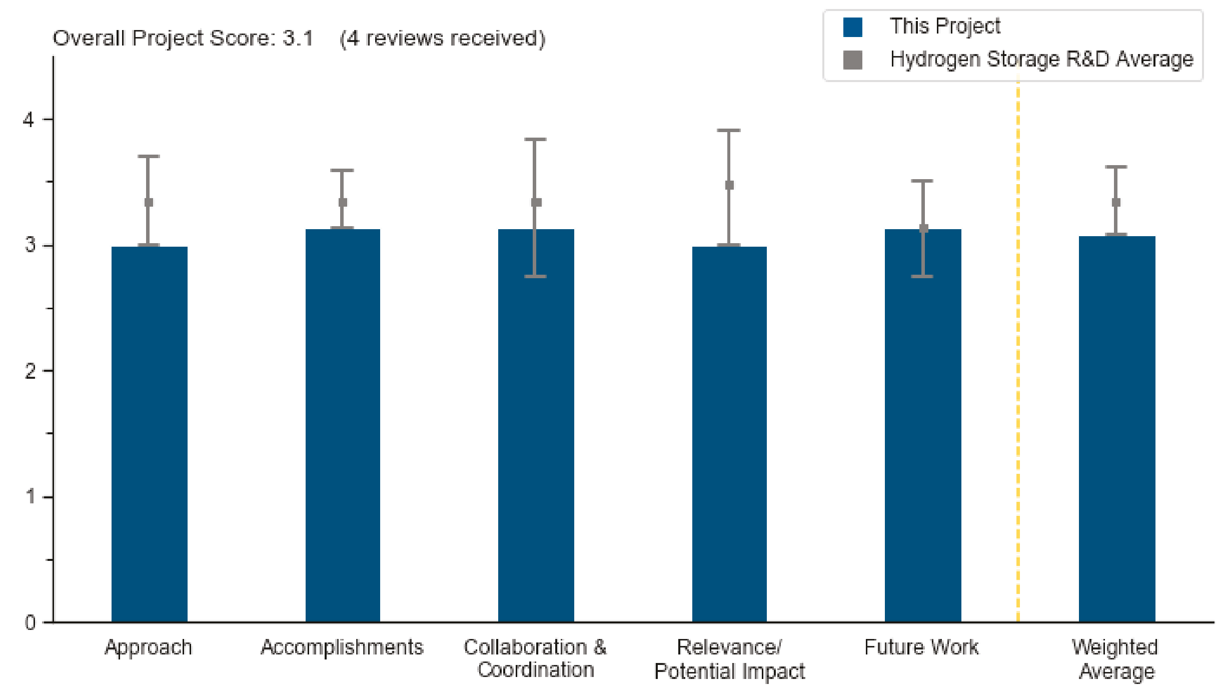
Project #ST-148: Novel Plasticized Melt-Spinning Process of Polyacrylonitrile Fibers Based on Task-Specific Ionic Liquids

Sheng Dai, Oak Ridge National Laboratory

Brief Summary of Project

The goal of this project is to develop a novel plasticized melt-spinning process based on nonvolatile task-specific ionic liquids (ILs) to replace the current solution spinning process. The four main research tasks are (1) investigation of how the molecular structures of ILs dictate plasticizing interactions with polyacrylonitrile (PAN), (2) study of how the chemical interactions of ILs with PAN can be used to control the cyclization degree in intermediate ladder structures, (3) integration of the information gained from the first two tasks to develop IL-assisted melt-spinning systems, and (4) demonstration of considerably enhanced production efficiency of PAN fibers. If successful, the developed technology is expected to result in significant cost reduction for carbon fiber.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Storage R&D projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The use of ILs in a melt-spinning process appears innovative and has been shown to reduce melt temperatures of commercial-grade PAN. An issue with the work scope is that this project, although needed and useful, may not be the most critical link in developing cost-effective carbon fiber for hydrogen storage applications. The effort devoted to understanding the stabilization process for PAN fibers is questioned. This is a well-known, or at least well-practiced, process, and Oak Ridge National Laboratory (ORNL) should already have a good understanding of this process. The morphology of the fiber-drawn PAN fiber precursor appears to be excellent.
- The novel approach is an excellent idea to improve the processability of the PAN precursor and understand the effects of the IL on the fiber properties. Being able to melt-spin PAN would be a benefit, lowering the processing costs to be similar to gel spinning. The approach is very logical and appears to be well executed.

- The approach to producing a new melt-spinning process for PAN using ionic liquids is unique and fits well into the U.S. Department of Energy project portfolio. It is stated that the cost will be reduced by using this process, although a technoeconomic analysis is yet to be completed. However, it is not clear from this presentation how the project is tackling the system weight and volume barrier.
- The approach is to reduce the cost of spinning PAN into fiber by using melt spinning through addition of ILs for plasticization. It is not apparent that this approach will reduce the cost of the carbon fiber; it could make it more expensive. The ILs are relatively expensive and may be recovered for reuse through fiber-washing. Since the fiber must be washed after melt spinning, it is not apparent that this is any better than wet spinning. The project requires a cost model to validate the potential for cost savings. It is not clear at this time whether the IL could result in weaker or stronger carbon fiber.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The author demonstrated >15°C decrease in PAN melt temperature (later stated to be >100°C reduction) and good spin morphology and is processing a commercial range of fiber diameter. A patent for the process is being prepared. Carbon yield greater than 50% was achieved. More progress on the technoeconomic analysis was expected, but the analysis should be ready by the end of FY 2019. The 525 Solutions Inc. analysis of IL costs in the context of the presentation listed a cost advantage that was not converted into process-cost benefit.
- The project is progressing very well and has demonstrated progress on investigating fiber morphology. The fiber surface and core quality will directly affect the carbon fiber properties that will inhibit the fiber property performance. The project has demonstrated the ability to make good-looking, quality fiber that will help toward the project's and DOE's goal of reducing cost with high-performance fibers.
- The progress toward meeting the project objective is good. The solubility and resulting rheology changes made it possible to melt-spin PAN fiber. Washing the fiber showed it may be possible to recover 80% of the IL. It is not clear how any residual IL in the carbon fiber might affect its mechanical properties. While a cost model is being developed to determine the cost of the IL, there needs to be a focus on cost for the new carbon fiber.
- PAN melt temperature has been reduced by an order of magnitude past the milestone goal. The project is well on its way to meeting the next set of milestones. It is unclear how the system weight and volume barriers are being addressed. For the technoeconomic analysis, only the cost of the IL is estimated. It is unclear (quantitatively) whether the overall cost will be reduced. Additionally, from an original equipment manufacturer perspective, these ILs would not be considered a capital expenditure.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- Based on the success of the project, the team appears to be well coordinated. In subsequent reviews, it would help to identify during the presentation, and in the presentation, what part of the work was done with the collaborators.
- ORNL's role was not described in sufficient detail. This project could have the best potential for technology transfer in the near future. It would be helpful to establish a metric from some type of industrial participation before the end of the project.
- There is some collaboration with an IL supplier for technoeconomic analysis. It is unclear if this is really an effective collaboration. Cost analysis of the IL is not sufficient to show whether there are any cost savings over fibers made from traditional PAN. The collaborations within ORNL appear to add good value to the project, though.
- 525 Solutions Inc. is under subcontract to develop technoeconomic analysis and scale-up for IL.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is very relevant to DOE goals and has the potential to have impact on the cost and performance of the carbon fibers related to pressure vessels.
- This project is an incremental but necessary area of improvement for the melt spinning of commercial PAN fibers and associated processing and environmental improvements.
- It is well known that compressed hydrogen technology cannot meet all of the DOE targets, so a project focused on this technology could not be said to significantly advance toward the DOE project goals and objectives. However, this project does align with the Hydrogen and Fuel Cells Program objectives and has the potential to advance progress toward the DOE goals.
- It is too early to determine whether the approach has a pathway to reduce carbon fiber cost. It is also too early to know what type of carbon fiber may be generated using this technology and whether the IL approach will help or hinder the performance.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The future work plans appear adequate for the current stage of the effort: developing a better understanding of IL variants and effects on PAN rheology. The project needs some focus on a comprehensive cost model. The project also needs to validate that residual IL will not disrupt carbon fiber morphology, leading to weaker fiber.
- The project's future work aligns with the overall project objectives. It is, however, still unclear how system weight and volume are affected, and the technoeconomic analysis of the IL by itself seems to add little value to the DOE portfolio.
- The future milestones, future work, and current stage of the project were clearly defined. The possible use of TechPAN is questionable without a clear supply route defined.
- The proposed future work is on target for what needs to be completed.

Project strengths:

- The project is well planned, and it is clear that the principal investigator is a leading expert in ILs. Additionally, the selected ORNL team members are all great complements to one another. The systematic approach and analysis make the project valuable to DOE. For the non-expert, the results are fairly easy to understand after some time with the material.
- There is excellent work on performing high-quality spinning and carbonized fibers. The melt-spinning approach appears to be on track as a viable option to gel-spinning fibers.
- The IL approach did allow for melt spinning of PAN. The cost benefits and carbon fiber properties are yet to be determined. The results could be a strength or a weakness.
- The project's strengths include a reduction in melt-spinning temperature.

Project weaknesses:

- The project is laser-focused on the material aspect, which is both a good and bad thing. Because of that, it is not always clear how the research is addressing the barriers seen on slide 2. For instance, it is clear that the cost is being addressed in a general way. However, the technoeconomic analysis looks at only one aspect of the cost, and it seems that maybe using the IL will actually increase the cost because of this additional component.
- The IL approach did allow for melt spinning of PAN. The cost benefits and carbon fiber properties are yet to be determined. The results could be a strength or a weakness.
- The project's weaknesses include that the team is doing economic analysis at this stage of development, when contact is being made with potential licensees.

- The project needs to have economic data.

Recommendations for additions/deletions to project scope:

- Recommendations include that the project team (1) needs a comprehensive cost model, and of particular concern is the time required to wash the fiber; and (2) needs to determine the effect of residual IL in the fiber on the mechanical properties of the carbon fiber.
- The approach of the technoeconomic analysis needs to change to focus on the cost of the PAN fibers or the carbonized fiber, using traditional PAN as a baseline. Determining the cost of the IL alone does no good in determining whether using ILs results in cost savings.
- The project team should delete the TechPAN work and concentrate on melt spinning of commercial PAN. It may be good to look at any benefits of textile PAN precursor, although melt spinning is already performed.

2019 – Fuel Cell R&D
Summary of Annual Merit Review of the Fuel Cell R&D Subprogram

The Fuel Cell R&D subprogram includes a diverse portfolio of fuel cell technologies to enable low-cost, durable, and high-performance fuel cells for a range of applications. Early-stage research and development (R&D) areas in fiscal year (FY) 2019 include catalysts and electrodes, membranes, fuel cell performance and durability, and assessments. Catalyst and electrode R&D comprises efforts on development and utilization of low-platinum-group-metal (low-PGM) and PGM-free catalysts, with the latter being the focus of work by ElectroCat (the Electrocatalysis Consortium). Membrane R&D includes polymer electrolyte membranes (PEMs), as well as alkaline membranes. Fuel cell performance and durability is the purview of the Fuel Cell Performance and Durability Consortium (FC-PAD). The Fuel Cell R&D subprogram has a portfolio that includes work on medium- and heavy-duty fuel cell applications. The subprogram also includes fuel cell system modeling and analysis, as well as efforts to develop components for unitized reversible fuel cells.

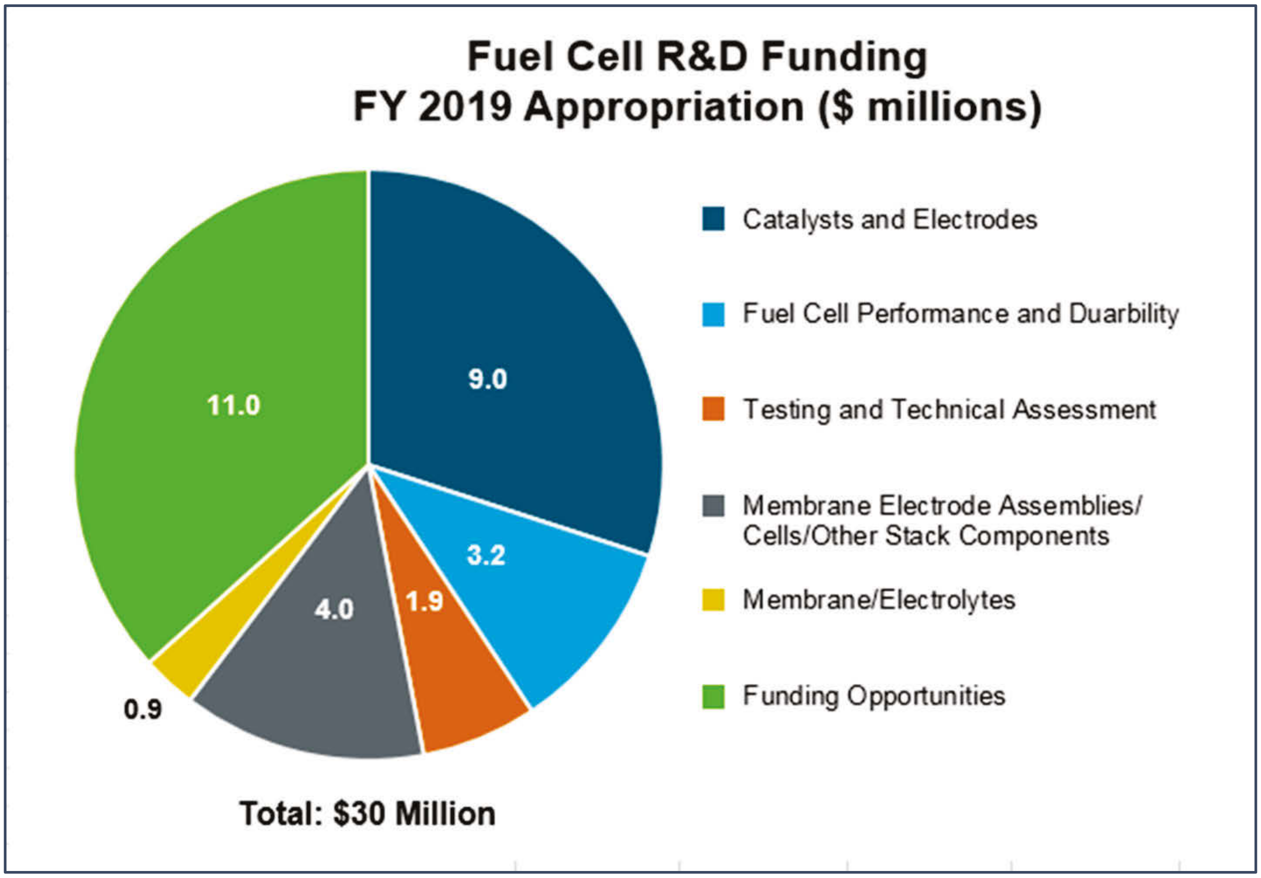
Summary of Fuel Cell R&D Subprogram and Reviewer Comments

The Hydrogen and Fuel Cells Program (the Program) reviewers noted that the Fuel Cell R&D subprogram has a comprehensive, well-structured, and focused project portfolio, with elaborated metrics and milestones, focused on low-technology-readiness-level (low-TRL) research with long-term impacts. The reviewers agreed that the general focus of the various initiatives are in line with the fuel cell industry's long-term needs and that early-stage R&D addresses the primary issues and opportunities. Program reviewers also specifically noted that the consortia approaches with ElectroCat and FC-PAD are well organized to reach the Program's goals and are providing opportunities for more efficient utilization of cross-laboratory capabilities. Furthermore, reviewers agreed that consortia should continue to focus on materials properties work in regard to fuel cell catalysts and fuel cell durability, both of which were repeatedly highlighted. ElectroCat was specifically noted as showing excellent progress in PGM-free catalyst development and performance in MEAs, while working on understanding and mitigating durability issues. Reviewers highlighted the increased emphasis on technology reliability and cycle life as positive. The subprogram was encouraged to continue to support and develop stronger links between the consortia and industry. Reviewers remarked that the consortia- and funding-opportunity-announcement-directed approach to funding will yield highly focused projects. Reviewers stressed the importance of cost reduction in fuel cells, especially in medium- and heavy-duty fuel cell applications. There was agreement that the increased focus on medium- and heavy-duty applications is a strength of the subprogram and will be critically important in advancing adoption in these sectors of industry; the Program was encouraged to continue focusing on these applications. Project reviewers were also impressed with specific project-level highlights and accomplishments, as detailed in the project review reports that follow this introductory summary. Certain individual projects were judged to have unclear or insufficiently defined pathways for hitting their targets and goals within the subprogram and, therefore, to require additional focus.

Forty-eight projects were reviewed, receiving scores ranging from 2.5 to 3.5, with an average score of 3.17. Each of the individual project reports in this section contains a project summary, the project's overall score and average scores for each question, and the project-level reviewer comments.

Fuel Cell R&D Funding

The Fuel Cell R&D subprogram received $30 million in FY 2019. The subprogram focuses on early-stage applied R&D to reduce fuel cell costs and improve performance and durability, as depicted in the figure below. The funding is expected to achieve increased activity and utilization of low-PGM catalysts, PGM-free catalysts for long-term applications, ion-exchange membranes with enhanced performance and stability at reduced cost, improved integration of catalysts and membranes into membrane electrode assemblies (MEAs), and advanced fuel cell performance and durability. Future work is expected to focus on meeting performance, cost, and durability targets for fuel cells with continued work through the consortium approach, further reducing PGM content in catalysts, and expanding the knowledge base to advance fuel cell performance and durability. Approximately $11 million was allocated toward funding opportunities that will support H2@Scale initiatives, including advancing reversible fuel cell stack technologies and prototype systems, as well as medium- and heavy-duty fuel cell applications.


Fuel Cell R&D Funding
FY 2019 Appropriation ($ millions)
9.0
3.2
1.9
4.0
0.9
11.0
Catalysts and Electrodes
Fuel Cell Performance and Duarbility
Testing and Technical Assessment
Membrane Electrode Assemblies/
Cells/Other Stack Components
Membrane/Electrolytes
Funding Opportunities
Total: $30 Million

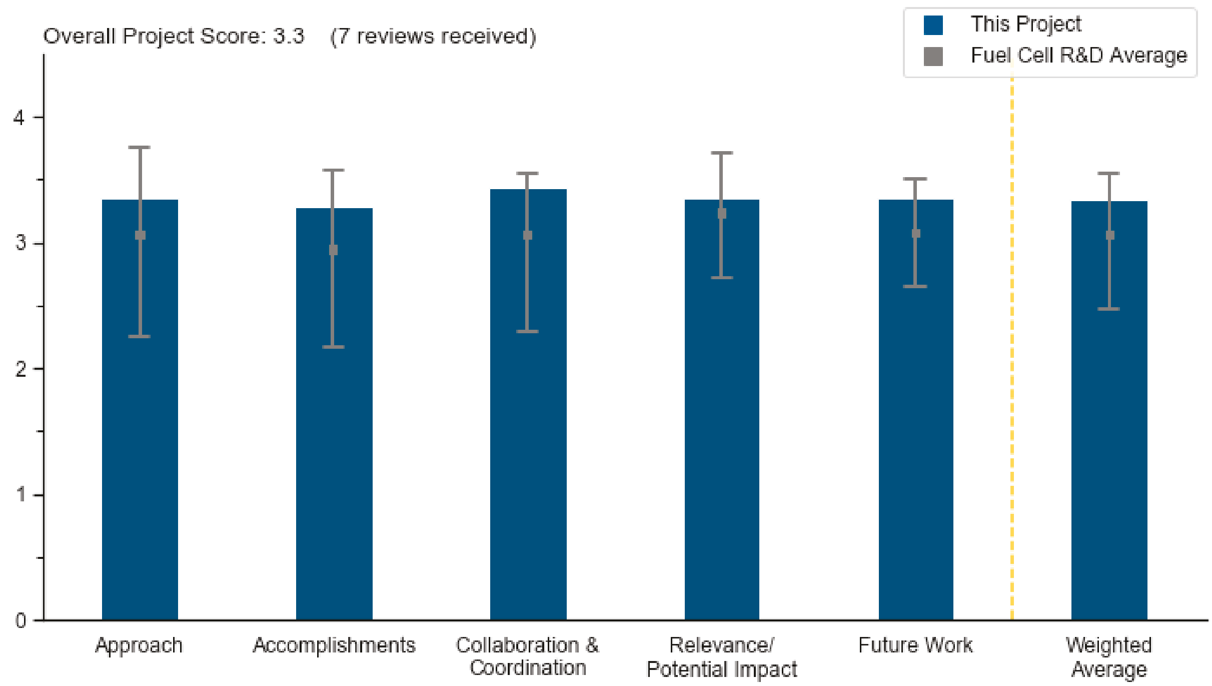
Project #FC-017: Fuel Cell System Modeling and Analysis

Rajesh Ahluwalia, Argonne National Laboratory

Brief Summary of Project

The objective of this project is to develop a validated system model and use it to assess design-point, part-load, and dynamic performance of automotive and stationary fuel cell systems. Argonne National Laboratory (ANL) will support the U.S. Department of Energy (DOE) in (1) setting technical targets and directing component development, (2) establishing metrics for gauging progress of research and development (R&D) projects, and (3) providing data and specifications to DOE projects on high-volume manufacturing cost estimation.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This work is highly relevant to DOE technical targets and provides a needed stack/system element to help ensure research is moving in the right direction. The approach involves development and refinement of a polymer electrolyte membrane fuel cell (PEMFC) system model, including the latest results from other projects. The approach of investigating various design options, heavy-duty vehicles (HDVs) in particular, and using modeling to predict performance and cost makes sense and is helpful.
- ANL uses a variety of modeling techniques to shed light on important aspects of fuel cell design, including platinum-group-metal (PGM)-free catalysts and electrodes, alloy catalyst performance and durability, and design specifications related to heavy-duty applications. This project has excellent continuity through the years and uses robust approaches to modeling and interpreting fuel cell design choices.
- The approach to modeling is sound and has produced good results year after year. These results are important for understanding systems and can have an impact on moving performance forward, but in an indirect way. The attention to different topics is broad and leverages other efforts, although it is not clear how they are delineated or whether they should be independent projects or nested in other activities such as

the Electrocatalysis Consortium (ElectroCat) and Fuel Cell Consortium for Performance and Durability (FC-PAD), where they support other efforts.
- This work is an important part of the Hydrogen and Fuel Cells Program, and it supports many other activities, such as FC-PAD, ElectroCat, and technoeconomic modeling (e.g., Strategic Analysis, Inc.'s [SA's] work). The principal investigator (PI) does a good job at prioritizing areas of focus.
- The work is quite valuable. It hinges on a wide range of collaborations with complementary projects and interactions with numerous partners and organizations. Given the amount of data on cells in transient and dynamic conditions, a complete system dynamic model would be valuable for shedding some light on barriers related to system thermal management and transient operation.
- The approach used in the project is very good. Evaluating the impact of different materials, designs, and some operations is needed to achieve the overall objectives of the project. Now the whole challenge is to prove the validity of the developed tools.
- While not directly working on technologies that could reduce the barriers, the project's modeling and analysis is effectively integrating the efforts and assessing and/or suggesting promising and relevant pathways to pursue.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has many investigations and results. The project progresses well toward the set objectives and the diversity of studied aspects. It also progresses well toward the DOE goals.
- ANL has made significant contributions to understanding important aspects of fuel cell design and the effects of these design choices on performance and durability. The work performed in the last year on PGM-free catalysts and electrodes is very important and useful in helping to guide design of these catalysts and electrodes.
  - That said, the reported results are based on only a single catalyst system (the atomically dispersed Fe-N-C catalyst supplied by Los Alamos National Laboratory). Certain results reported, including the extremely high Tafel slope, seem surprising and may not be accurate.
  - Furthermore, it is likely that related catalysts (for instance, the cyanamide- and polyaniline-based catalysts, or catalysts produced by other ElectroCat partners) may have different properties.
  - Therefore, there is some risk that PGM-free catalyst researchers could go down the wrong path in catalyst and electrode design if they base their design choices on the ANL-reported results.
  - This problem is exacerbated by the fact that there is no experimental validation of the predicted performance enhancements shown in slide 13.
  - Therefore, ANL should be encouraged to perform similar analysis on other PGM-free catalysts.
  - ANL should also try to get experimental validation of the predictions (which would need to be done through external collaboration).
  - The modeling work on kinetic and transport parameters using PtCo data supplied by General Motors is helpful in increasing understanding of the loss mechanism for state-of-the-art catalysts.
  - The analysis of operating conditions and durability related to HDV applications is very helpful in guiding researchers in this increasingly important area.
- The addition of HDVs to the analysis framework is clearly interesting and needed. Quantifying the durability tradeoffs of loading and alloyed versus non-alloyed Pt catalysts will be critical in determining what approaches would be best explored experimentally to validate model findings.
- The results involving PGM-free catalysts are not as compelling; the results highlight how far away the technology is from meeting targets and then also show how activity needs to increase by more than an order of magnitude, with higher loadings and increased active-site densities in engineered electrodes, without presenting any rationale for how this would be accomplished or if it would be possible.
- ANL's accomplishments are relevant, and the team provides excellent data, but it will be interesting to see model validation to give further support to this effort. When presenting the performance and cost targets, a sensitivity analysis of the different parameters should be added to evaluate the most sensitive ones. Investigation of a PGM-free catalyst in the study is relevant, but several types should be used, in particular at least one PGM-free and Co-free catalyst. The project's investigation of HDVs this year is interesting,

and the first results are useful. Nevertheless, close collaboration with FC-PAD seems necessary to use relevant accelerated stress test (AST) and load cycles for durability estimations.
- Many results are presented here. However, the PI should also strive to make stronger conclusions. The results are almost always presented as “preliminary results” or “prone to changes” and really impactful conclusions are never made. For example, it is unclear what decay mechanisms FC-PAD should be focused on, or what HDV hybrid configuration should be focused on.
- ANL has demonstrated progress toward DOE goals. For future work, additional details on the methodology for reaching DOE targets in performance and cost would be helpful, along with details on the mechanisms for improving power density.
- The project continues to meet annual project goals.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The PI does a great job of engaging with multiple other project teams and a variety of entities. However, a major improvement would be to increase the likelihood of these other projects’ success. An example here would be to model range-extender fuel cell electric vehicles (FCEVs) and show how they can have a significant and positive impact on durability and vehicle efficiency. This may encourage the assessment of range-extender light-duty vehicles (LDVs) (as well as others) by SA, which may result in success in showing reduced cost and/or durability.
- The level of collaboration and coordination, with both industrial and academic relationships, appears appropriate for this type of project. Collaboration with FC-PAD and ElectroCat should be further enhanced, in particular to integrate durability data from single cells and stacks as well as performance from new catalysts and HDV applications.
- The collaboration with other consortia, industries, and working groups seems effective. Collaboration with SA seems relevant, and it may be that additional collaboration with end users could be relevant to obtaining real operation data at stack and system levels.
- The project is well integrated with DOE national laboratories, FC-PAD, and the PIs and projects under the DOE and U.S. DRIVE Partnership portfolio.
- The collaborations from this effort are significant and good, but they are leveraged interactions with other projects, and the ability of this project to specifically request experimental findings to validate models is a minor weakness. If this project is just to validate experimental findings, this lowers the project’s impact but improves its collaboration.
- There is overall good collaboration. More experimental collaboration on validation of model predictions, especially for the PGM-free work reported this year, would be helpful.
- The project is based on a strong interaction with other institutions and partners.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The developed system model is very relevant, as it is generic and takes different scales into account. Therefore, it is of great interest to DOE, as it supports setting technical targets and redirecting component development. The model also allows for assessing performance and degradation toward DOE objectives, and the collaboration with SA allows for proving relevant data for estimating high-volume manufacturing cost.
- While not working directly on technologies that could reduce the barriers, ANL’s modeling and analysis effectively integrate the efforts and assess and suggest promising and relevant pathways to pursue. The durability model, if fully realized, would be a significant addition.
- Examining system designs and modeling the effects of design decisions on performance and cost are helpful to building understanding and informing R&D decisions. The new work on heavy-duty applications is timely and relevant.

- The project is relevant in its role of integrating evolutions of component and sub-component performance and durability as system architectures and subsequent system performance and durability. This project has a strong impact in helping SA better estimate the status of cost. However, the impact might be even higher if the model could have been validated at stack and/or system level, not only at single-cell level.
- The project fits very well within the FCTO Multi-Year Research, Development, and Demonstration Plan.
- The project supports efforts to achieve DOE targets through modeling studies and collaboration. The project itself does not meet or attempt to meet DOE targets.
- To have a higher impact, the P.I. will need to make more solid and impactful conclusions.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- It is necessary to (1) examine and evaluate the behavior of the different solvents in the gas diffusion layer and catalyst (carbon and ionomer) environment, (2) explore advanced characterizations, and (3) continue the very interesting work on break-in and conditioning. The proposed future work should be separated into two levels: the first one, which is the "immediate future work" deriving from the conclusions of the actual achievements, and the second level, which is the recalibration of the objectives with regard to the new findings, eventually updating the work directions (taking into account the impact of the current achievements and how performance and durability can be improved).
- The proposed future work includes further support of the SA cost modeling, along with modeling of electrode and catalyst effects for PGM-based and PGM-free catalysts, further HDV modeling, and improved integration of durability into the system analysis. All of this work will be helpful to DOE and to fuel cell researchers.
- Further efforts in medium-duty vehicle (MDV) and HDV markets clearly make sense. Trying to incorporate durability considerations in systems analysis is a challenge, but it is also required. The other proposed future work is a continuation of existing projects and has the ability to leverage other funded efforts.
- The proposed future work is pretty much a continuation of the project mandate of updating technology assessment. Durability model progress and validation can be of significant benefit.
- The future work is well planned. A more detailed modeling for fuel cell systems would be valuable as a future contribution. This should include balance-of-plant (BOP) and thermal management dynamics.
- The proposed future work is good. The project team should add range-extender LDVs.
- The proposed future work is in line with the overall targets.

Project strengths:

- The tool is very powerful in the sense that it is versatile and multiscale (i.e., component, stack, system). It is also being updated with new achievements. The project is collaborating with SA to have up-to-date cost estimation with new material and designs. This year, the investigations of operation modes (approaches to limiting degradation during shutdown and start-up from sub-freeze temperatures as well as idle) are very relevant. The same goes for AST and conditioning (even if the operating conditions for conditioning are not clearly specified and validated).
- The ANL team is highly experienced and skilled in performing analyses of PEMFC components and systems, and ANL works in a well-coordinated manner with the SA team.
- The team has excellent continuity, as they have been working in this space and refining their modeling techniques for many years. Every year, the team expands the envelope of design factors analyzed, making the project increasingly useful.
- The project's strengths include the team's analysis expertise, access to world-class diagnostics, and close association with the DOE and U.S. DRIVE fuel cell community.
- The project's strengths include experience and skill in the area and established methods and approaches, as well as connections to the community and different projects.
- The project can count on a wide network of collaborations, strong capabilities in fuel cell testing, and knowledge in degradation mechanisms.

- The project's strengths include picking good things to analyze and its good engagement with a range of collaborators.

Project weaknesses:

- The project has a very interesting approach to the system modeling; however, the choice of investigations could be discussed, such as investigating operation at high pressure while the trend is to simplify the system, therefore operating at lower pressures. Operating at slightly higher temperatures with new membranes could avoid the investigations around water management.
- ANL should include more sensitivity studies to identify what key improvements can enable substantial improvements in performance and durability. The model should be validated at a stack and/or system level. It is difficult to rely on a model based solely on experimental single-cell testing results.
- The project so far seems to be lacking more insight on the system simulation side, which could be easily validated given the insight available to the authors from their experimental work.
- There is no specific funding for experimental measurements or direct connection to experimental validation within this funded effort.
- More experimental validation of model predictions is needed.
- The impact on the FCTO is less than it could potentially be.

Recommendations for additions/deletions to project scope:

- It is recommended that the project team pursue the work on operating modes such as the impact of different shutdown procedures, conditioning, and idle. The mechanisms behind those operation modes should be investigated. In general, the input and specifications should always come from real operation at system level. This allows for more efficiency in materials investigations. It could be of great interest if the consortium releases recommendations for the most relevant and safest protocols. Investigations of system operation with the BOP components are very relevant. However, investigations should be oriented toward the desired simplified model and its impact on the stack components—for instance, operation with lower pressure and higher temperatures (membrane materials). ANL should also assess the impact of characterizations on durability since they are also part of the real operation. The model should be updated to integrate these operation modes.
- The project team should focus on longer-durability applications in which cost or durability is a major tradeoff, as well as crossing the line to include systems analysis for cost considerations. These applications would best be studied by leveraging SA's efforts but using the models developed here to feed into the cost studies, building on the technoeconomic analyses.
- It would be preferable to see focus on the durability model. Both this and the SA projects are now addressing MDV/HDV fuel cell applications. Both teams would benefit from more clearly defined targets for these systems.
- ANL should investigate a PGM-free and Co-free catalyst in the study.
- The presentation slides do not need to be so busy. The project team should pick just a few key conclusions and show key results that support these major conclusions. The rest should be backup material.
- Additional insights could be provided on the feasibility of the improvements suggested for performance and cost targets.

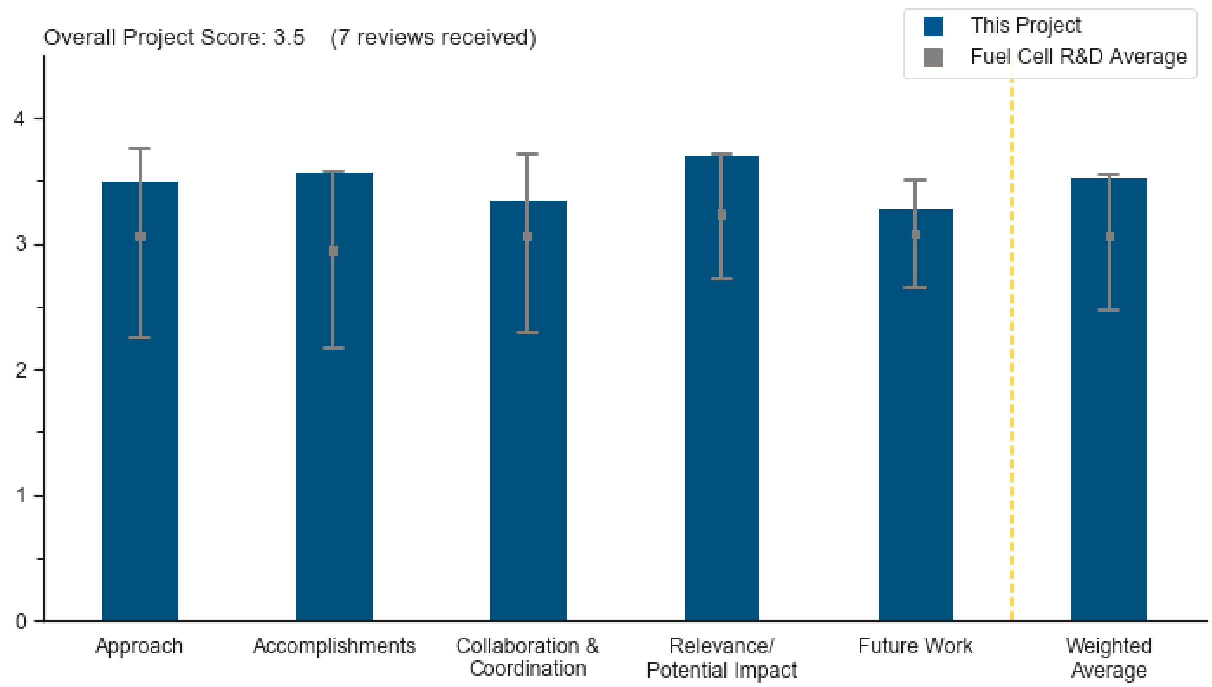
Project #FC-135: FC-PAD: Fuel Cell Consortium for Performance and Durability

Rod Borup, Los Alamos National Laboratory

Brief Summary of Project

The Fuel Cell Consortium for Performance and Durability (FC-PAD) coordinates activities related to the denoted development areas and supports industrial and academic developers. This effort aims to advance performance and durability of polymer electrolyte membrane fuel cells (PEMFCs). Researchers will develop the knowledge base and optimize structures for more durable and high-performance PEMFC components; improve high-current-density performance at low Pt loadings; improve component durability; and develop new diagnostics, characterization tools, and models.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Addressing durability and performance of fuel cells is not a simple task. It needs investigations of different disciplines (thermics, fluidics, material science), with different expertise, at different scales (component, cell, stack, system). It needs also to combine all the generated knowledge in such a way that allows comprehensive interpretations. The approach of gathering the needed capabilities at national laboratories and combining them with different funding opportunity announcements (FOAs) and other collaborations is excellent. The matrix organization between components and cross-cutting thrusts seems very efficient, covering almost all the components of a cell (other stack components need to be addressed as well). The FC-PAD organization succeeded at clearly defining and structuring the sub-objectives.
- The combination of modeling work and expertise, a suite of in situ characterization techniques, and technical expertise has resulted in a more detailed understanding of fuel cell performance and durability. The systematic approach that has been taken, along with the targeted collaborations, has been very successful to date.

- The approach of coordinating the investigation of the performance and durability of fuel cells through a partnership between national laboratories and other organizations in a five-year project is excellent. This project appears to have a very structured approach, combining the strengths and capabilities of the different national laboratories involved.
- The alignment of the national laboratories' efforts in this area is an excellent approach to complement the strengths of each. The result is a generally comprehensive strategy investigating modeling, characterization, cell testing, and durability testing.
- This very strong team is taking a well-crafted approach to improving the science behind component-level integration in PEMFCs. The only area where the work could be clarified from an approach perspective is to be clearer about how samples and information are being efficiently shared among team members.
- The approaches in the different subareas of the membrane electrode assembly (MEA) are appropriate and are addressing the key areas that need to be better understood. Having a coordinated effort among all the parties, in particular the national laboratories, will increase the likelihood of a successful outcome. The way the division of the effort is organized is also excellent. Communication must remain the top priority of such an effort, as it seems to be. The only concern is the groups going off on different, unrelated tangents.
- The approach is sound. Two areas of improvement are recommended for consideration: (1) It should be clearer how the project objectives are set based on input that goes beyond the Fuel Cell Technical Team and encompasses the broader fuel cell international community. For the work to stay relevant, it is paramount that a large number of stakeholders, especially from the industry, can have a say in setting the goals. (2) The project aims at addressing a large number of technical challenges. It seems that this approach may somewhat dilute the resources; further prioritization might be beneficial.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The degree of detail and results presented at the review was exceptional. All topic areas showed significant progress in everything from microscopy to electrochemical testing. The modeling should progress nicely as the data become available. The activities are focusing on the right metrics. Regardless of the ultimate outcome, a wealth of knowledge will result that then can (or will) be used to design and engineer the next-generation MEA. The accomplishments are still mostly macroscopic in nature. In time, this should pave the way to more mechanistic, molecular-level investigations.
- To date, progress has been excellent in terms of development of models, detailed characterization of targeted aspects of the MEA, and analysis of the impact of MEA characteristics, including loading, carbon type, ink solvent, etc. The project team has developed useful insight to this point.
- The team is making tangible progress in every area: ionomer and ink processing, catalysts, etc. This is very good work.
- The results presented deliver clear value, especially the work performed to understand the catalyst layer manufacturing properties; this is seen as directly transferable to the industry.
- The objectives of the project are clearly defined and structured, and they are well-aligned with DOE goals. The project is progressing properly toward the realization of these objectives. Certain aspects have been validated, but the accomplishments toward DOE goals cannot be discussed yet. Further validations are still needed.
- The project's accomplishments and progress are effective. The project clearly addresses the DOE targets in terms of performance and durability of MEAs and their components. The impressive results are reflected in 24 publications again this year. However, as there are so many results, they need to be well-structured within a one-hour presentation in order not to be overwhelming. To facilitate the reviewers' work, either fewer acronyms should be used, or a dedicated glossary slide should be integrated.
  - To capitalize on all this knowledge, there should be a dedicated action (on the website) in the consortium to gather all the data resulting from FC-PAD.
  - The platinum-group-metal (PGM)-free catalyst investigated contains cobalt. From a critical raw materials perspective, this means that this issue is not solved. Therefore, FC-PAD should also investigate PGM- and Co-free catalysts.

  - Accelerated stress test (AST) protocols should be developed to investigate component degradation mechanisms. FC-PAD should also investigate degradation mechanisms occurring in stack operation.
  - The ink study has shown interesting results. However, all the experiments referred to electrodes produced by spraying technique. As this technique is not the most-used industrial technique of electrode coating, complementary techniques (slot-die casting, microgravure, screen printing) should also be investigated to quantify the materials and process impacts on durability.
  - FC-PAD investigation and knowledge may also apply to applications other than PEMFCs (e.g., anion exchange membranes [AEMs] or electrolysis).
- The break-in procedure is clearly ineffective to have had such poor performance, but it is difficult to judge what is going on without knowing what the procedure was. The work on conditioning effects is nevertheless useful and important to guide both the ability to get maximum performance out of a given design and to guide factory acceptance testing. It is also important to characterize and understand new material sets as they are introduced. The ink solvent effects are important, and the work is providing useful and interesting results with linkages to expected ionomer behavior. One caution is that ionomer-to-carbon/solvent systems are difficult to generalize, and conclusions should not be applied too broadly. The work is valuable to guide the types of investigations that can be applied to different systems. The characterization of aggregates and agglomerates is very interesting and useful. The study on interactions between carbon pores, water, and Pt locations provides useful work and linkages to the model. For the catalyst AST, which was examined for the loading study, it would be useful to plot the change in the catalyst's specific activity to separate out the change in surface-area kinetic effect from the change in Co-associated kinetics. It is useful to pursue membrane degradation modeling. In reference to Ce migration and its effect on membrane properties and thin films, the results are interesting and deserve further investigation.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- There is excellent collaboration with other national laboratories. The amount of collaboration with each of the FOA-1412 projects is likely more properly assessed in their presentations.
- The structure of FC-PAD is based on collaborations. This aspect seems to be very well-thought-out and done either in the frame of the FOA (interactions with the DOE-awarded FC-PAD projects led by 3M, General Motors, United Technologies Research Center, and Vanderbilt University), in which regular follow-up conference calls and in-person meetings are set, or out of the FOA frame, including international collaborations. (It is not clear though, how the intellectual property management and information/data exchange are managed in the latter cases.)
- The collaboration between the project's partners is intense and emerges clearly from the presentation. The project team is encouraged to seek more input (or make the input more visible) from the larger community in the prioritization of goals. This work is valuable and must remain relevant to the whole industry.
- The collaboration between the different partners is well structured and well managed and appears very efficient. Enhanced collaboration with the National Renewable Energy Laboratory (NREL) manufacturing team will enable greater understanding of degradation mechanisms, including process impacts on these mechanisms. Collaboration with Argonne National Laboratory and Strategic Analysis, Inc., will be needed to investigate medium-duty (MD) and heavy-duty (HD) vehicle applications.
- The collaboration is excellent based on the coordinated results reported at the review. The project team must ensure that communication among all parties remains the top priority. An area of concern related to collaboration is the dependence on certain suppliers and the subsequent materials selection. Comprehensive studies are being carried out on just a few suppliers' products (gas diffusion layer [GDL], catalyst, carbon source [e.g., Vulcan®], ionomer, etc.). As related to collaboration, the supplier collaborative effort should be expanded. Not all Pt/C catalysts are the same. It is unclear how to improve this activity, especially if the material is proprietary.
- The team has shown good collaboration with partners, both funded through the FOA and unfunded. One of the consortium's goals was to highlight the utility of the national laboratory teams in addressing research

issues and challenges that may be facing industrial and academic researchers. This may be more of a comment for DOE rather than the team associated with this project, but it would be helpful if there were a detailed plan to make these resources available to those outside the national laboratories and the FOA associated with this consortium.

- The rating here might not be fair, but the team did not do a particularly great job in the presentation of describing how the team is integrated. For such a large project, it is easy for all of the members on the team to have their own pet projects, with limited coordination between the individual members. Next time, it would be very helpful for there to be a slide dedicated to this beyond just an organization chart.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Durability and cost are the two main aspects that have been identified by the Fuel Cell Technologies Office (FCTO) Multi-Year Research, Development, and Demonstration Plan (MYRDDP) as key still-missing points for fuel cell commercialization and deployment. In that sense, the work done by FC-PAD is absolutely necessary, not only to assess the advancement toward those two objectives but also to generate innovative breakthrough technologies and materials that are needed to meet MYRDDP objectives. FC-PAD's mission is to generate the necessary knowledge to understand (operation and behavior, components, faults, degradation, interactions, and impacts of operating conditions) and, based on this knowledge, direct the research toward innovative components and elaborate and test them in real operating environments. With that, the mission includes being able to provide clear directions to durability improvement (with cost reduction) to at least reach the MYRDDP objectives.
- The project is totally relevant. The MEA's limitations, performance, and cost factors are clearly impeding, or will impede, the acceptance of the technology by both the producers of the components and fuel cells and the customers. Removing the cost/durability issue will be the primary "win" if the technology can be demonstrated to achieve lifetime, cost, and durability targets.
- Durability, particularly of MEA components, is of critical importance for PEMFC commercial viability. This project details and studies many of the aspects of MEA design that can limit durability. The work completed to date has provided useful insight into many of the mechanisms of degradation and will likely have an impact on future efforts to improve durability.
- The project looked at components under several lenses. It will be important to dedicate efforts to integrate the information and interpret the data at system level. In fact, as stated by the presenter, the belief is that the interfaces between components are the key and must be looked at with a holistic and systematic approach.
- FC-PAD is of very high relevance for the FCTO in achieving MYRDDP targets. Concurrently achieving cost and durability targets is the real key driver.
- The project is providing key insight into all the highest-priority performance and durability mechanisms.
- It would be nearly impossible to find another project more aligned with FCTO targets.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed future work is in coherence with the addressed conclusions. It is in fact necessary to examine and evaluate the behavior of the different solvents in the GDL or catalyst (carbon and ionomer) environment, to explore advanced characterizations, and to continue the very interesting work on break-in procedure and conditioning. The proposed future work should be separated into two levels: the first level, which is the "immediate future work" deriving from the conclusions of the actual achievements, and the second level, which is recalibrating the objectives with regard to the new findings and eventually updating the work directions (taking into account the impact of the current achievements and how to improve performance and durability).
- The proposed work in the near term is appropriate, as the activities reported are not complete. These activities must continue in all areas. From such results, the modeling should evolve into a tool that may dictate changes in the MEA. This is the most valuable outcome. Materials, architecture, conditioning,

particle sizes and distributions, loadings, etc. should all be scrutinized in the results of the current work in order to derive the model. The proposed work supports this. After the current activities have been carried out, the electrode effort should review the hydrophobic/hydrophylic character in the membrane and electrode interface, as well as in the body of the electrode. The microlayer should also be re-evaluated. The following topics should be incorporated in the test plan:
    - Interface chemistry and architecture, especially of the cathode
    - Impact of the fluoride ion released in the first 100 hours and its impact on the electrode properties, in particular the wetting character
    - Impact of various pre-treatments on the carbon used for the catalyst support, GDL, and microlayer
    - Use of carbon other than Vulcan
    - Electrode structural changes and their impact on performance using 3D printing vs. spray vs. doctor blade-like application methods
    - Hydraulic properties of the electrode, microlayer and GDL (possibly using the National Institute of Standards and Technology neutron facility)
    - Energetics of the proton-ionomer dynamics
    - A revisit of the older proton mobility question of McBreen, performed in the 1970s, especially on the cathode
- The project’s future work is detailed and well-structured.
- The proposed future work seems to be aligned with industry needs. It is recommended that the project focus the scope even further and consider the interfaces between components as part of the work.
- The proposed future work is mostly straightforward; it would be very helpful if there were more focus on predictive rather than descriptive approaches.
- Regarding requirements for HD applications and research directions, there are a significant range of HD requirements, and not all can tolerate lower power density. The space (or size) of the system can be very important. Cost will also continue to be critical, thereby driving a need for high area utilization of the fuel cell and high current density. Since the durability is critical, the oxygen transport limitations at high current density also become very important later in life as the Pt surface area is reduced. Membrane durability modeling, ionomer film aging, and Ce effects are all areas that should be continued but are not explicitly mentioned in the path forward.
- The move to MD/HD vehicle application is relevant but will induce an adaptation of the ongoing studies, materials, and operating conditions used for the testing. The move has to be well-prepared. Specific AST protocols will have to be defined. Collaboration with the NREL manufacturing team should be foreseen in order to include some manufacturing process aspects (e.g., ink viscosity and coating technique) in the comprehension of degradation mechanisms.

Project strengths:

- The project’s strengths include clear objectives, excellent organization for efficient multi-laboratory coordination, different competencies (elaboration, testing and characterization, modeling), means, and different collaborations (e.g., laboratories, universities, and industries). All these points make the project solid and efficient.
- The project’s strengths include its highlighting of the critical aspects of MEAs that have directly impact on durability, its detailed experimental and computational analysis of relevant MEA operational processes at a range of length scales, its efficient use of DOE resources, and its adequate integration of research partners.
- The composition of the consortium, the coordination of the project, and the well-defined role of the different partners involved are real strengths. There is a strong focus on publication of the results in a large number of publications to share as much as possible with the international community.
- The multi-laboratory and multi-level approach to studying a broad range of higher-priority degradation and performance mechanisms is a key strength. The outstanding characterization capabilities really drive the in-depth understanding.
- This project has a very strong team and a very clear pathway for development toward FCTO goals.
- This is a well-articulated project with excellent connections between the national laboratories.
- This project is an outstanding coordinated effort by some of the best folks in the country.
- Experimental resources at the laboratories and knowledge of materials and electrochemistry all converged and were coordinated.

Project weaknesses:

- There are no project weaknesses, per se; however, the coordinated effort needs more than one person to manage such a large and important project. The project team needs someone to assist in "seeing the big picture." So much data is being generated that it is necessary to have not just a coordinator of the efforts but multiple people with a higher-level, broader perspective overseeing the technical results. This might already exist.
- It is difficult to find any weaknesses.
- It would be helpful if, in the presentation, the team would dig a little deeper regarding how information moves between partners to realize the strengths of all of the partners. It is clear that good work is being done, but the presentation did not make it clear whether we are seeing the result of several excellent pet projects, or a large volume of information (and possibly materials) is changing hands between the partners. The team is also focusing on a very narrow set of materials, which (although it can provide fundamental insight) can stifle innovation. The modeling work, or at least how it is presented, appears to be very descriptive, and it was not clear what has been done to enable the team to be structurally predictive in the future. The team is not clear about how the information is being used for the predictive synthesis of materials and/or electrode structures.
- FC-PAD is doing tremendous work investigating different components with test/characterization and modeling; this is necessary and should be pursued. However, the real operation vision of the work is missing; in the end, what is needed is an operating system with optimized durability and cost. Now optimizing the components needs to be done in their real operation environment. A global optimization is not the sum of single-component optimizations, especially in a complex, multiphysics and multiscale system like a fuel cell system in which a large number of interactions exist. Optimizing components should be done—but with a stack- and system-level input. The validations should also be done at stack and system level. Even if investigations are done at component level, the problem must be set at stack and system level (including hybridization architectures). For instance, using AST for a component such as a catalyst cannot validate degradation under real operation of the cell (in a stack inside a system) because the degradation mechanisms of each component are not fully independent. There are interactions, and the degradation might be completely different under real operation.
- The presentation's slides lack clarity for some protocols and conditions, such as the break-in procedure. This is a clearly ineffective break-in procedure to have such poor performance, but it is difficult to judge without knowing what the procedure was. In general, although there is a lot of good data, there are a number of places where plots are not sufficiently labeled, conditions are not always given, there are not enough legends, and fonts can be too small to read. The value of the ordered array electrodes is not clear. Modeling to support this work is recommended. The performance with fill carbon is improved but still not good. The value of this work has not been established.
- A weakness of the project is its very large scope, which may lead to some loss of focus in the different activities. Using only sprayed electrodes appears also to be a weakness, as it is not the most representative coating technique for electrodes and leads to the absence of investigation of the manufacturing parameters' impact toward degradation.
- The project needs more industry input, deeper focus on fewer tasks, and a more holistic approach to study interfaces.

Recommendations for additions/deletions to project scope:

- The difficulty of the task is that investigations must be done at different scales, and degradation metrics must be defined at all steps. The researchers should, however, keep in mind that the final durability objective is located at the final object level (stack/system). Connection between durability at material level and stack/system level should always be clearly defined, because the final aim is stack and system durability. The work is great and should be pursued; the problem should be set slightly differently. The specifications should also come from system and stack, and for real operating conditions. Collaboration with higher technology readiness level (TRL) consortia (stack- and system-level partners) is recommended in order to have input for characterization, testing, and real operating conditions. It is the same for validations, which should be done at system level. The model should also be multiscale going from component to system, and fault and degradation propagation between components and scales should be integrated into the models. The metrics to assess how well the ASTs perform should be clearly defined and located at stack/system level. ASTs should be updated to mimic degradation such as it results from real operation. One way to improve durability is to take advantage of the recovery phenomena (the real operation will certainly include some idle-modes recovery). Therefore, mechanisms behind voltage recovery should be investigated; additionally, how those mechanisms are correlated to aging and operating parameters should be investigated. The influence of different shutting-down protocols (with or without nitrogen) on these performance recovery phenomena is unclear. The parameters defining voltage recovery intensity (soak time, temperature, shutdown procedure) are also unclear. All these aspects are of great interest to improving durability in real operation. Work can be done at low TRL, but the requirement should come from system and stack to be more realistic.

  - Globally, and as a summary, durability in a fuel cell system could be linked to the following: choice of materials (investigated in FCPAD) and architectures; stack assembly, terminal plates (durability, cost, performance), and gaskets (durability under operating condition, leaching pollutants and their effects), as well as stack assembly techniques (pressures); and effect of system operation with real operating cycles, different hybridization schemes). These aspects should be investigated concomitantly; optimizing one single aspect independently of the others is hard to validate in a complex system with a lot of interactions, such as in fuel cell systems. It is recommended that the project team open the consortium to other partners to take into account system consideration, and slightly update the organization of FC-PAD to adjust the problem inputs and validations.

- The next level of research should go into a deeper dive regarding the electrode dynamics. For example, now that there are "visuals" such as the ionomer in the electrode(s), the actual function of that ionomer film or particle, whatever it is, is still a question. This needs to be done on many different levels. For example, it is unclear what the impacts are of voltage, current, or hydraulic effects on the electrode as a function of the distance from the membrane. It is also unclear whether there should be a hybrid approach to an ionomer/polytetrafluoroethylene (PTFE) electrode based on the results. Answers to these questions might possibly provide additional knowledge for developing a better electrode structure. In addition, with the current resources, it is unclear whether it is of value to understand the energetics of the ionomer–proton transport concept within the membrane (but away from the surface of the membrane). One could ask what the driving force is of an ionomer particle that may or may not be in physical contact with other ionomer particles or films in the electrode—a particle that is microns away from the membrane—to transport a proton. Even if a proton could make it to the far reaches of the electrode, it is unknown how much energy it takes to jump from an ionic-like solution in the pores of the electrode to sulfonic acid sites of the ionomer. It is also unknown what the delta H of solvation is, as well as the transition from a liquid phase to the bound ionic phase. It is unclear whether this impacts performance or whether the ionomer positioned away from the membrane acts only as a wetting site. Lastly, and related to the above, there is a question of how electrode architecture differences affect the key metrics. Perhaps there should be exploratory electrode structure activities.
- The project team should evaluate the effectiveness of AST protocols in predicting component and cell lifetimes in real devices. The team should also use its tools and knowledge to better direct where the technology is going. Of the materials and approaches the team has tested, it is unclear which are very unlikely to meet targets. The team should also develop a robust synthesis and structure a database of material sets. It is unclear whether the project team can leverage what FC-PAD has done or is doing to facilitate more rapid growth in other areas, e.g., AEM fuel cells and electrolysis. Specific to AEM fuel cells, this seems to directly fit into the scope. Granted, three years ago, no one would have seen that AEM fuel cells would get to >3W/cm^2 on H_2/O_2 and 1000+h durability. However, now they have, and there are at least as many fundamental questions as AEM fuel cells. Some of these questions are even more troublesome, with no clear existing pathway for electrode design approaches, ionomer–catalyst interactions, water management, CO_2, etc.
- The project team should initiate close collaboration with the NREL team working on electrode manufacturing in order to include these aspects in the comprehension of induced durability impact. The project should also investigate a PGM- and cobalt-free catalyst.

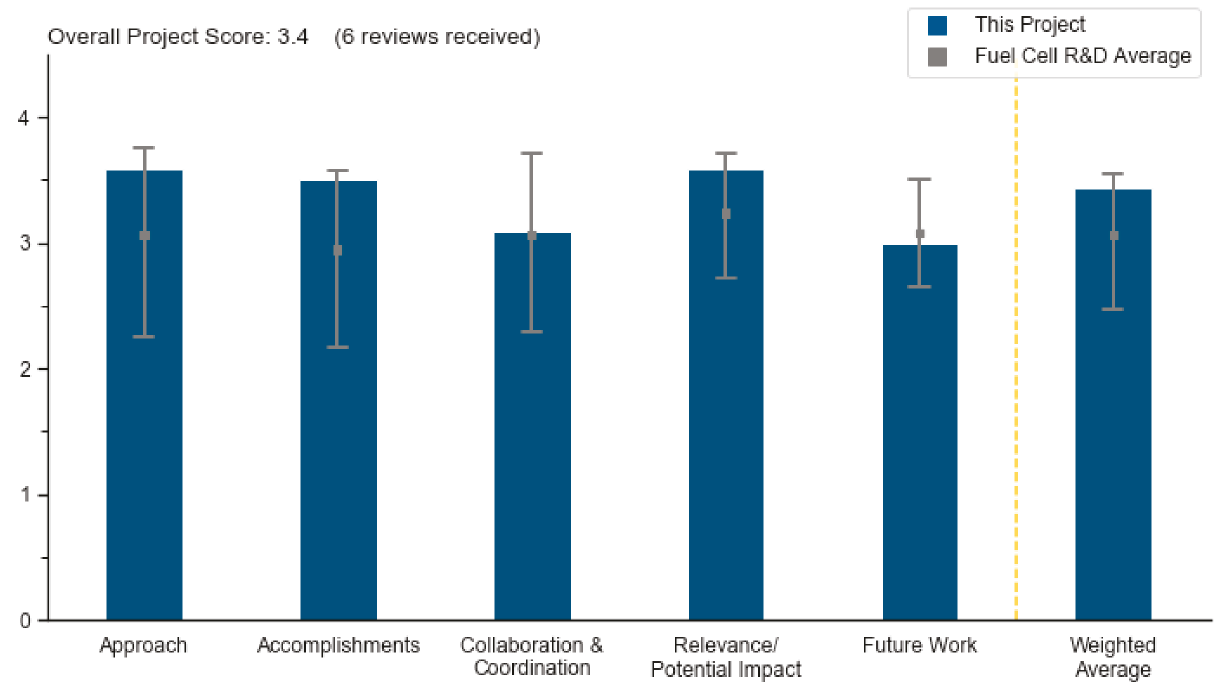
Project #FC-140: Tailored High-Performance Low-Platinum-Group-Metal Alloy Cathode Catalysts

Vojislav Stamenkovic, Argonne National Laboratory

Brief Summary of Project

A primary focus of the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (the Program) is development of highly efficient and durable Pt alloy catalysts for oxygen reduction reactions (ORRs) with low Pt content. This project will go from fundamentals to real-world materials to achieve rational design and synthesis of advanced materials with a low content of precious metals. Researchers are taking a materials-by-design approach to design, characterize, understand, synthesize/fabricate, test, and develop tailored high-performance low-Pt-alloy nanoscale catalysts.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The catalyst development approach at Argonne National Laboratory (ANL) is unparalleled in terms of the team's abilities to develop and characterize catalysts across the range from fundamental studies of well-defined single crystals to practical scalable thin films and nanoparticles.
- The materials-by-design approach is excellent for improving catalyst performance and durability. Many high-activity Pt alloy catalysts are synthesized in this project, while much effort was focused on understanding Pt or alloy metal dissolution rate.
- The technology based on a materials-by-design approach for the synthesis of low-Pt-alloy nanoscale catalysts is specifically focused on overcoming critical barriers. The approach is feasible and well integrated with other related efforts in the field of designing durable low-Pt architectures.

- The materials-by-design approach taken to designing and characterizing low-platinum-group-metal (low-PGM)-alloy catalysts is comprehensive, including design, synthesis, characterization, scale-up, and fuel cell optimization.
- ANL's approach is novel and has a good chance of "engineering" a catalyst material with better Pt utilization. The approach could be improved if there were more focus on the processes that can make the 5–10 g scale of material, rather than sub-gram-scale batches. The challenge of sub-gram-scale batches is that scale-up is almost always required to make a membrane electrode assembly (MEA) with controllable properties such as loading. The one sample that was made at a 5 g size (a sample of PtNi) showed the best fuel cell performance.
- The approach to project targets is effective, and DOE targets could be met.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- It is encouraging to see the scale-up of most of the catalyst in gram levels and very good performance in 50 cm^2 MEAs from these scaled batches. The dissolution dependency study is also very helpful to understand and improve the durability further. ANL exceeded DOE 2020 technical targets for 50 cm^2 MEAs for PtAu, PtNi 5 nm, PtCo 2 nm, PtNi 5 nm, and PtNi/PtCo intermetallic. So far, seven patents have been awarded and six have been filed, which is one of the best outcomes of this project.
- Excellent progress has been made toward stabilization of Pt from dissolution through integration of Au, first at the thin-film rotating disk electrode (RDE) level, and then extended to nanoparticles in MEAs. Additional work could be considered to develop the fundamental understanding of the impact of Au, which may allow integration of other non-PGM materials. Progress toward development of highly active nanostructured PtNi has continued, with very high activities obtained in RDE. However, activity of the PtNi nanoframes in MEAs remains much lower than RDE assessments, and the large decrease in mass activity during conditioning (as seen on slide 18) suggests a very serious durability issue that needs to be resolved. The hydrogen and air performance was quite good for the low-Pt loading used. Another area of note was intermetallic development. Fundamental thin-film RDE studies showed the enhanced stability and activity expected. The transition to nanoparticles yielded good mass activities, but durability (the key expected benefit) was not reported.
- This project has yielded significant insights into structure–function relationships and has yielded several promising classes of catalyst.
- The principal investigator (PI) clearly demonstrated successful progress toward project and DOE goals through the accomplishment of a majority of milestones.
- More fuel cell results are shown this year as compared to last year. Some of the approaches do not appear to pan out in fuel cell performance gains; for example, the higher-mass-activity catalysts do not demonstrate superior performance in fuel cells. It is sometimes difficult to make comparisons, even within the project team's presentation, since at times the researchers run experiments at 250 kPa of air and sometimes at 150 kPa of air.
- Many catalyst systems of PtNi and PtCo have been studied on the stack level for this project. ANL met DOE goals for mass activity and loading for PtNi/high-surface-area-carbon (HSAC) and 2 nm Pt_3Co/C, but did not address the durability goal on the stack level.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- The project lead collaborated on different technological thrusts with several research groups from national laboratories, academic institutions, and OEMs.
- There is very good collaboration among the team members, which is evident from the results. Now the team is making high-performing catalysts in gram batches, so they are encouraged to share with interested parties, especially with original equipment manufacturers (OEMs) for evaluation. The National Renewable

Energy Laboratory's (NREL's) MEA testing capabilities are well known, but evaluation from outside this team will provide more interest in the industry, considering future technology-to-market (T2M).
- The collaboration on fuel cell performance is limited to one partner, NREL, for fuel cell testing. Again, small batch sizes of catalysts limit the amount of collaboration that can be done since sample size is too small for controllable, repeatable fuel cell testing.
- The laboratory has already developed some high-performance catalysts. Collaboration with the industry sector would be more efficient to transfer technology.
- There is broad collaboration among national laboratories. There could be more indication of interactions with outside researchers and OEMs.
- The project's collaborators consist primarily of other national laboratories. The project would be strengthened by additional collaborations with universities and/or industry.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Though fuel cell electric vehicles are in the commercialization phase, cost still remains the biggest challenge. High-activity, high-durability catalysts are a must for reducing the cost further. This team has developed many high-performing catalysts while also providing insight about durability.
- The project does have the potential to optimize Pt utilization since it is a true engineering approach to catalyst design.
- ANL's achievement is relevant to DOE goals. Research and development of ORR catalysts in this laboratory may have potential impact on high MEA performance for the fuel cell stack.
- The project is directly addressing one of the top key commercialization barriers, the activity and durability of the ORR electrocatalysts.
- There is high potential for impact in terms of new catalysts with high durability and low cost.
- The project is critical to the Program and for the fuel cell community in general.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- Taking into account that the project is close to the end, the proposed future work is clear and logically focused on the achievement of final project goals.
- The project has strong future plans in terms of characterization, optimization, and scale-up. Additional effort on theory and structure–function relationships is desirable.
- The proposed future work seems reasonable. It is recommended that the project team add best-candidate-catalyst MEA testing with an institution outside of the project team.
- The proposed future work is appropriate, as it directly aligns with addressing key barriers.
- There are too many catalyst systems that have been investigated so far in the laboratory. The proposed future plan would be more feasible if only the best catalyst and the best scale-up method were investigated. Secondly, RDE-inductively coupled plasma (RDE-ICP) seems to have no clear relevance to the MEA performance.
- The proposed future work sounds like simply more of the same. It lacks the focus to translate to improvements in fuel cell performance. Mass activity is reaching targets, but power density is still far off. More focus should be put on addressing this limitation.

Project strengths:

- PIs at ANL are world leaders in the Pt and Pt-alloy catalyst field. Other team members are supporting ANL's scaling-up efforts, analysis, and MEA testing, which almost completes the circle. The capabilities of each team institute are tremendous for accomplishing the technical challenges.

- The project's strengths include the following aspects: 1) the method for the scale-up is critical for the manufacturer; 2) the use of HSAC for the support benefits of mass transfers at high current density; and 3) the demonstration of the catalysts' performance on 50 cm^2 MEAs.
- This project brings deep fundamental understanding and unique, highly practical analyses to bear against the key barriers of cost and durability.
- The team is very creative in terms of catalyst design, synthesis, characterization, and scale-up.
- The project's strengths include a good engineering approach with a high degree of fundamental studies of the catalyst materials.
- The project is based on a solid scientific hypothesis and solid approaches and is led by a PI with substantial expertise in this field.

Project weaknesses:

- The project's weaknesses include the possibility that (1) the effort to study so many catalyst systems may lead to few gains from each one, (2) there are few durability tests on MEAs with Pt_3Ni/HSAC and 2 nm Pt_3Co/HSAC, and (3) the performance gap between RDE and MEA is still unknown.
- A third-party (outside-project-team) MEA evaluation is missing. This might not be needed from the point of view of the statement of project objectives but is surely important from the T2M perspective.
- The team seems to lack the ability to translate promising catalyst materials to true fuel cell performance potential. A different approach is required to tackle this limitation.
- The project would be strengthened by increased funding to enable increased development scope and rate.
- The project's connections to OEMs for validation are lacking. The theory-backed design could be better demonstrated.

Recommendations for additions/deletions to project scope:

- The NREL team has demonstrated that current commercial catalysts can show mass activities between 0.7 and 1.1 A/mg Pt after the conditioning protocol. Though those high activities of commercial catalyst do not translate to performance, ANL needs to think about how to surpass the MEA performance of the commercial catalysts.
- The PI should consider putting less of an emphasis on increasing the activity of porous PtNi nanoparticle structures and emphasizing stabilization. The PI should consider conducting analyses to understand the impact of catalyst-specific material factors (if any) on the large discrepancy between RDE activity and the MEA.
- Changes to the project scope should be (1) that the project should focus only on one or two of the best catalysts for MEA testing and (2) that RDE-ICP should do more to monitor the loss of Ni or Co.
- An increased emphasis on downstream customers and upstream theory-backed design is recommended.
- There should be more emphasis on scale-up and collaboration with partners with MEA manufacturing experience.

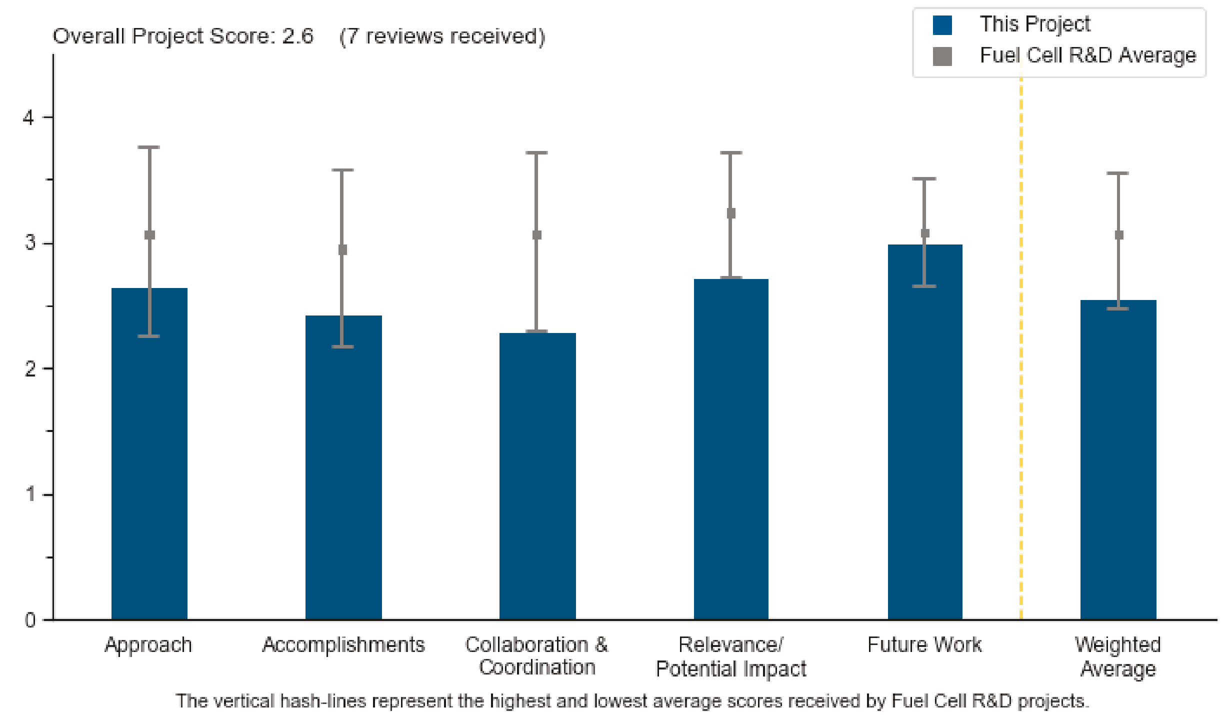
Project #FC-141: Platinum Monolayer Electrocatalysts

Jia Wang, Brookhaven National Laboratory

Brief Summary of Project

This project aims to synthesize high-performance platinum monolayer electrocatalysts for the oxygen reduction reaction consisting of a platinum monolayer shell on stable, inexpensive metal, alloy, metal oxide, nitride, or carbide nanoparticle cores. Three low-platinum catalysts will be developed that will meet U.S. Department of Energy (DOE) technical targets for 2020.

Project Scoring



Question 1: Approach to performing the work

This project was rated **2.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project seeks to develop Pt-monolayer catalysts that can meet DOE's technical targets for durability, activity, and cost simultaneously. The iterative approach of synthesis, rotating disk electrode (RDE) screening, and characterization (scanning transmission electron microscopy [STEM], x-ray diffraction [XRD], etc.) has led to two catalyst types: $Pt_{skin}(PtNi)_4N)_{core}$ and Pt-NbO_xC. As part of the approach, down-selected catalysts are to be submitted to partners for membrane electrode assembly (MEA) testing, an important activity that was absent this year.
- The approach of this project toward DOE goals is generally effective. The core components for the monolayer Pt atom on nanoparticles are essential, and the modification of support indirectly affects the stability of nanoparticles.
- The project has continued to address the development of novel and promising catalyst concepts (PtNiN and Pt-Nb_xC), the key advancement being the formation of Pt thin skins over Ni-enriched nitride cores, where the Pt skin is stable.
- With respect to material sets being examined and final targets, the approach was presented and appears to align with reasonable goals. However, no outline of the tasks and milestones was presented. It is not clear if

the plan is feasible if this information was not presented. One concern is that the project seems to be focusing on RDE results for optimization. There needs to be MEA testing in parallel to avoid optimizing the catalysts for RDE performance and ending up with a material that does not work well in an MEA environment.

- The proposed project focuses on the barriers: improving the activity, especially the durability, of Pt-based catalysts in polymer electrolyte membrane fuel cells. The two chosen approaches are not fundamentally infeasible; however, one of them ($PtNbO_x$) was given up, and the lack of the MEA data on the other one (PtNiN) makes a fair judgment impossible.
- The project focuses on catalyst development and characterization, with promising RDE results, but with limited effort on MEA translation and demonstration. It would be good to have a Ni dissolution study.
- Brookhaven National Laboratory (BNL) did not show any MEA results from the last year. This is a major weakness in the approach. There is also little to justify the selection of chosen catalytic systems.

Question 2: Accomplishments and progress

This project was rated **2.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project focus was on characterizing and optimizing the high-mass-activity PtNiN catalyst while also determining the cause for low MEA activity of the NbO_x-based catalyst. To this end, XRD and analytical STEM were heavily employed. Two key accomplishments involved developing a new intermetallic catalyst and demonstrating that the high activity and electrochemical surface area (ECSA) of the PtNiN catalysts could be retained on a Vulcan support following the catalyst accelerated stress test (AST) in RDE. The latter approach shows great promise for meeting support AST targets. The lack of progress or attention to MEA performance issues was a major omission from this year's progress and accomplishments.
- The PtNiN on Vulcan shows good ECSA and activity stability in RDE catalyst AST. The Ketjen support was explored to control particle size and promote internal Pt for higher beginning-of-life (BOL) mass activity; the activity stability is lessened relative to Vulcan but still meets the project targets after the AST. Unfortunately, this year has not seen an update in terms of MEA-level performance.
- Screening of catalysts was done, and an improvement in catalyst activity was based on RDE performance, which is on track for DOE targets.
- Identification of the no-go on $PtNbO_x$ is still meaningful. The RDE measurements and characterizations on the PtNiN are comprehensive and complete. The RDE performance of PtNiN is good and informative. However, so far there are no MEA data.
- The project has good characterization of an interesting set of materials and presents exceptional RDE mass activity. There is no need to further optimize activity of these materials in RDE. The durability in RDE is not a good measurement of true durability because it is at a lower temperature than an MEA and metal leaching from the catalyst would not have as much impact. Unfortunately, the MEA results clearly trail those of peers in this area for reasons that have not been determined. This should be the focus of all future testing.
- The lack of MEA testing is severely limiting the usefulness of this project. The well-established lack of correlation between RDE and MEA results means that there is no way to know whether any of the catalysts under development hold any promise for fuel cells. The only MEA results mentioned, which are on slide 5, appear to be from the previous year. The use of lattice contraction as measured by XRD to assert that Pt skin formation occurs on PtNiN is questionable. Data from synchrotron studies (extended x-ray absorption fine structure [EXAFS]) or energy dispersive x-ray spectroscopy (EDX) are needed. However, the EDX data on slide 9 do not show any evidence of Pt separation. Therefore, the putative nanoparticle structure does not seem accurate.
- Most DOE targets have been met only on RDE tests. MEA performance should be the final goal.

Question 3: Collaboration and coordination

This project was rated **2.3** for its engagement with and coordination of project partners and interaction with other entities.

- The team is strong and covers necessary aspects of the proposed work. In particular, this proposal involves international collaborations. Although no MEA data have been provided yet, General Motors (GM) is the ideal choice and will deliver reliable data. The presentation did not make the roles of the Korean and Japanese groups clear.
- Since last year, the list of partners and collaborators has dropped significantly, and engagement with existing industry partners appeared minimal. A key deliverable of this project is to provide catalysts showing high activity and durability in RDE to collaborators for verification in MEAs. Without that coordination, this project provides little value toward meeting DOE technical targets.
- Most or all of the results seem to be from the BNL group. Support for MEA testing is desperately needed, but either GM did not provide MEA testing or the results of the testing were not shown.
- Some MEA results from GM were presented, but more MEA iterations are needed to improve MEA performance. It was not clear if any other institution collaborated significantly on this project.
- This year has not seen a major update in MEA performance, which is a role of the project partners. It is unclear what the partners (e.g., GM) have contributed.
- MEA testing could have more collaboration with GM and Toyota.
- The project's collaborations are not strong, and collaboration contributions to the project are not clear at all.

Question 4: Relevance/potential impact

This project was rated **2.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The potential impact of this project is high. The high BOL mass activity with the Ketjen support and the highly stable mass activity of the PtNiN catalyst may be a promising pathway to meeting DOE platinum-group-metal (PGM) targets for performance and durability.
- The project's goals for developing stable core–shell catalysts that can meet DOE activity targets are relevant to the DOE Hydrogen and Fuel Cells Program (the Program) objectives.
- The project's accomplishments are relevant to DOE goals. The future work could have the potential to increase the performance of catalyst durability.
- The development of highly active and durable low-PGM catalysts is highly relevant to DOE's mission, especially with the shifting focus to heavy-duty applications. However, to be relevant, the high RDE performance must be transferred into MEA, which has yet to be achieved over the life of this project.
- Based on the excellent RDE activity results, this project shows potential for making progress toward DOE goals for low-PGM-loading catalysts. The likelihood of achieving those goals is low if the project does not focus more on MEA testing.
- During its long history, this project has consistently failed to show good performance in MEAs. Analysis in recent years has demonstrated that RDE testing is barely relevant to fuel cells. Without good MEA results, this project is not very relevant.
- The Program's goals and objectives are based on MEA performance, which is missing from the presentation.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- At a high level, the proposed future work appears to be logical. More details on the MEA optimization and who will be performing the work need to be presented to increase confidence that the MEA optimization will be successful. The Nb-nitride materials are being pursued for risk mitigation, but there should be an early decision point for whether to continue exploring Nb-based materials, because so far the results are not promising.

- There may not be much future work since the project is ending. If further work continues, the proposed MEA testing will be the most important part. The proposed future work on corrosion-resistant supports does not seem like a good idea for now since testing the catalyst performance and durability is much more important.
- The primary focus should be on MEA optimization; additional focus on catalyst optimization by RDE or corrosion-resistant supports should be shelved until the factors limiting MEA performance are identified.
- The proposed future work is mostly important here since it proposes to focus on the MEA testing, which is eventually all that matters. Making a nitride catalyst on a corrosion-resistant support is also plausible.
- There is only a short duration left in the project. The proposed MEA testing should be a key focus to identify any major hurdles for future development of these catalysts when implemented in fuel cells.
- MEA validation should be performed, and a dissolution study could be beneficial.
- Validating the catalytic performance in MEAs should be the top priority.

Project strengths:

- The project continues to push the forefront of low-PGM catalyst development, incorporating the advanced characterization tools available in the Office of Basic Energy Sciences user facilities in order to explore underlying mechanisms for high performance and manifest durability in RDE.
- The project has met the DOE targets on RDE for activity and durability. The Ni_4N core is relevant to the stability of the Pt monolayer, and NbO_2 could contribute to the anti-corrosion of carbon.
- The strength of this project is the novel PtNiN catalyst particle structure and resulting mass activity and AST stability.
- Overall, the project is investigating interesting materials, has excellent characterization of the materials, and has excellent RDE results.
- The RDE measurements and the characterizations are comprehensive, complete, and informative. The fundamental science is good.
- The project's strengths include characterization.
- The team has access to good characterization capabilities at BNL, though they could be better utilized.

Project weaknesses:

- The project's weaknesses include the following: 1) the size homogeneity of PtNiN nanoparticles could be improved through the modification of the synthetic method, 2) it is unknown whether there is a Ni leaching problem, and 3) DOE targets have not been met on the MEA level.
- As of yet, no MEA data are available to justify the approach of PtNiN. RDE performance is good only for electrochemical characterizations and screening and is not that relevant to DOE targets.
- The weakness of this project is a lack of parallel MEA testing and apparently weak collaborations.
- The project's weaknesses include weak collaborations and mediocre progress, especially lacking MEA translation of the developed catalysts.
- The key weakness of the project is the lack of integration with MEAs through the project partners.
- The lack of collaborative MEA testing is the primary weakness of this project.
- Lack of any MEA testing severely hurts this project.

Recommendations for additions/deletions to project scope:

- More focus on MEA optimization is needed for the project to be successful. The materials are active enough in RDE; no more RDE activity optimization is required. The Nb-nitride materials are being pursued for risk mitigation, but there should be an early decision point on whether to continue exploring Nb-based materials, because results so far are not promising.
- The project is ending. Based on the lack of progress demonstrated in recent years, there does not seem to be any reason to continue the work. However, if DOE chooses to fund this work again in the future, there should be assurance that a funded partner will be performing extensive MEA testing. The unfunded collaboration with GM does not seem to be providing any MEA results.

- Identifying an invested, engaged partner who will work to overcame challenges of MEA integration should be the highest priority of this project. Los Alamos National Laboratory was listed as a partner last year but was notably absent on this year's slides.
- It is highly recommended that the project run MEA testing on the PtNiN catalysts. Any further characterizations, reasoning, and catalyst optimization should be based on MEA performance. It is reasonable to give up $PtNbO_x$.
- It is recommended that BNL pursue MEA validation and optimization.

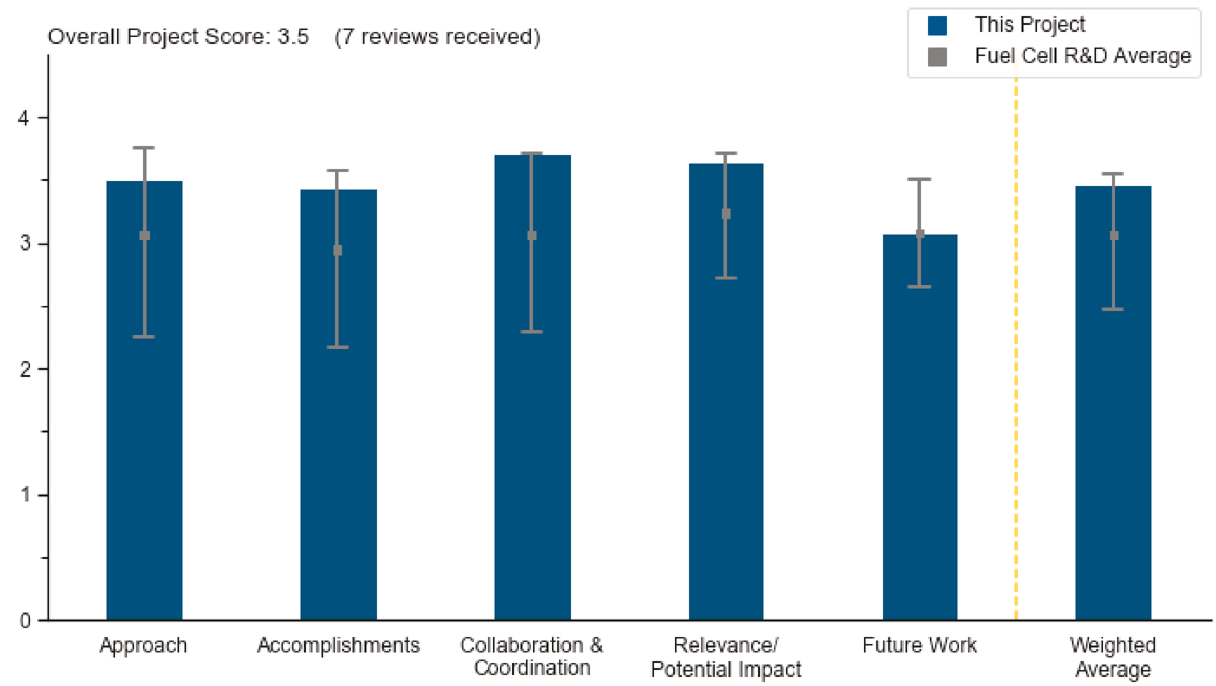
Project #FC-144: Highly Accessible Catalysts for Durable High-Power Performance

Anusorn Kongkanand, General Motors

Brief Summary of Project

This project aims to reduce overall stack cost by improving high-current-density performance in hydrogen–air fuel cells that meet U.S. Department of Energy (DOE) heat rejection and Pt-loading targets. Investigators will maintain high kinetic mass activities and mitigate catalyst degradation using supports with more corrosion resistance than the current high-surface-area carbon (HSAC). The project takes a four-pronged approach: (1) improve oxygen transport with new carbon support, (2) reduce electrolyte–Pt interaction, (3) enhance dispersion and stability of Pt-Co particles, and (4) improve understanding and control of leached Co^{2+}.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project team utilizes a combined approach, examining catalyst supports and alloyed catalysts and improving transport to the catalyst using ionic liquids (ILs); this is supported by a novel characterization tool for understanding the origins of performance improvements. The approach is technically sound and could lead to key improvements, such as increased oxygen transport, H+ conductivity, and Pt electrochemical surface area (ECSA). The project’s findings have the potential to lead to results that could help meet activity and durability membrane electrode assembly (MEA) targets under low-loading conditions. In addition, looking at cation effects, which leach out of the catalyst, or at Ce, which is used as a radical scavenger on the ionomer conductivity, is also important toward achieving the DOE targets.
- The project has an effective approach to understanding opportunities for improved catalyst utilization and performance. The areas that have been selected have provided meaningful results and are promising for

further development; these areas include the accessible carbon supports, the ionomer and IL interface understanding, the ordered intermetallic alloys, and the effects of the cations.

- The approaches adopted are appropriate and comprehensive, covering most important aspects of the topic—including the catalyst, the IL, the ionomer, and the carbon—to improve performance. In addition, modeling has been applied to understand the oxygen and proton transport issues so as to understand the fundamentals and the experimental results obtained.
- The project is making good use of developing different carbon supports to make catalyst particles accessible. The project seems to have moved to ordered intermetallic alloys, which is an approach similar to the Voja and Spendelow projects; maybe a consensus is forming on desiring ordered intermetallics. The IL approach is curious, especially considering that, in the past, Fuel Cell Technical Team (FCTT) members (or General Motors [GM]) have indicated they do not believe that ILs will be stable in electrode layers.
- The project's approach is focused on achieving DOE performance goals at high current density (HDC) by optimizing carbon supports, the electrolyte–Pt interface, the catalyst's activity and durability, and the mitigation degradation effects from transition-metal cations.
- The project takes on a major question about fuel cell behavior at low loadings, and the limitations of low loadings, while giving possible solutions.
- The approach taken by this team to address some of the HCD performance issues and methods used to quantify those losses is commendable. However, it is not clear that the IL that has been used in this project is the best available system for this effort. It is not clear what the fundamental ionic properties are or whether the IL has had any durability issues during the various cycling protocols employed.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The intermetallic ordering work is very promising. The IL's effect on stability is quite interesting, and it is good to see that these tests were done. The effects and understanding around them should be studied further. Although the project boosted the utilization of Pt to high levels, it was not able to achieve the rated power target at 150 kPa. The results were nonetheless impressive. However, using a system with such low catalyst loading, below the DOE target, may not provide the best value in terms of lifecycle cost. Focusing on systems with target platinum group metal (PGM) levels is recommended. The accessible Pt-Co stability is a concern, but the trade-off with the higher current density performance still makes this approach worthwhile. Regarding the Co loss effect, the result is relatively as expected. However, the lattice strain mapping is providing some good insight. The catalyst aggregate model and scanning transmission electron microscopy – computed tomography (STEM-CT) work are providing some good insights and are appropriate for better understanding the interactions within the catalyst–ionomer interface. The oxygen diffusivity through the water-filled pores will also feed into this work. The modeling work is a valuable aid in understanding and should be completed.
- The project has made progress toward the goals, has met most of the milestones, and is on track for the others. There is a nice set of variables and parameters investigated in terms of their impact on cell performance as well as investigation of the underlying cause of those changes using novel characterization tools and modeling studies.
- The project team has made very good progress toward achieving DOE targets on PGM total loading and utilization. All targets except the rated power at 150 kPa have been met.
- All the important milestones and go/no-go targets were achieved. Ionomer-related progress is not significant in either practical or fundamental terms.
- The use of ordered PtCo intermetallic catalyst appears to be a significant advantage in terms of durability and lower loss in mass activity (at least with the PtCo/KB). However, the PtCo/KB seems inferior at beginning of life to the PtCo/HSAC-f, and the support corrosion metric has not yet been determined; probably both fail that metric, and thus reliance on system mitigation will still be required. The Pt/Co ratio study and the contrary effects on low current density and HCD are nice contributions. The measurements related to Co dissolution and amount of Co in the ionomer phase raises questions about the effect of the ionomer-phase Co. Further questions that should be explored include whether it reduces the proton conductivity, and thus increases losses, and whether the oxygen resistance is higher for transport through

this Co-contaminated ionomer phase owing to lower water uptake. The measurements are good, but more understanding should be undertaken. The lattice strain mapping should be supplemented with extended X-ray adsorption fine structure (EXAFS) for better understanding of the catalyst surface. This catalyst development project appears to have developed primarily into an MEA development project.
- The project has raised more questions than it has answered, but this is always the case with good research. The finding that the best catalysts are those in pores without direct ionomer contact is something that most would not have guessed, and it will be the basis for much research going forward. Similarly, it is hard to understand how the ILs are limiting catalyst dissolution.
- Sensitivity studies on MEAs addressing durability and HCD performance should be done to understand what the effect of loading on HCD performance is before and after durability accelerated stress tests.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration among partners is evident in the publication list. The accomplishments in characterizing the Co migration and the use of advanced tools, such as STEM-CT and nano-CT to measure diffusivity through water-filled pores, is very effective.
- The team has strong collaborations with both unfunded and funded partners on a variety of techniques and topics. The partners' contributions to the project are clearly defined, and a clear strategy exists for the team to work together to accomplish project goals.
- The project is coordinated very well by GM, with collaboration between Cornell, Carnegie Mellon, Drexel Universities, the National Renewable Energy Laboratory, and 3M.
- This is a very strong team with significant collaboration with a number of groups, including other industries, national laboratories, and academics.
- The collaboration is great. The work from different groups is relevant and well integrated.
- The organization's collaborations appear well managed and valuable.
- This project is truly using some of the best people and facilities in the world doing what they do best. Generally, such a high number of collaborators should be discouraged, but the project team seems to be making it work well. However, it is very difficult to tell how much each group is contributing.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The work being performed on this project clearly aligns with the needs expressed in Fuel Cell Technologies Office and DOE research, development, and demonstration goals. The project is addressing the mitigation of cost and performance limitations in low-loaded catalyst layers by investigating a wide parameter set (from carbon types to ionomers and ILs) that has the potential to meet DOE targets.
- The project is well aligned with DOE goals and objectives and has the potential to advance DOE goals by improving fundamental understanding of processes occurring at the fuel cell cathode and integrating this knowledge into real-world polymer electrolyte membrane fuel cells.
- The work is highly relevant, addressing a key technical challenge of HCD performance and durability in an MEA that is impeding progress toward lower catalyst loading.
- The impact of this project will be very high. The project team is not only finding practical improvements but changing the models of how the community thinks these systems work.
- Higher-mass, active, durable catalysts are needed to enable higher levels of vehicle commercialization.
- The project team has made good progress on optimizing the catalyst and demonstrating the benefits of porous carbon for the HCD performance of low-PGM catalysts. However, it remains unclear how the porous carbon helps. The development of ionomers is mild, while this is an important part for the HCD performance.

- The potential impact of this approach for understanding transition-metal migration and durability is significant. However, in this approach, the team should also keep durability in focus and conduct sensitivity studies at higher loading. The impact on MEA cost is understood, but durability is critical.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- There should be more follow-up on some of the questions raised by the project's findings. This is especially true for how the ILs are working and will be retained, as well as the mechanism of conductivity within the pores. It would be interesting if the team had a carbon expert and could better tailor the catalysts to a structure that is more optimal with the new understanding.
- The proposed future work appears to be appropriate, covering fuel testing, materials (especially ionomer optimization), and fundamental understanding.
- The project's proposed work is well balanced and combines fundamental and practical aspects of fuel cell development.
- The project team should use target PGM loadings rather than the 0.075 mg/cm^2 loading. The other future work identified is appropriate.
- Future work tasks are well outlined, although it is not clear what type of "new ionomer" development and IL optimization will be carried out.
- For future work, the project team should consider a higher-loading MEA along with a low-loaded MEA for durability. This would help with clearly understanding the impact of this approach. Additionally, implementing a new IL this late in the project would not be an efficient use of funds or time. The team should focus on understanding the impact of the IL system already being used on durability. Exploring "catalyst synthesis paths for intermetallic ordered PtCo with well-controlled size" also seems to be a task starting too late in this project. If this was a new scope in the project from the 2018 Annual Merit Review, then the team should consider dropping this effort.
- It does not make sense to spend significant effort on optimizing IL application when there appears to be no idea of whether these are stable in the electrode matrix and/or durable. The project's response to 2018 reviewer comments regarding IL stability seems ill-considered and rash. Evaluating the IL stability in the matrix seems a critical task in terms of spending more effort related to this, especially when FCTT (specifically GM) has criticized use of IL in the past because it will not be stable. Evaluating the leaching of IL from the electrode matrix is, in part, not as difficult as evaluating effluent water from the fuel cell for the IL, and the task seems a bit straightforward and semi-trivial. Repeated cyclic voltammograms monitoring the capacitance and ECSA may also provide insight as to the stability of the ILs in the matrix.

Project strengths:

- One of the project's strengths is attacking the problem from various angles, which provides an enhanced parameter and material matrix (ILs, porous carbon, ionomer, and annealing effects) that allows for identification of design parameters for improved cell performance. Other strengths include the examination of the cation effects and Co loss studies, a number of characterization studies that clearly contribute to the project, and linkage to foundational work (imaging, strain mapping, etc.).
- The project team is great. The leading organization, GM, is well equipped and extremely experienced in this topic. The expertise of the team's collaborating partners is the right hammer for the nails to be addressed in each strategy. As a result, the team knows what barriers are likely to be overcome by what strategies and has the resources and capabilities to implement those strategies. The project has made steady progress, meeting all the milestones and go/no-go targets at a good pace. Optimizing the catalysts and demonstrating the benefits of porous carbon for HCD performance are important achievements.
- The project combines fundamental and practical aspects of fuel cell development. The project team has implemented state-of-the-art experimental techniques, such as lattice strain mapping, confocal X-ray fluorescence, and advanced modeling, to understand the root cause of insufficient fuel cell performance.
- The project collaborators provided excellent diagnostics, characterization, and modeling approaches to supplement the main studies and increase fundamental understanding. There was also identification and development of concepts and approaches that have proved fruitful.

- There is a strong approach and relevance with great results and implications, as well as strong teaming, with each group working toward its strength.
- The ordered intermetallic PtCo is showing improved durability and mass activity; this is similar to other projects led by Voja and Spendelow.
- The project's strengths lie in the team's expertise in understanding Co migration techniques and correlating that to fuel cell performance curves. Using IL in the MEA, although a novel approach to understanding the Pt–ionomer interface, does not seem to provide value without durability testing. If there is no efficient method for characterizing IL during durability tests, then this effort should be dropped for the rest of the project.

Project weaknesses:

- It appears that the ionomer-related progress lags behind. It has been known that the major limitation of low-PGM catalysts for HCD performance arises largely from the Pt–ionomer interface, such as local oxygen resistance and site-blocking by the ionomer. However, most improvements lie on the catalyst side, probably by improving the catalyst's inherent activity and durability. Although it was demonstrated that porous carbon helps, there is no clear evidence for how this occurs, and the improvement has not been related to the ionomer-related barriers. There are no images in the atomic scale showing the interfaces between the Pt nanoparticles and the porous carbon in the atomic scale. It is appealing to see that the project will make improvements on the ionomer and the Pt–interface parts and will directly address the local oxygen transport resistance associated with deeper understanding of corresponding fundamentals.
- This project seems to be focused only on PtCo catalysts. Perhaps exploring other Pt-M alloy catalysts using a similar approach may have shed more light on the transport mechanisms and impact on HCD performance. The IL seems to serve only as a diagnostic tool for understanding the Pt–ionomer interface. The project does not seem to have addressed the influence of the IL used in these studies, and it is unclear that the results would be different if a different IL had been used.
- The principal investigator has no idea whether the IL is stable and/or durable in these electrodes. It is unclear why the IL benefits do not occur with the HSAC-f support; there is a lack of fundamental understanding on effect. The CO displacement measurements indicating that adsorption of SO^{3-} is lower is not correlated to mass activity measurements. If lower surface adsorption occurs with the ILs, the mass activity should increase, similarly to rotating disk electrode measurements in $HClO_4$ compared with H_2SO_4.
- Something related to one of the project's strengths is that, because of the many interrelated phenomena, it is not clear how to isolate certain effects and identify the dominant factors controlling the performance.
- The project is relying on a PtCo catalyst that has limited potential for improvement.
- As the project developed, the team was not very agile at changing scope or pursuing some of the questions that have been raised but rather has stuck to the script.

Recommendations for additions/deletions to project scope:

- There are no major recommendations, but the scope should be managed carefully to identify the key contributors to the catalyst layer performance and stability. For example, annealing reduces Pt loss, but perhaps it would also affect the CO dissolution. It is also unclear what the major contributor to the PGM utilization is: annealing or carbon support.
- The strain effect in PtCo has been well understood and documented. There is no need to proceed with the fundamental parts and characterizations. It is recommended that atomic-scale imaging be applied to explore the Pt-carbon-ionomer interfaces, which would be best under operando conditions. Efforts made on the catalyst side are excellent; more efforts should be dedicated on the ionomer and interface sides.
- This project needs to evaluate the stability and durability of ILs in their electrodes before more significant work is put into optimizing these electrodes. The lattice strain mapping should be supplemented with EXAFS for better understanding of the catalyst surface.
- The project team should do more work to understand how the IL retards catalyst dissolution. There should be some custom synthesis of carbons to optimize the number of appropriate pores.
- It is recommended that the project drop the scope on new catalyst synthesis paths for PtCo-ordered structures with controlled size and stop all IL work, as there is no method to characterize the IL once it is incorporated in the MEA.

- The part of the project related to introducing a new 3M ionomer does not look very promising.
- Recommendations for additions or deletions are not applicable at this point in the project.

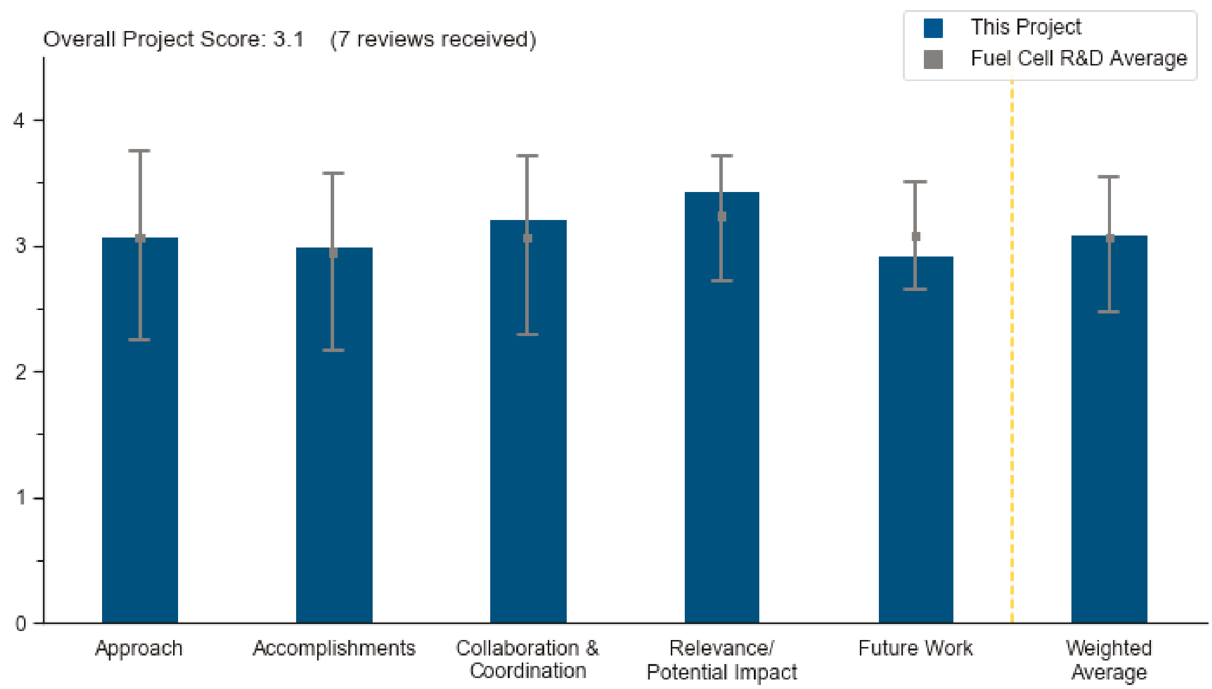
Project #FC-145: Corrosion-Resistant Non-Carbon Electrocatalyst Supports for Proton Exchange Fuel Cells

Vijay Ramani, Washington University

Brief Summary of Project

Carbon's high electrical conductivity and low cost make it an excellent electrocatalyst support, but corrosion leads to kinetic, ohmic, and mass transport losses. This project is synthesizing doped non-platinum-group-metal (non-PGM) metal oxides as non-carbon alternatives. Along with being corrosion-resistant, the project supports would have high surface area, exhibit strong metal–support interaction with Pt, and demonstrate high electrocatalyst performance.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Investigating support materials that offer improvements to corrosion resistance over carbon would benefit fuel cell systems. Combining modeling with synthesis and experiment is a viable approach to finding new materials and systems. The choice of doped tin oxide seems very reasonable based on the conductance properties. The choice of and focus on Nb and Sb were not really presented; the doping levels and methods investigated were also not presented in detail.
- It is interesting that this project is looking at such a unique approach by pursuing non-carbon supports. This seems to be a high-risk–high-reward project. The plan to address barriers appears to be working, based on test results.
- The connection to theory seems lacking, and the addition of atomic layer deposition (ALD) seems strangely complicated. Overall, the project has a good synthetic approach, with barriers to overcome and down-selects in the right places.

- The approach includes experimental and theoretical modeling of non-carbon-based catalyst supports (non-PGM metal oxides) to develop high-surface-area supports with good electrical conductivity. Most of the approach discusses TiO_2 and doped TiO_2 supports. Data are related to Sb-doped SnO_2 and Nb-TiOx-aerogel supports.
- This project addresses the need for non-carbon supports to mitigate support corrosion during shut-down/start-up of fuel-cell-powered vehicles. From the research performed since the last U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (the Program) Annual Merit Review (AMR), it appears that the project did not focus on achieving its mass activity target. It is not clear from the presentation what Pt-based alloys will be prepared to meet the mass activity target. The presentation does not mention how the project will address the load cycling accelerated stress test (AST) and meet the DOE target of <30 mV loss at 0.8 A/cm^2 after 30,000 cycles.
- Both aerogel and xerogel approaches are good for porous media. The only concern is the scale-up for aerogel, which requires the use of supercritical drying. It is not clear that scale-up for aerogel is realistic. The stability of Sb-doped SnO_2 may also be a concern. It is not clear that Sb-doped SnO_2 is stable in the fuel cell operating condition.
- Alternative supports for carbon can yield benefits in support stability; however, equally important are the catalyst stability and catalyst activity. The approach to the work seems to be lacking in these areas.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made good progress with respect to improving the performance of non-carbon supports in membrane electrode assembly (MEA) tests. The non-carbon supports appear to work with respect to improving catalyst start–stop durability. In the future, load-cycling data should be discussed to confirm that these catalysts and supports are also effective for the drive-cycle requirements. It is good that the project is presenting cost modeling results; however, the team needs to consider the system mitigation cost, not a stack replacement, as the baseline. It is known publicly that Toyota and General Motors have system mitigation strategies that would not require a stack replacement. Determining the cost of this mitigation may not be easy, but some type of estimate should be derived to determine the real value of the non-carbon support.
- In the past year, there were meaningful improvements in mass activity and performance, one of this project’s major limitations in the past. It seems that performance is getting close to that of Pt/C while offering significant potential durability benefits and that one of the big advances was improving the catalysis by modifying the synthesis pathway to include Pt in aerogel formation. This was not discussed in much detail in terms of why and what was learned and what this could mean for additional advances. The catalyst cost analysis showed clearly that antimony-doped tin oxide (ATO) was not a critical cost concern compared to Pt, but the system cost analysis was not particularly compelling, as most systems will not tolerate stack replacements. This perhaps changes when considering heavy-duty applications in which these materials may offer even more durability advantages.
- The observed durability is excellent and the performance good, despite the apparently lower kinetic performance due to Pt deposition issues. It is likely the move to alloys will help with this.
- Rotating disk electrode results show better mass activity for Pt/aerogel-NbTiOx. However, the MEA performance is well below that of Pt/C. Even worse, the durability of the Pt/aerogel is substantially worse. Comments were made that this is due to loss of conductivity, which is likely going to happen under other conditions as well. Thus, these materials do not seem overly promising for long-term durability. It seems like work can end on these materials.
    - The in-cell mass activities of Pt/Pt-aerogel-ATO do not appear comparable to Pt/C (slide 15, beginning of polarization curve). While they show better performance at very high current densities, those performances are not comparable to state-of-the-art (SOA) Pt/C electrodes (they get <0.4 V at 2.0 A/cm^2, whereas the SOA is ~>0.6 V at 2.0 A/cm^2).
    - The carbon corrosion results (slide 15) do show that these materials have improved durability in comparison to Pt/C. However, the degradation over 1,000 and 5,000 cycles is substantial. The real competition is not Pt/C with shut-down/start-up cycles but Pt/C with mitigation strategies incorporated into the vehicle system to avoid high potentials. While a material solution is preferred, it needs to be competitive with the overall system strategy; this is not.

- The cost modeling assumptions are simply inaccurate. Original equipment manufacturers (OEMs) are not going to make systems in which the catalyst has substantial degradation; OEMs are putting in system mitigation strategies to limit the shut-down/start-up voltage excursions. Thus, current Pt/C MEAs do survive 5,000 cycles; the issue is the additional system complexity, which equates to some cost and probably some loss of efficiency—but nowhere near that associated with replacing the stack. Thus, the cost modeling assumptions are simply incorrect, and it is an erroneous conclusion to state that the Pt/ATO is cheaper than Pt/C. The Toyota Mirai is working very well with Pt/C.

- The support stability for aerogel–niobium-doped titanium oxide (NTO) is questionable; mass activity loss is about 50% after only 500 cycles (slide 11). Aerogel–NTO is not as stable as carbon-based support. It is not clear why the project still focuses on the aerogel–NTO support. Beginning of life of Pt/aerogel–ATO polarization curves is much lower than that of Pt/C within the 0.9–0.6 V range. It would be good to know the cause. The H+ conduction seems to be an issue. The principal investigator (PI) may consider improving the H+ conduction within the catalyst layer. Mass activity loss is quite significant: 50% for Pt/aerogel–NTO. The loading is high: 0.2 $mgPt/cm^2$. Backpressure is high: 100 kPa.
- Incremental improvements toward addressing mass transport limitations were presented, but catalyst activity is still significantly behind. The cost analysis did not seem to consider the industrial engineering controls to avoid high voltage spikes. If engineering controls are considered, it is not clear whether the cost analysis with the expensive support will be an attractive alternative.
- Not much progress has been made since the 2018 AMR. The technical target/current status table on slide 5 is identical to the one presented in the 2018 AMR.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- This project appears to have effective and strong collaborations.
- The teamwork is very impressive.
- Collaboration levels seem mixed. Nissan Technical Center North America (NTCNA) is strong. The University of California, Irvine, seemed to have a good start at the University of New Mexico but was delayed by the PI move; what remains is unclear. The Fuel Cell Consortium for Performance and Durability (FC-PAD) interactions are not clear; it seems that some stability testing would be helpful.
- The team has broad relevant skills appropriate for the project. What seems to be missing is an industrial participant that would potentially be able to supply the developed materials at commercially relevant scales.
- Collaborations seem appropriate, although additional collaborations might prove useful, especially in the area of mass activity. The project could use help preparing Pt-alloy catalysts.
- Interactions with NTCNA in terms of testing and MEA optimization should be beneficial.
- This project involves two universities and an OEM. Interaction with FC-PAD is suggested.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Higher-mass active catalysts with stable supports to eliminate degradation mechanisms such as corrosion and particle coarsening would be a tremendous benefit to fuel cell commercialization.
- This is an interesting project that is investigating unique non-carbon supports. The technology may be unlikely to be adopted for automotive MEAs in the near future because it is relatively immature; however, these supports could prove useful in electrolyzers or other types of fuel cells that require harsh operating conditions and in which carbon corrosion is a bigger concern.
- The potential of this approach and the achievements greatly advance Program goals.
- Replacing standard catalyst material supports with high-performance and more durable replacements would have a significant impact. Initial durability testing using ASTs has shown promise. Performance is not yet

to a fully competitive level, and whether ASTs developed for current systems are relevant for these new systems is not clear.
- Using metal oxides as a catalyst is a good approach for long-term durability of polymer electrolyte membrane fuel cells (PEMFCs). However, the cost of metal oxides may prevent their application in PEMFCs, despite the benefit of the support stability.
- If successful, the new supported catalysts will benefit fuel cell development. However, as fuel cell manufacturers continue to advance their technologies, the new low-PGM electrodes using this class of supports might not be relevant.
- The project focuses on corrosion-resistant metal oxide supports. Metal oxide supports have been suggested as catalyst supports in the literature. However, to date, none of the proposed metal oxide supports meet the DOE target for catalyst durability and support stability.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The future work all seems appropriate; the project should concentrate on catalyst development related to mass activity and durability. Cost analysis should not be a priority for this project; however, if any is done, realistic assumptions related to how OEMs are actually operating cars should be incorporated (i.e., new catalysts are a trade-off with system mitigation strategies). Future work should include use of higher-activity alloys, such as Pt-Ni and Pt-Co. Future work should also include understanding the support electrical conductivity degradation and whether that reduction in electrical conductivity will occur at steady-state operating conditions.
- The Pt alloy investigations make sense to increase mass activity. Varying the ALD conditions to try to further improve Pt distribution seems reasonable, as this seems to have had a strong impact on this year's performance improvements. Gaps include a lack of detail in future work plans and a discussion that includes mechanistic understanding of the processes affecting properties.
- The goals of improving mass activity and electrodes make sense. Additional support approaches from the University of California, Irvine, also make sense. However, density functional theory (DFT) at this stage of the project makes no sense, especially as the effectiveness and connection between the early DFT and results is tenuous. Pt ALD seems like an overly complicated approach to Pt deposition and is poorly suited to the high loadings of Pt needed.
- Preparing Pt-alloy can lead to improved mass activity and meeting the project milestone of achieving 0.3 A/mgPGM. However, the PI did not specify the type of Pt-alloy catalysts that the project will prepare in the third year.
- The future work is logical and appropriate. Examination of 0.95–0.6 V cycling should be presented to enable an understanding of whether Pt adhesion to the support is an issue for these materials.
- The proposed future work is appropriate.
- Pt alloy development should have started earlier in the project. It is doubtful the project will be able to accomplish good activity performance in such a short time before the final deliverable. There is no mention of catalyst durability testing. While the support stability seems reasonable, the Pt stability on the metal oxide supports might be affected.

Project strengths:

- This project is attacking catalyst durability through a unique approach relative to other projects. The team has made significant progress at improving the performance of the non-carbon support catalysts in MEAs and has obtained encouraging initial results with respect to durability.
- The metal oxides are a good approach for catalyst support stability. The aerogel and xerogel approaches are effective for obtaining high surface area, which is critical for support. This project is a good exploration of non-carbon catalyst supports with stability superior to carbon.
- The project has strong new results for a more corrosion-resistant support system. Performance is approaching that of Pt/C, with improved durability.
- Catalyst stability is excellent, even with low mass activity. There is a close connection between Washington University and NTCNA.

- Collaboration with NTCNA adds strength to the project, as Nissan has provided significant contribution to the research. The PI is well experienced in PEMFC research.
- The strength of this project is the development of materials that should not be susceptible to corrosion during normal operation or shut-down/start-up (e.g., carbon corrosion).
- The team is developing more stable supports, as compared to Vulcan® XC carbon.

Project weaknesses:

- The cost analysis is overly flawed with assumptions. Pt/C is never going to be operated straight away like this. The catalysts, to date, are not competitive with SOA Pt/C, let alone PtCo/C. The Pt/C polarization curves (e.g., slide 15, iR-corrected) are not representative of what can be achieved with Pt/C; the fact that those are iR-corrected but the Pt/C slope is rather large shows there is a problem with that baseline. The supports have not adequately improved catalyst durability to remove vehicle durability mitigation strategies; thus, they are still in a developmental phase. The durability needs to be improved rather dramatically, it appears, in both electrical conductivity and Pt activity stability.
- Catalyst AST testing (0.6–0.95 V, 3,000 cycles) should be included to assess the usefulness of the materials under realistic conditions. The cost model needs to have a more realistic comparison to system mitigation strategies, not stack replacement. Performance at low current density needs to be addressed.
- The project does not focus on catalyst durability under load cycling between 0.6 V and 0.95 V. The metal-oxide-supported Pt and Pt-alloy catalysts tend to show poor activity after a few hundred or few thousand cycles owing to Ostwald ripening and agglomeration processes.
- The catalyst development needs more fundamental aspects. More characterization of the Pt/aerogel–ATO/NTO catalyst is encouraged to build the property–structure–performance relationship to better guide MEA development.
- Mass activity of catalysts is poor, possibly stemming from poor Pt deposition. The proposed remediation via ALD is dubious. The utility of DFT and implementation of DFT are unclear, even at project closing. FC-PAD is underutilized (for stability, DFT, and analysis of Pt quality issues).
- The catalyst mass activity seems to have reached a maximum with these supports. With fuel cell engineering controls, the need for this work is not clear since the catalyst’s corrosion-resistant attributes do not justify the sacrifice in catalyst activity.
- The project lacks details and mechanistic discussion or understanding regarding critical processes related to performance and durability.

Recommendations for additions/deletions to project scope:

- More mechanistic studies are needed to quantify degradation rates and mechanisms. The project should conduct additional in situ testing (Sb, Sn leaching and effluent analysis), ex situ testing (conductivity studies as a function of thermal or electrochemical oxidation), and post-mortem analysis (Pt size, migration/coalescence).
- The project should emphasize the direct mass activity comparison with SOA PtCo/C catalysts and evaluate the catalyst in terms of durability, in terms of both Pt mass activity and corrosion. Appropriate metrics for durability are not comparisons with Pt/C but whether a catalyst with improved durability can replace Pt/C with the various mitigation strategies present in operating systems.
- The project should remove DFT and focus on improved synthesis of supports and Pt-alloys (that will likely stabilize on oxides). Also, there should be more interaction with FC-PAD for stability and support degradation analysis.
- In cost modeling, the team needs to consider the system mitigation cost, not a stack replacement, as the baseline. Load-cycling data should be reported to confirm that these catalysts and supports are effective for the drive-cycle requirements.
- Understanding the interaction of metal oxide support and catalyst will be valuable for support and catalyst stability.
- The project should perform load cycling ASTs for at least one of the promising catalysts.
- Catalyst ASTs are needed, in addition to the support ASTs.

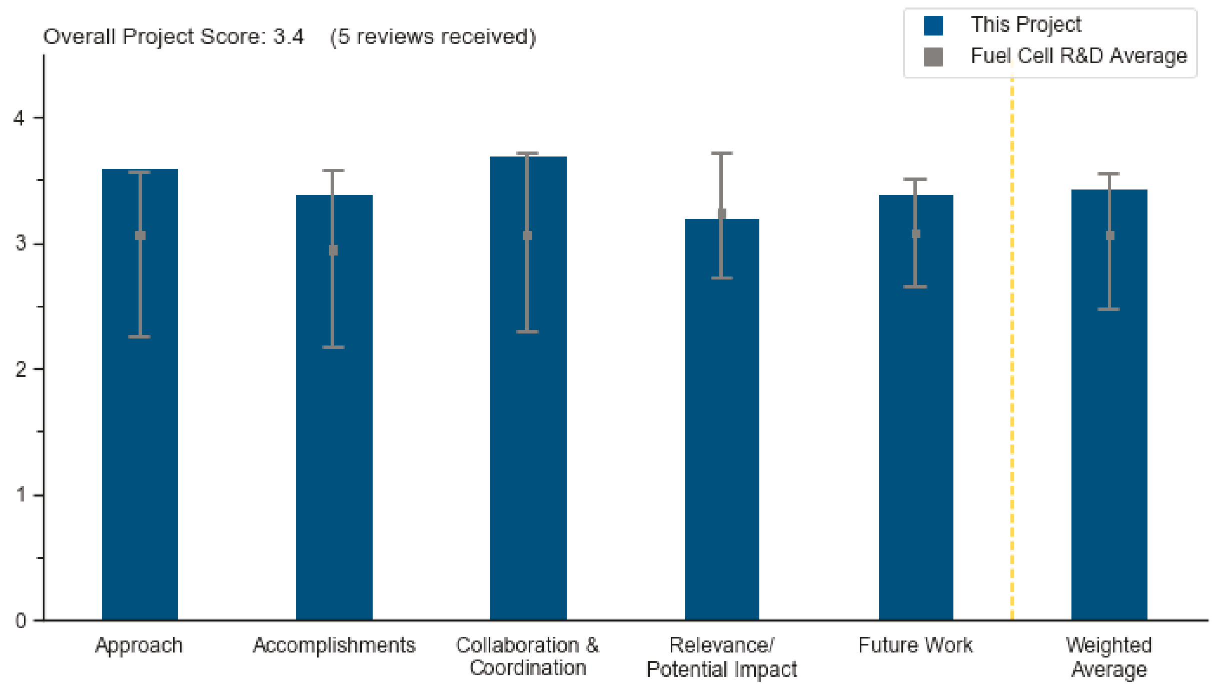
Project #FC-146: Advanced Materials for Fully Integrated Membrane Electrode Assemblies in Anion Exchange Membrane Fuel Cells

Yu Seung Kim, Los Alamos National Laboratory

Brief Summary of Project

This project is developing advanced materials for fully integrated membrane electrode assemblies (MEAs) in anion exchange membrane fuel cells (AEMFCs), enabling fuel cell cost reduction without sacrificing performance. The improved anion exchange membrane (AEM) materials are based on highly conductive and stable hydrocarbon polymers. The project also aims to address challenges with integrating catalysts and AEMs into high-performance MEAs. The approach involves (1) preparing AEMs without aryl-ether linkages in the polymer backbone and (2) developing different ionomeric binders for anode and cathode.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has done a very good job of systematically defining and solving new challenges in the AEMFC field, some of which (such as phenyl adsorption on Pt, cation co-adsorption, etc.) have not been tackled or discussed, essentially, by any other groups. This project has been timely in many aspects and has been one of the truly successful projects in the field globally.
- The project addresses key barriers of durability, performance, and cost of alkaline membranes and AEMFCs. Key barriers of stability of the backbone polymers and cationic groups have been identified and are being addressed. Key issues concerning interactions of the ionomer and ionomer degradation products with the catalysts have been identified and are being addressed.
- The approach addresses critical limitations of AEMFCs. An initial focus on membrane stability, followed by a shift to addressing cell performance and durability, addresses critical barriers; the project is well integrated with other AEM efforts.

- The project's approach is a logical progression from membrane production and testing, to AEMFC performance evaluation, to AEMFC durability testing.
- The main idea behind bringing in AEM materials was to create fuel cells with inexpensive electrodes, which means no platinum group metals (PGMs). A significant portion of this project's attention seems to be on the interaction of the ionomer and Pt. Maybe, if a non-PGM catalyst were employed, no phenyl/phenol-Pt or cation-Pt interactions would be important. If phenyls create problems, the polyphenylene polymer appears to be the worst choice for AEMs. Also, it would be good to pick a "champion" ionomer and go through all the tests with that polymer. Showing good durability data with an AEM of conductivity of 10–20 mS/cm at 80°C (which is practically useless material from the perspective of fuel cell power output) is not fair and will not lead to any practical conclusion.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has developed a new route to complete quaternization in ionomers; now conductivity loss due to interaction between catalyst and ionomer is addressed, and the project has a very stable membrane. The project team identified performance limitation caused by cation co-adsorption and designed an ionomer to minimize adsorption. The team is finishing 5000-hour durability and observing better performance at high current density, thanks to a lower potential for oxygen reduction reaction. The project is on track to meet final project milestones and complete deliverables. This is the final year of the project, which is an extension of the original three-year project. The project is 98% complete toward an end date of September 30, 2019, and nearly all money has been spent.
- Significant progress has been made, especially in the area of determining degradation modes and some of the causes for poor AEM or MEA performance. The project has worked to determine that the reason for the conductivity loss and degradation of Diels Alder PolyPhenylene (DAPP) membranes is cross-linking due to unsubstituted Br reacting with hydroxide, followed by dehydration and ether formation in the Hexane-6-TriMethylAmmonium (HTMA)-DAPP membranes. This has led to pre-cross-linked material with higher durability for AEM materials. The results indicating phenyl oxidation to phenol and poisoning by the phenol group are important for future durable membrane design and high performance in AEMFCs. Work from this project has been instrumental to increasing understanding of AEM durability issues and catalyst alkaline–ionomer interactions. As seen on slide 6, showing alkaline stability results using a logarithmic scale for the conductivity is misleading, masking degradation and making it look like materials are more stable than they are. The initial decrease in conductivity (over the first 1000 hours) for the HTMA-DAPP shown in this slide is substantial and could be as high as 50%, but it is difficult to determine from the logarithmic plot. Because of the choice of a logarithmic scale for the Y axis, it is difficult to see if there is continued degradation after the first 1000 hours. The neutron reflectometry results are interesting, but it is not clear how the simple molecule analogs relate to the real-world situation. In membranes, the cations are tethered to a polymer backbone, and the tether and polymer backbone will have a large influence on how densely the cationic groups can pack near the Pt surface.
- Good progress has been made in regard to improving performance and the durability mechanism. However, the loss in performance after 500 hours is a concern, and the target is unlikely to be met with remaining project funds.
- The only target that has yet to be met is durability. Otherwise, very good progress has been made.
- Practically all project milestones have been met on time.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- The project partners appear to be collaborating well with each other. The project lead has been collaborating with others in the AEM community, including other national laboratory, academic, and industrial collaborators, and has been a leader in the AEMFC community.

- The collaboration seems strong, with team partners contributing. There are also a number of other non-funded partners with some level of interaction.
- It appears that this team has worked very well together and that team members have all made significant impacts on the project.
- Many collaborators, materials, and much knowledge is flowing in both directions.
- Strong inter-laboratory cooperation is evident.

Question 4: Relevance/potential impact

This project was rated **3.2** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This has been one of the most successful AEMFC projects out there. The team has pushed the performance and improved the stability of ionomeric components ex situ. Even though they have not yet met the durability target, a couple of years ago, 500 hours of AEMFC durability with 12% degradation would have been unheard of. Even now, it is very good, and only a few other groups are known to have had the ability to accomplish it.
- AEMFCs are an appropriate low-technology-readiness-level area for DOE to investigate. They offer the potential to operate with reduced- or zero-PGM loadings, potentially leading to reduced costs and a large potential impact. This project addresses key AEMFC issues of durability and MEA performance. The applicability of AEMFCs to automotive applications is unclear, as there are issues with carbonate formation and extra system complexity needed to scrub CO_2 from air.
- The commercialization of AEM materials with Xergy, Inc., and Aldrich is impressive and should be impactful to the community.
- Relevant progress has been made in developing AEMFCs with higher performance. There is a continuing need, however, to develop more durable cells that can produce high levels of performance with non-PGM catalysts.
- The reviewed research can be classified as basic. Except for the ionomers developed at Rensselaer Polytechnic Institute, everything will be of moderate practical importance toward achieving the general goal of bringing AEMFCs to the market.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work addresses critical issues, including improved durability, non-PGM catalysts, and carbonation.
- The one remaining task cuts right to the heart of AEMFCs now: durability.
- The project is nearing completion. The proposed work is appropriate for the time remaining in the project.
- The proposed future work is appropriate to finish the project by September 20, 2019.
- Investigating the degradation of pathways due to the presence of Pt is a waste of time. It would be better to try some non-PGM catalysts. Also, fuel cell performance tests with O_2 oxidant should be done with air, or at least with synthetic air (with no CO_2), instead.

Project strengths:

- The project addresses the stability of AEM membranes and the performance and durability of AEMFCs. These objectives are critical barriers. Good progress was made in particular with improving cell performance and meeting the majority of milestones.
- The project has developed stable AEMs, identified causes of performance degradation, and developed mitigations for those causes. New ionomers have been commercialized and will be available through Aldrich. The project has numerous collaborations.
- The project team has done exceptional work determining degradation mechanisms.
- This is a very strong team, and they have made very good progress.
- The project is strong, but not too strong.

Project weaknesses:

- The membrane durability remains a concern, and targets will likely not be met. Future work can potentially address other AEMFC limitations, including non-PGM catalysts and carbonation. It is also unclear how or to what degree steady-state operation projects to lifetime durability.
- The project has no real weaknesses, though it may tend to oversell the technology slightly (for example, using a logarithmic plot when showing degradation).
- The team does not show compelling evidence that the real cause for in-cell degradation is the cathode ionomer oxidation.
- There is too much focus on the effects of Pt. Non-PGM electrode-based AEMFCs are what is needed.
- The project's weaknesses include the delays to the project schedule. Ongoing questions remain about the long-term stability of AEMFCs.

Recommendations for additions/deletions to project scope:

- The team might benefit from reaching out to another group outside of this project with a more cathode-stable ionomer–electrode formulation, in order to reach the durability target. Also, it is unclear or unstated whether the cells are operated with wet KOH at the beginning of life or whether the KOH is completely removed before operation. If the former, it could be that it is the KOH mobility outside of the cell area that is decreasing performance with time. Finally, the team could also try to run the durability experiments with air (both with and without CO_2). This can often help with durability by either (1) making the reacting environment less oxidative (lowering oxygen concentration), or (2) the presence of a small amount of CO_2 at 80°C leaving a few carbonated groups, which are less nucleophilic than OH-. One of these approaches might also improve stability enough to reach the target. Also, there is disagreement with the previous year's reviewers about CO_2. That would be a distracting task from the primary goals and skills of the team.
- The project is nearing completion. No additional scope is suggested. This is an area that would be appropriate to continue, but perhaps with more of an emphasis on electrolyzer conditions.
- The project team should focus on the best-performing ionomer type only and test it thoroughly.
- The project is nearly complete, and changes to the project scope are not recommended.

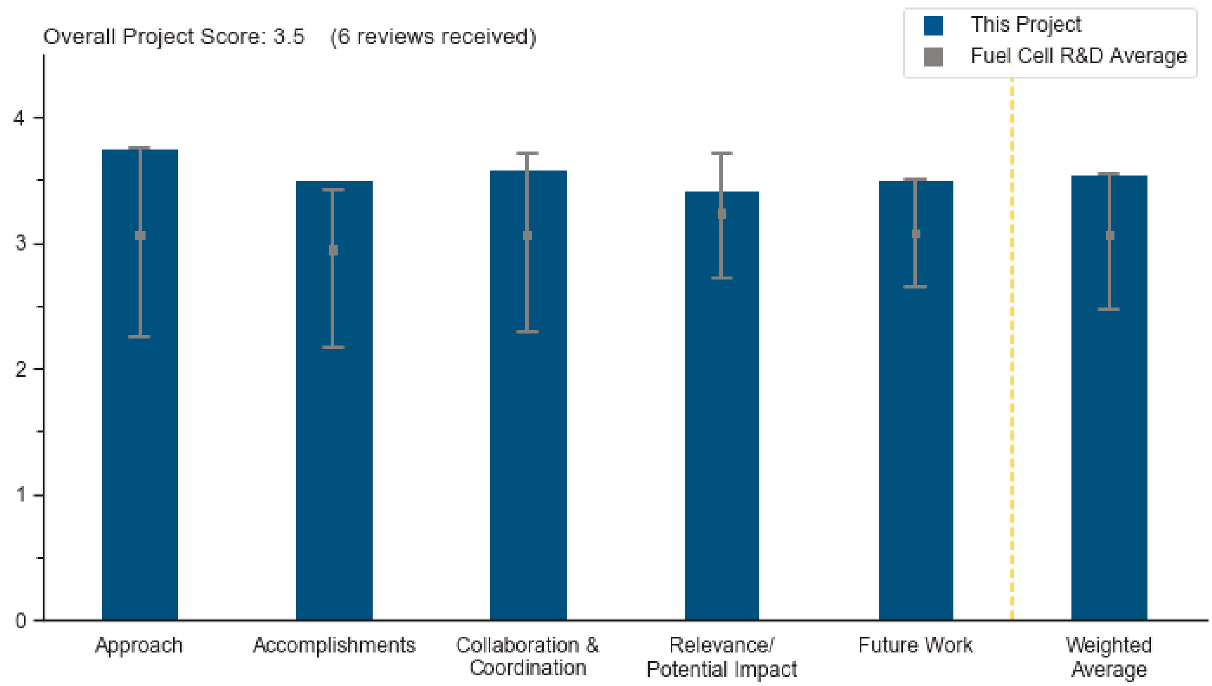
Project #FC-147: Advanced Ionomers and Membrane Electrode Assemblies for Alkaline Membrane Fuel Cells

Bryan Pivovar, National Renewable Energy Laboratory

Brief Summary of Project

Anion exchange membrane fuel cells (AEMFCs) offer promise for improved performance and decreased cost. This project aims to develop novel perfluoro (PF) anion exchange membranes (AEMs) with improved properties and stability, employ high-performance PF-AEM materials in electrodes and as membranes in AEMFCs, and apply models and diagnostics to AEMFCs to determine and minimize losses (water-management-, electrocatalysis-, and carbonate-related). Researchers will synthesize, characterize, and optimize AEMs and fuel cells for performance and durability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project identifies durability, cost, and performance as key barriers for AEMFCs. The strategy to use perfluorinated materials to address water management is notable, as water management is a key issue affecting performance in AEMFCs. This project is also addressing the impacts of CO_2 and carbonate formation, another key barrier often neglected in AEMFC studies. The approach of using perfluorinated materials may be detrimental to cost but should be beneficial for water management.
- The team is clearly extremely experienced and competent enough to carry out this work; this is evident in the approach. This is an extremely challenging project, given inherent issues with AEMs and their application to fuel cells. The team has done an excellent job sequencing through different synthesis paths for the polymer and developing different configurations for membrane electrode assemblies (MEAs). The data are encouraging.

- It may be that, just like with polymer electrolyte membrane (PEM) systems, the path to practical AEMFCs will lead through perfluorinated backbone ionomers. The project team does the syntheses, optimizations, and modeling very well.
- The project has a systematic approach from membrane to MEA and fuel cell testing. The project team has developed a combined experimental and modeling approach with key collaborations and partnerships.
- The project is well designed; the critical barriers and technological risks are understood, and the mitigation strategies have been proposed.
- The project team has made great progress.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The AEMFC performance and durability demonstrated by the project's principal investigator (PI) are in the top 3% of the world's best achievements in the field. A majority of milestones have been successfully completed.
- The demonstrated performance, methodology, and identification of problems and avenues for improvements were excellent.
- There has been excellent progress in MEA developments and investigating different catalyst approaches (gas diffusion electrode vs. catalyst coated membrane). The team has done good work looking at water management in AEMFCs, particularly modeling work and experimental validation with segmented cells. The status of the Gen-3-type membranes (tethered with all C linkage) is unclear, specifically whether a go/no-go decision was made for this path or if this option is still being pursued. Gen 2+ work is important since data has shown the RN(Me)3+ cation degrades, but progress in Gen 2+ seems slow, and not much progress is apparent since last year. International Electrotechnical Commission conformity is a bit low, and durability data for longer durations is needed. It would be nice to know what cation is being utilized in the Gen 2+ work.
- The project is 85% completed toward project goals and ends on September 30, 2019. The Gen 2+ membrane shows material degradation in KOH testing, which could complicate conductivity measurements. There are interesting modeling results from Lawrence Berkeley National Laboratory (LBNL) that point to water management as key to stable performance. There is more work to be done on experimental validation of the CO_2 modeling results.
- All the past milestones were met. The fact that the team attempts to employ CO_2-free air in the fuel cell experiments is a plus. Now, let the project move toward non-platinum-group-metal (non-PGM) electrodes, as promised to the public years ago. Modeling CO_2 effects and water management indicates that the team is attacking truly important barriers.
- To the extent that the project laid out key performance metrics and achieved them, the work is excellent. The team achieved 600 hours of continuous operation and good current densities. However, there is still a gap in requirements for commercial systems.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- The in-project collaborations appear to be working well. Collaborations with the AEMFC community are apparent, especially through the electrode work. National Renewable Energy Laboratory (NREL) has been supplying its Gen 2 membrane to multiple institutions.
- The collaboration between NREL, LBNL, Colorado School of Mines, and 3M was mutually beneficial and accelerated the project's progress.
- It is evident that the team worked well together. Each team member appears to have done its part, and NREL has coordinated activity well.
- There is excellent collaboration between three national laboratories, a university, and an industrial partner.
- There has been good collaboration with all partners and other projects.

- There is an effective use of collaborators' strengths.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- AEMs offer a route to lower the cost of fuel cell systems (an anticipated reduction in precious metal catalyst content and costs). This is of vital strategic importance in DOE's overall strategy to support a transition to hydrogen fuel cells in order to meet global targets for CO_2 reduction and eliminate dependence on fossil fuels. The project is clearly relevant and has high potential impact. There are, however, multiple routes to achieving this goal. DOE should explore many alternatives simultaneously. It would be important to understand why this chemistry is a good candidate to be in that down-selected group. The perfluorinated backbone is a big plus. It would be good to know if there are other considerations.
- AEMFCs are an appropriate low-technology-readiness-level area for DOE to investigate. They offer the potential to operate with reduced- or zero-PGM loadings, leading to reduced costs and a large potential impact in some applications. The applicability of AEMFCs in transportation applications is questionable, as there are added complexities of dealing with carbonate formation. Some analysis of the necessary cost and size of an automotive system to remove CO_2 from the air stream may be beneficial for guiding decisions on directions for AEMFC work. This project addresses key AEMFC issues of durability and MEA performance.
- Durable ionomer and the important studies of CO_2 and hydration are surely well aligned with the Hydrogen and Fuel Cells Program and DOE research, development, and demonstration (RD&D) objectives. This project has the potential to advance progress toward DOE RD&D goals.
- AEMFC development is critically important for advancing inexpensive fuel cells with completely PGM-free anodes and cathodes. The project under review fully supports the goals and objectives in this research area.
- The performance of AEMs continues to be of concern, but at least now NREL has demonstrated good performance is possible.
- The project team has developed new insight into mechanisms of performance degradation in AEMFCs.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The project's future work involves continuing the development of better polymer structures based on learnings from the first two rounds of synthesis, integrating modeling analysis into component development, and further development of electrode assemblies. This is consistent with the overall project approach.
- The proposed future work identified continued integration of modeling efforts with cell testing as a key next step in developing this class of AEMFCs. The proposed work elucidating performance losses in the MEA will be beneficial.
- The team has a clear understanding of how to address remaining challenges and barriers through the proposed future work.
- Based on the figure summarizing the effects of AEM improvements versus electrode improvements, it can be concluded that the focus should be on the ink and electrode optimization.
- The project is nearing completion. The proposed work is appropriate for the time remaining in the project.
- While the modeling and the weaknesses of ionomers is well described, the path to improvement is not clear.

Project strengths:

- The project's strengths include its combined theoretical and experimental approach, its good use of collaborator strengths, and its identification of weaknesses in Gen 2 material and engineering of a solution in Gen 2+.

- The project's focus on perfluorinated membranes provides unique properties that other AEMFC projects lack, including the benefits of perfluorinated systems in water management.
- The project's strengths include its excellent analysis and expansion on understanding of AEM-based fuel cell performance and electrodes. The project has a strong team and collaborations.
- The PI demonstrated a significant breakthrough in AEMFC technology by successful development of the team's approach, passing critical milestones and go/no-go design points.
- The team understands the challenges with AEMs and has performed excellent work with 3M to develop these materials and test them in fuel cells. The team is very experienced and accomplished.
- This is a very strong project; it has a great team and great results.

Project weaknesses:

- AEM development is inherently challenging. From the data, it looks like a membrane reinforcement strategy would have been a plus, to integrate into the component development. It would have been beneficial to have seen some data with alternate (non-platinum) catalysts. Ultimately, testing should be standardized on CO_2-free air, versus hydrogen or oxygen. It is hard to compare the data with data seen outside this project in the commercial sphere. But these are minor issues; the fundamental project effort has been excellent.
- The project needs to do more experimental validation of predictions related to water management and CO_2. Membrane materials still demonstrate mechanical failure in KOH.
- AEM stability is still very low. AEM performance lags far behind that of PEMs, while PEMs improve. It is not certain that AEMs really make sense in PGM fuel cell applications.
- The project has made no effort to test non-PGM electrodes.

Recommendations for additions/deletions to project scope:

- From the data, it looks like a membrane reinforcement strategy would have been a plus, to integrate into the component development. It would have been beneficial to have seen some data with alternate (non-platinum) catalysts. Ultimately, testing should be standardized on CO_2-free air.
- A shift to electrolysis may make sense since the economic case may be better. Now that performance with Pt is proven, it is also recommended that the project incorporate PGM-free, at least on the cathode, to reduce Pt loading.
- The project should compare the performance of Gen 2 PF AEMFCs with PGM and non-PGM electrodes, using synthetic air (with no CO_2) as the oxidant.
- The project is nearing completion, and there are no recommendations for added scope. It may be beneficial to focus future AEM work on electrolyzer applications.

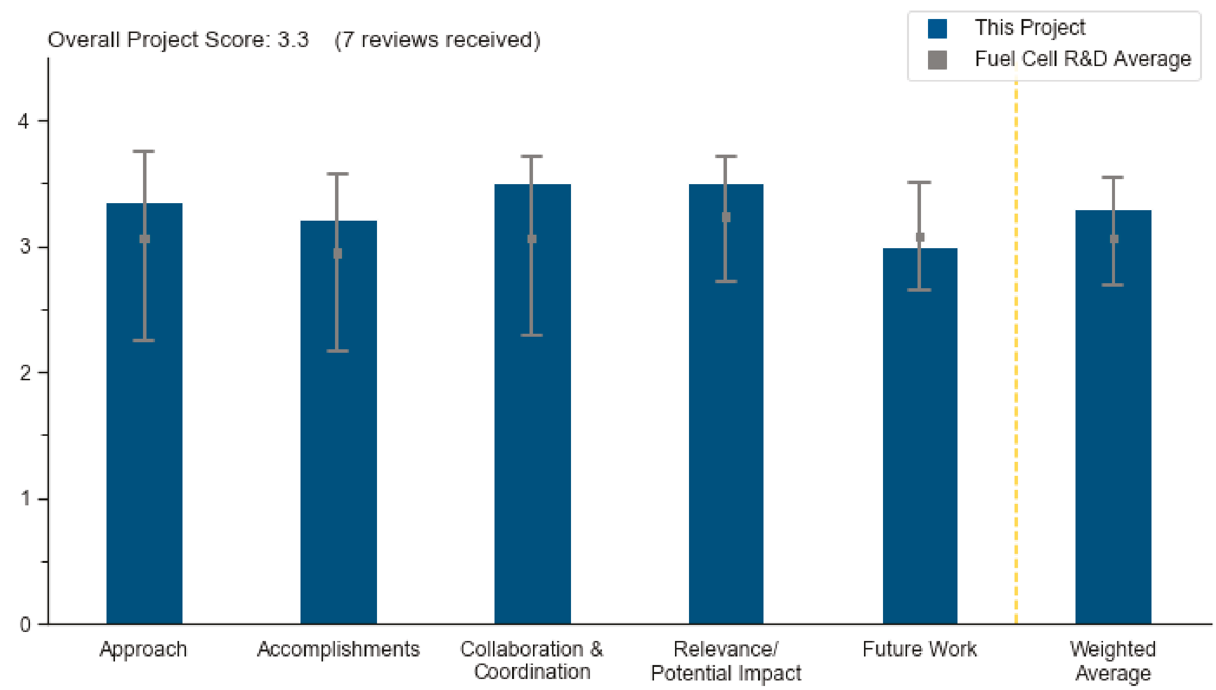
Project #FC-155: Novel Ionomers and Electrode Structures for Improved Polymer Electrolyte Membrane Fuel Cell Electrode Performance at Low-Platinum-Group-Metal Loadings

Andrew Haug, 3M

Brief Summary of Project

The objective of this project is to develop novel ionomers and electrode structures to improve polymer electrolyte membrane fuel cell (PEMFC) performance and durability. The focus of the ionomer development is on combining high proton conductivity with improved oxygen transport. The project also seeks to understand and optimize novel cathodes that utilize nanostructured thin-film (NSTF) catalysts in powder form. These powder catalysts are being integrated with the ionomers to develop an advanced cathode of high activity and durability. State-of-the-art novel characterization and modeling techniques guide these development efforts.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project scope addresses the cost, performance, durability, and robustness barriers as outlined in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (MYRDDP). Specifically, this project addresses the localized mass transport limitation of oxygen on the cathode side of the fuel cell. The project addresses this through the understanding and characterization of oxygen transport in ionomers and by designing new ionomers, integrating dispersed NSTF (dNSTF) into catalyst layers, and evaluating the benefit with respect to improving oxygen transport, while also maintaining performance and durability. The ionomer approach aims to improve ionomer conductivity and transport, allowing for a reduction in ionomer content, which could result in an overall reduction in local resistance. The project approach is in direct alignment with the MYRDDP and the goal of reducing mass transport limitation.
- It is good that 3M is taking a hard look at different ionomers. The researchers seem to have an open mind, and they have found that proton conduction, rather than oxygen transport resistance, is the limit. They use

their well-known NSTF catalyst for the work. The research deficit of the proposal is that the chemistry of the ionomers is not disclosed (IMIDE#1, etc.), so it is hard for the community to get a better understanding of the science behind the results. Overall, the project is making good progress toward U.S. Department of Energy goals.

- This approach is very insightful, especially coupled with the work General Motors is doing, as both are answering the oxygen transport problems at low loading from very different perspectives. The one thing that cannot be judged is whether this approach is cost-effective. The only mention of cost is when it is listed as one of the barriers. One of the great things about NSTF it that it was a roll-good item that could be directly transferred to the membrane. Now, there are multiple layers, higher loadings, and additional processes, all of which will significantly increase costs. It is also not clear how this helps solve the flooding problems generally seen with NSTF, but the catalyst seems to operate fine at high relative humidity.
- The approach is excellent; however, there is a concern about how the technology being developed here will be successfully utilized by the fuel cell community, since 3M recently announced that it is not going to make membrane electrode assemblies (MEAs). Since only 3M makes the NSTF catalyst, it is not clear how MEAs with NSTF are going to be produced. It should be clarified whether 3M will sell the NSTF catalyst as a product so that this technology might be usable.
- The approach addresses many of the elements of creating a catalyst layer, including the catalyst itself (dNSTF), oxygen transport through ionomer, and proton transport through ionomer. However, not much is mentioned in the slides about the carbon content of the layer or how water management might be addressed. The use of modeling eventually points to the higher coverage of whiskers with ionomer, but it is not clear whether this has led to better results in testing at higher current density. The approach emphasizes the improvement of kinetic parameters, such as mass activity and ECSA, to meet performance goals. The approach leaves considerable uncertainty as to how high-power targets are to be met, outside of the modifications to the ionomer.
- Electrode ionomer is an important area of work. However, the dNSTF was not well planned. It would have been better if the project had done some preliminary work prior to the start of the project. The risk and reward are quite low considering the relatively low mass activity, low electrochemical surface area (ECSA), and additional processing costs. It is unclear how productive it is for Michigan Technological University (MTU) to pursue modeling to investigate the root cause of the dNSTF problem, considering its non-uniform structure and performance perspective.
- Attempting to improve ionomer performance through increasing permeability and conductivity is worthwhile, as is investigating dNSTF in MEAs. The synergies of the two approaches are not clear.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made excellent progress toward the project goal. The researchers have met all of their milestones and targets. All tests are done in accordance with procedures outlined in the MYRDDP. However, not all of the targets are met with one membrane–ionomer–catalyst system, and some testing or targets are done at 70°C or 80°C, so it would be nice to see consolidation in the future work. On the ionomer side, imide-based ionomers have shown through this project that oxygen and H+ transport can be improved. Multi-acid-side-chain (MASC)-based ionomers do not appear to be characterized or reported here. The Fuel Cell Consortium for Performance and Durability (FC-PAD) characterization indicates the reasoning behind that, namely the local structure of the polymers on Pt, orientation, and swelling. This should be extended to other imides and MASC ionomers. On the catalyst side, dispersing NSTF is a logical extension of the approach, and it circumvents issues with NSTF while resulting in a new catalyst layer structure enabled by dNSTF.
- There are impressive results with respect to both the development and demonstration of new ionomers in catalyst layers and new catalyst layers with dNSTF. It is good to see that dNSTF may be able to overcome some of the major issues with conventional NSTF (e.g., those listed on slide 3 of FC-143: operational robustness, contaminant sensitivity, and break-in conditioning). For many years, some have been recommending this approach; 3M's response used to be that dNSTF would not be cost-competitive. The team should clarify how or whether this concern has been addressed.

- The team has made remarkable progress, having reached almost every DOE 2020 target, in some cases by a wide margin. At the time, these were very aggressive targets. Similarly, the team has completed nearly all of the project objectives while providing new insights into transport and degradation mechanisms.
- The project has made very good progress toward DOE goals. As of February 2019, the team has achieved the DOE goals and seems to be on track to meet all of the targets.
- The project has had some encouraging ex situ results on ionomer development. However, it is late in the project, and the benefit has not been realized in fuel cell performance. There are some interesting fundamental analyses by partners and FC-PAD. It is not clear how the project will implement the learnings, as it is late in the project. Data quality is a concern; it is unclear whether there was any measurement replication. The sample description is lacking. It is not clear what data belong to which MEA configuration. The targets were not met with the same or a similar MEA configuration. It is not clear whether there were any positive outcomes or learnings from dNSTF. If not, this should stop. The MEA diagnostics did not translate to fuel cell performance.
- The project has had some positive results surrounding the ability to go to lower ionomer-to-carbon (I/C) ratios, to reduce the transport resistance at high current density, and to achieve reasonable performance and durability metrics with dNSTF. The project still has a number of challenges, including voltage loss at 0.8 A/cm^2 and questions regarding conductivity within the electrodes that need to be further elucidated. It was difficult to relate the results to tasks, as the task topics showed up only in the summary at the end of the talk. Clearer comparisons of single variable changes that are focused on just ionomer changes or just catalyst changes would have been beneficial in assessing the impact of different factors on performance and durability.
- The mass activities are still below project targets. It is not clear if the gram-per-kilowatt measurements are bounded by $Q/\Delta T$. Good progress has been shown on addressing robustness. Some imide ionomers may still be a problem for electrode conditioning. The researchers were able to understand that high-current performance may be limited by proton transport. They were able to realize transport gains with more carbon and less ionomer. Support-corrosion accelerated stress tests (ASTs) show that the losses are within target. However, higher current density losses following 0.6–0.95 V cycling point to a need to address agglomeration and slow proton transport.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- 3M has done an excellent job leveraging its university and DOE collaborators. Combined with 3M's excellent test methodology (and a good gas diffusion medium), the results are very compelling.
- Nearly all of the collaborators made contributions, even though 3M certainly did most of the work. Argonne National Laboratory processed the electrode, while Lawrence Berkeley National Laboratory provided direction on which ionomers would lay flat on platinum. Tufts University (Tufts) evaluated electrode tortuosity and looked at the coverage of whiskers with CO-stripping measurements. MTU provided a model to support increasing ionomer coverage. The National Renewable Energy Laboratory measured mass transport resistances, while Los Alamos National Laboratory ran fuel cell tests that showed performance was limited by proton transport. The one collaborator whose role was difficult to find in this year's slides was Oak Ridge National Laboratory (ORNL). The presumption is that ORNL is called upon whenever images are needed. MTU's work supported what was found experimentally, but the polarization in the validation plot seems to reflect a shape different from the polarization that was measured.
- There are many project partners, including FC-PAD, MTU, and Tufts. It was great to see progress made by sub-partners this year, as highlighted by the project slides. Important contributions were made to project scope and the prime's capability to meet the targets. Regarding slide 10, it is not clear which ionomers Tufts analyzed by alternating current (AC)/direct current (DC) or what the conclusion is. The team should clarify with which perfluoro imide acid (PFIA) the I/C ratio was measured and why MTU performed water uptake at such high temperatures. More information should have been included here.
- The prime, 3M, appears to be getting many useful results from the project partners and FC-PAD.
- The team, including the FC-PAD members, has appropriate skills.

- The project lists nearly 50 individual contributors and 8 organizations; some of the capabilities seem to overlap, and from an organizational standpoint, it might be better and easier to stick to a tighter team. Having said that, there are strong contributions from all of the major players, though 3M and FC-PAD seem to be doing the lion's share.
- 3M does all of the development work. The project's partners and FC-PAD contribute only to fundamental analyses, and it is not clear whether or how much any of the learning was feedback to the materials development work.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project goes directly to the heart of one of the biggest challenges facing automotive PEMFCs: the limit of low-loaded catalysts with air. The project has provided much insight, especially considering transport in these systems. It also offers real strategies with demonstrated improvements. Not much more can be asked from a project.
- The work being performed on this project clearly aligns with the needs expressed in the MYRDDP. The project approach to attack oxygen transport limitations using both ionomer and catalyst layer changes has the potential to meet the DOE targets in terms of performance and durability at low loading. Importantly, the project focuses on both ionomer and novel catalyst structures to understand the issues and provide mitigation strategies.
- The project supports many of the targets familiar to lowering cost and enhancing durability for proton exchange membrane fuel cells with low amounts of platinum. The project uses a catalyst that can be produced at relatively high commercial volume, although 3M's commitment to producing fuel cell electrodes at high volume is questionable. The impact of ionomers on conditioning will affect the utility of the material, which will also affect relevance.
- The team is working on the key issues to enabling MEAs with ultra-low platinum-group-metal (PGM) loadings. However, it is not clear how some of the learnings might be used by the fuel cell community if only 3M has the NSTF catalyst and 3M is not selling the NSTF catalyst or MEAs.
- Based on the reported results and performance, the ionomer development efforts may have more relevance. They have shown the ability to go to lower I/C ratios and decrease transport resistance, and they have the potential to be applied to a variety of different catalyst systems. The dNSTF approach is clearly interesting, but it needs further development and may not be able to achieve state-of-the-art performance.
- This project supports the DOE's goals well. The only problem is that, ironically, the project has no corporate transition partner, as 3M has minimized its fuel cell business. Perhaps 3M will sell one of these wonderful new ionomers and advertise how to make good catalyst-coated membranes with them.
- Electrode ionomer development is important, but dNSTF appears to be an unproductive choice. Many unnecessary efforts were put into topics with low return on investment (ROI).

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The project's Gantt chart, milestones, and future work plans are clearly presented and show the pathway to ultimately achieving project targets, as well as new understanding about this important issue.
- The future plan is good with respect to completing the technical milestones. However, it is not clear how this technology is going to be successfully handed off to others for use in future MEA product development.
- Most of the "key items" have to do with processing, toward which the researchers do not provide much insight. The project is coming to an end, and one of the focus items is to reach the voltage durability target, which is the only one they have not yet met; this is a good focus.
- The future work contains many important areas (e.g., proton conductivity and improving the ionomer coverage of the whiskers), but it is balanced more toward enhancing performance rather than durability. With the losses at higher current density, more of the future work should be directed toward durability. The

project end date is September 30, 2019, so it may be wise to cut new material developments from the future work.

- The project ends in September, so the researchers are just wrapping up. It would have been helpful to hear about a transition plan and about how well the ionomers work with non-NSTF catalysts.
- It is quite late in the project. Effort should be put into realizing benefits in fuel cell performance. Electrode ionomer development is important, but dNSTF appears to be an unproductive choice. Many unnecessary efforts were put toward low-ROI topics. Some interesting fundamental analyses were done by partners and FC-PAD. It is not clear how the project will implement the learnings, as it is late in the project.
- The proposed future work is reasonable, but it does not provide prioritization and was not discussed during the presentation. The slide included is a "laundry list" of relevant activities that does not provide clarity of focus or direction on most critical issues.

Project strengths:

- The project's greatest strength is the uniqueness of the NSTF approach. These catalysts are different and behave differently from any other catalyst systems that others are studying and provide a very different perspective. Any model that one comes up with has to fit both this approach and more traditional Pt/C approaches. The unique NSTF, coupled with a strong team, has led to the ability to meet or exceed almost all DOE milestones while keeping to the project goals.
- The project is using a catalyst that can be made at a high manufacturing volume using scalable and repeatable vacuum processes. The primary investigator is knowledgeable in manipulating catalyst, catalyst-layer, and ionomer parameters to create higher performance. The project has made good use of all collaborations in the national laboratory network.
- The project has a good approach. NSTF catalysts are a clearly differentiated catalyst architecture, and therefore it is great to see that 3M is (finally) taking a different approach to potentially addressing the major issues with NSTF catalysts. The new ionomers are great new materials for the fuel cell community.
- The project's strengths include its strong collaborations and its utilization of both sub-partners' and FC-PAD's capabilities and expertise. The project has an interesting and promising approach for both ionomers and catalysts/catalyst layers to achieve targets.
- The project's strengths include its advanced ionomer development, in which 3M is a world leader, and the NSTF catalysts that offer a unique platform of interest for advanced fuel cells.
- The project has very good and very credible results. The members of the large team are all contributing appropriately.
- The project's strengths include its ability to develop perflouro polymers.

Project weaknesses:

- The project should make more use of FC-PAD's capabilities to understand the role of ionomer structure on properties, the impact of ionomer in catalyst layer structure on performance, and durability at low loading.
- There are limited synergies between ionomer development and dNSTF approaches. The presentation included significant data, but it was difficult to distill differences between the results.
- Only 3M makes the catalyst, and it would be difficult to imagine it being made by other suppliers. Most stack manufacturers will likely continue to rely on dispersed powders unless something very convincing emerges from this project. There are still some remaining issues with conditioning that appear to relate to ionomer choice. This could be a significant barrier to implementation. The project still needs to show compelling power density and durability. Without these, the odds of implementation in a commercial fuel cell system could be very low.
- Cost analysis is not in the project or not reported. This is troublesome because it is difficult for an outside observer to tell if what the team is proposing is practical. Along those lines, adding Ir, the rarest of PGM catalysts, as a solution does not seem like a very viable pathway, but maybe it is so low an amount that it does not matter.
- The useful ionomers are not disclosed, and it is not clear that anyone could ever get them. It is also not clear whether the ionomers work with catalysts that are not NSTF.

- The project's collaborations are weak. It is unclear if having partners and FC-PAD was helpful or simply a distraction to 3M.
- The path forward, with respect to technology handoff, is not clear.

Recommendations for additions/deletions to project scope:

- 3M should provide the new ionomers to others so that other groups can see whether higher performance can be obtained using other conventional catalysts. This could greatly increase the interest in these new ionomer options. 3M should clearly communicate what the path forward is with the NSTF catalyst. NSTF seems to have great promise for electrolyzer applications. However, if 3M is not going to sell MEAs or NSTF, the team should consider how electrolyzer developers will utilize NSTF, as well as how fuel cell developers will potentially use NSTF catalysts.
- It is recommended that the team work on a transition plan to commercialize the ionomer and advertise the results. If 3M does not want to make the ionomers, perhaps 3M can license them to another company.
- The project is in its last six months, so there are no additions to suggest. Removing new material developments would be wise in the late stages of the project. The project should remove most of the activities that are not related to lowering conditioning time and enhancing power density and durability after 0.6–0.95 V cycling.
- There should be more tie-in of materials that meet component-level targets into AST and performance testing—for example, the high-oxygen-permeability ionomers in MEA testing. There should be more characterization of the catalyst layer produced from dNSTF regarding what it looks like and how it is unique or different from conventional catalyst layers.
- Clearer comparisons should be made between single variable changes, and the impacts on performance and durability for each of the systems should be studied.
- The project is wrapping up and is rightfully focusing on increasing durability.
- It is not clear if there were any positive outcomes or learnings gained from dNSTF. If not, the work should stop.

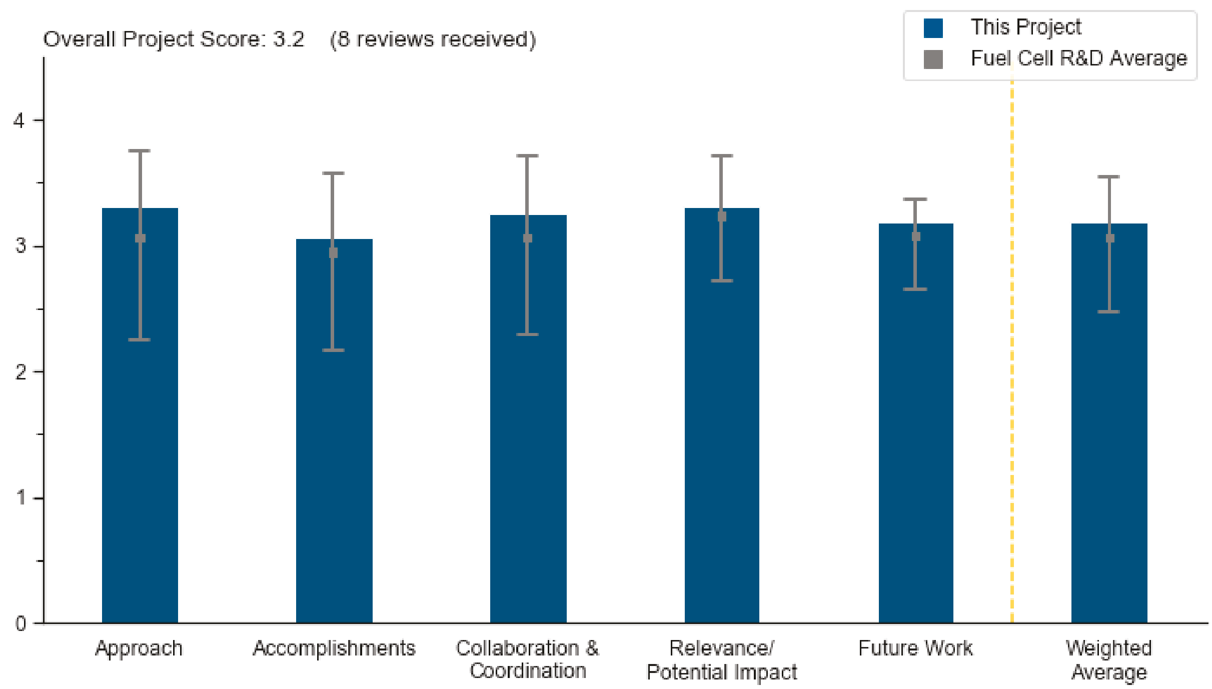
Project #FC-156: Durable High-Power Membrane Electrode Assemblies with Low Platinum Loading

Swami Kumaraguru, General Motors

Brief Summary of Project

This project seeks to improve the durability of a state-of-the-art (SOA) membrane electrode assembly (MEA) by identifying and reducing the stress factors affecting electrode and membrane life. Project tasks include (1) MEA optimization of a low-loaded electrode through down-selection and integration of MEA components, (2) durability studies of the developed MEA, and (3) development of a predictive model for degradation in different operating conditions.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The proposed approach is clearly described and based on a multi-step, multi-factor improvement design matrix. The milestones and go/no-go decision points are adequately selected and allow for the estimation of progress being made toward Office of Efficiency and Renewable Energy final targets from the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan.
- The project strives to identify benign operating conditions that will enable enhanced MEA durability through the use of in situ and ex situ testing, analysis, and modeling. The overall project approach appears sufficient to meet the project objectives.
- The project has performed very comprehensive study under realistic operating conditions. Various voltage cyclings are performed to develop fundamental models of mechanical stresses for combined degradation. Tasks are very well distributed among the team members. The team is starting with SOA MEA, which eliminates many variables in the study and provides more confidence in the results.

- The approach is detailed and well suited to identifying the detrimental conditions to avoid in MEA operation. The use of two-factor analysis of the load cycling experiments can provide some very useful insight and should be pursued further.
- The project has a sound approach; particularly appreciated was the use of "design of experiments" to accelerate the testing campaign.
- The approach addresses the two major classes of failures: those caused by voltage cycling and those caused by either low or cycled hydration. The project includes variations in voltage cycles and deeply analyzes aspects of membrane degradation that are a tier below the operating condition stressors, such as cerium migration and hydrogen crossover. Interactions of voltage cycling and hydration with temperature are well addressed. One question that could be raised with the approach is whether all cerium-containing additives behave alike. It is unclear whether the results shown here would be repeated for any cerium additive package. Given that many milestones from budget period 2 still remain incomplete, there does arise a question of whether the project scope is too large. The voltage cycling runs could be completed, but it is uncertain that the membrane degradation modeling will be completed. There is also a model based on Pt and Co dissolution that needs to be completed. The Pt dissolution model does not have an equation for conversion of PtO to Pt2+.
- The voltage cycling of significant run variations may end up providing valuable results, but at this point in the project, not all data appear to make sense. This is an extensive and methodical way to generate the test data, but improved understanding on repeatability and error-checking (or at least insight into this) would be appreciated in order to ensure that the data will be meaningful when the testing is done. As mentioned last year, the use of only one material set does raise concerns that relationships may change. No indication of the material set was provided. This should be provided in at least general terms. It is recommended that the team run tests on air and hydrogen to more closely mimic actual operation, as there will be changes in the catalyst layer's local conditions and some effect on mechanisms. These are not expected to be significant enough to invalidate the approach, but this will need to be checked.
- The project's strengths revolve around the SOA materials, performance, and durability of the systems being investigated. The approach itself seems strongest in budget period 1, with decreasing clarity and impact in subsequent budget periods. The meaning of the task numbers given on accomplishment slides is not clear, and those tasks do not connect to budget period task numbers. All the areas of interest at least have scientific relevance, but most are not directly tied to overcoming barriers and will instead help provide fundamental understanding.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Some important and practical results have come from this project: the realization that mechanical stresses accelerate chemical degradation (even at the cell outlet), the understanding that convection is the primary transport mechanism for cerium cations, and the understanding that cerium content affects the uniformity (or lack thereof) of membrane-thinning over the cell. The trends of electrochemical surface area (ECSA) loss and Co migration with higher relative humidity (RH) cycling were probably understood in the community prior to the work done by this project. Conclusions are still needed from the voltage-cycling experimental design. The project is still having difficulty understanding operating condition effects on gas crossover since the crossover rate appears to be independent of initial cell shorting.
- The go/no-go result of the effect of RH is not a new result. Previous DOE projects have demonstrated the strong effect of RH on cathode degradation. The project has interesting results on Co distribution in the MEA cross-section. In regard to the membrane highly accelerated stress test (HAST) work, the combination of accelerated testing with the diffusive crossover maps and Ce X-ray fluorescence (XRF) maps is very interesting and is providing useful insights. The follow-up work on Ce transport modeling and understanding mechanical stress impacts on chemical degradation is also valuable. For the membrane thickness effect on chemical degradation, the effect of the open circuit voltage (OCV) value on the membrane degradation rate should be considered. The OCV value will vary with membrane thickness. Further understanding of the local shorting effects is valuable.

- Very good progress has been made so far in studying various H_2–N_2 cycling to understand the effect of operating conditions. The effect of RH was studied extensively, with detailed analysis of losses. Significant progress has been made on model development and HAST testing.
- The project's progress has been strong in meeting DOE goals. Performance and durability have been demonstrated largely at the SOA level and at the level of DOE targets.
- The competition of main milestones and go/no-go points is on excellent track. The improvements made in the activity and durability of novel MEAs are significant.
- The team has made good progress on assessing the impacts of different MEA operating conditions on performance degradation. The demonstration of the impact of RH on Co dissolution, alloy catalyst performance, and ECSA loss is a very useful result.
- After two years, it appears the project may be behind from the perspective of milestones and total funds spent, assuming annual budget periods and go/no-go points. The membrane and Ce-additive-specific work appears to have made very good progress and is on track, but the H_2–N_2 and hydrogen–air voltage cycling appears behind, and the review slides on the model appeared primarily to provide the framework, with relatively few results and conclusions.
- The team is on track to deliver project goals.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- Collaboration with the Fuel Cell Consortium for Performance and Durability (FC-PAD) is well established, although this is a General Motors (GM) project for the most part. The National Renewable Energy Laboratory is engaged on cell testing, and Argonne National Laboratory is included on degradation modeling. The collaboration with Giner, Inc., appears to have yielded results that speak to the primary mechanism for cerium transport (convective). The collaboration with the University of Texas at Austin (UT Austin) has provided the results showing greater cobalt movement to the membrane with higher RH cycles.
- This project significantly benefited from close collaboration with FC-PAD, which allowed the team to demonstrate steady progress toward final project goals.
- The work distribution across partner organizations appears reasonably coordinated and appropriate for each organization's capabilities.
- The structure with FC-PAD and subcontractors leads to good collaboration.
- The team has made good use of outside resources.
- Although collaboration with project partners was mentioned, the presentation did not highlight the specific role played by each of the partners. The team is encouraged to prioritize the information so that the partners' work becomes more evident.
- The collaboration group is limited, but GM's breadth makes this less necessary. There are clear roles for the sub-tier partners but limited capability for bringing in outside strength beyond FC-PAD participation.
- The contribution of the UT Austin is not very clear. GM has done most of the work. The contribution of Giner, Inc., is evident from the results. FC-PAD's collaboration also seems less substantial.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Operational durability is of critical importance for polymer electrolyte membrane fuel cell integration. Activity and durability, especially for catalytic materials, are often inversely proportional. Improving the durability of MEA performance through the optimization of operational conditions has a higher chance of immediate success than an approach focused on the development of new materials.
- There is no question the project is highly relevant. At this stage in fuel cell development, material sets exist that can enable a degree of commercialization, as evidenced by vehicles that are actually on the road. However, much of the scientific phenomena that would enhance system mitigations, and therefore system durability, still remains unexplored. This requires a low-technology-readiness-level (low-TRL) kind of

effort to enhance high-TRL applications. This project attempts to do exactly that by probing the phenomena that got "left behind" as developers were racing to produce vehicles. The only question regarding relevance might be with respect to how well the project can expect to complete its goals before time expires. There is still much work to do, and the scope is very large. Although the project does focus on one particular material set, the material set is adequately representative of what the community is using.

- The combination of high power density and good durability with low Pt loading is clearly one of the main challenges that are left to be solved in reducing fuel cell cost and enabling the industry to grow. This work addresses the challenge directly.
- The results have been promising and strong when considering cell performance and durability. Other efforts, such as modeling studies and Ce migration, are relevant but do not provide the same value to the project as MEA optimization.
- The project team is aiming to achieve DOE's performance and durability targets. With GM being the principal investigator (PI), most of the tests are performed under realistic operating conditions and, most importantly, using SOA MEAs.
- The project is critically important for the DOE mission toward development of inexpensive and robust MEAs with low-platinum-group-metal content.
- The project is directly addressing MEA durability, which is one of the most significant barriers for the widespread deployment of fuel cell technology. The overall approach should provide significant benefit to the field. However, one concern is that the SOA MEA components are not disclosed, and as such, the results generated will be only indirectly useful. Without knowledge of the components, other research groups wishing to extend the results generated in this project will likely need to generate their own datasets with their own materials.
- The work is highly relevant. There is no doubt that much of the work will be of high value. However, the overall potential impact is difficult to assess at this point in the project.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed future work is in line with what is necessary to successfully complete the work. The focus should be on measuring the true intrinsic dissolution rates of Pt and Co at realistic conditions, such as the presence of Nafion™ and the effect of RH. The project team may want to look at different carbons, as they could affect metal dissolution and ECSA loss.
- The project still has an overwhelming amount to accomplish. The voltage cycling experiments need to be mapped, the dissolution rates of many species need to be measured, and a model needs to be made for membrane degradation, among many other things. The future work certainly acknowledges all of this. The future work mentions a durability improvement in the accelerated stress test. It would seem enough for this project to clarify the relationships between stressors and resulting material failures. Durability improvements would seem more the domain of actual developers in vehicle products, especially now that the technology status is based on vehicles.
- The planning of future work is logical and based on previously reported progress, including several risk-mitigation scenarios.
- The proposed future work is logical and aligned with the project plan.
- The scope of the work is appropriate but does little to suggest significant additional advances beyond those already demonstrated within the project; it is not certain these are even included in scope. The focus of the future work is on developing models and improving fundamental understanding, but these seem to be topics of a more academic focus rather than ones that advance the current SOA.
- The proposed future work seems reasonable for achieving the project goals.
- The future work seems to center around a new simulation model. The scope of the model is not entirely clear. It is recommended that the project team make the model validation plan and strategy very clear for the next meeting.
- The project team should provide more explicit data on the test station variability, as well as which DOE runs will be repeated and how many times.

Project strengths:

- GM's vast experience with MEAs and their degradation is the biggest strength of this project. The team is well established, too. Understanding combined degradation in order to help develop fundamental models that can predict the degradation is a really good approach. The team is looking into various H_2–N_2 cyclings instead of just using the established durability protocols.
- The work is relevant and is applied to high-priority degradation mechanisms. The HAST membrane work is very valuable. Although not shown in the presentation, the understanding of the oxygen transport mechanisms as the electrodes degrade likely will be applied and of value. The dataset is being generated on an MEA that meets DOE Pt-loading targets.
- The project is led by a vehicle manufacturer keenly aware of the relationships between operating stressors and material failures. This manufacturer understands that mitigations can be generated in system operation to prevent material failures. Not all developments have to come from improving materials. The project is well connected to the national laboratory network for analysis and modeling. The project has appropriately divided failure modes into two categories: those that arise from voltage cycling and those related to membrane failures.
- The PI demonstrated deep understanding of degradation processes in catalysts and catalyst layers, derived from a quite complicated design of experiment. The obtained knowledge will facilitate the completion of milestones and the final project goal.
- The project's strengths include detailed analysis of intrinsic mechanisms of instability in MEA performance, two-factor analysis of MEA operating conditions, and effort centered on finding the true dissolution rates at relevant conditions.
- The key project strength is in the project approach: utilizing in situ and ex situ testing, advanced characterization, and modeling.
- The project's strengths include the materials used, as well as the performance and durability demonstrated.
- The experimental approach is sound.

Project weaknesses:

- The project workload is extreme, which has resulted in a heroic list of tasks in the future work section. The project sometimes finds relationships that were already understood in prior work (e.g., ECSA losses increase following cycling at higher RH). The final product of the project may prove difficult for other developers to use in designing system mitigations.
- The project's weaknesses include its design-of-experiment data-generation format, which makes it difficult to assess emerging trends. The project is also specific to only one material set, and no information is provided on the material set being used. The team indicates that these are being provided with no restrictions on analysis, so more information could be provided in the DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR) material.
- It is recommended that the next AMR presentation be more focused on covering collaborations and high-level project takeaways.
- The primary project weakness is that it is using proprietary materials that will not be disclosed, limiting the direct usefulness to the field.
- It does not seem like the future work offers much opportunity for further advancing the performance and durability of fuel cells.
- The collaboration and contribution of other team members and FC-PAD are not very clear.

Recommendations for additions/deletions to project scope:

- Once the project has made sufficient progress in establishing the feasibility of the overall project approach, the team should consider assessing other catalysts and MEAs comprising disclosable material sets; this should be done earlier in the project rather than at the end of the project, as stated on slide 27.
- The project team should provide information on the material set used, test some variations on the material set once the degradation model has been developed, and include air–H_2 testing.

- The project team should look at different carbons—for example, high surface-area carbon versus Vulcan®—as porosity can affect particle sintering and dissolution.
- No additions are proposed. Any work associated with improving durability should be eliminated. This project should be designed for understanding the relationship of operating stressors and material failures. If repeated tests to observe crossover trends with local shorting do not show trends, then this part of the project should be eliminated.
- Much of the modeling work and fundamental studies seem of limited value. It is not clear what else could be done to further advance performance and durability, but approaches along these lines would provide more value.

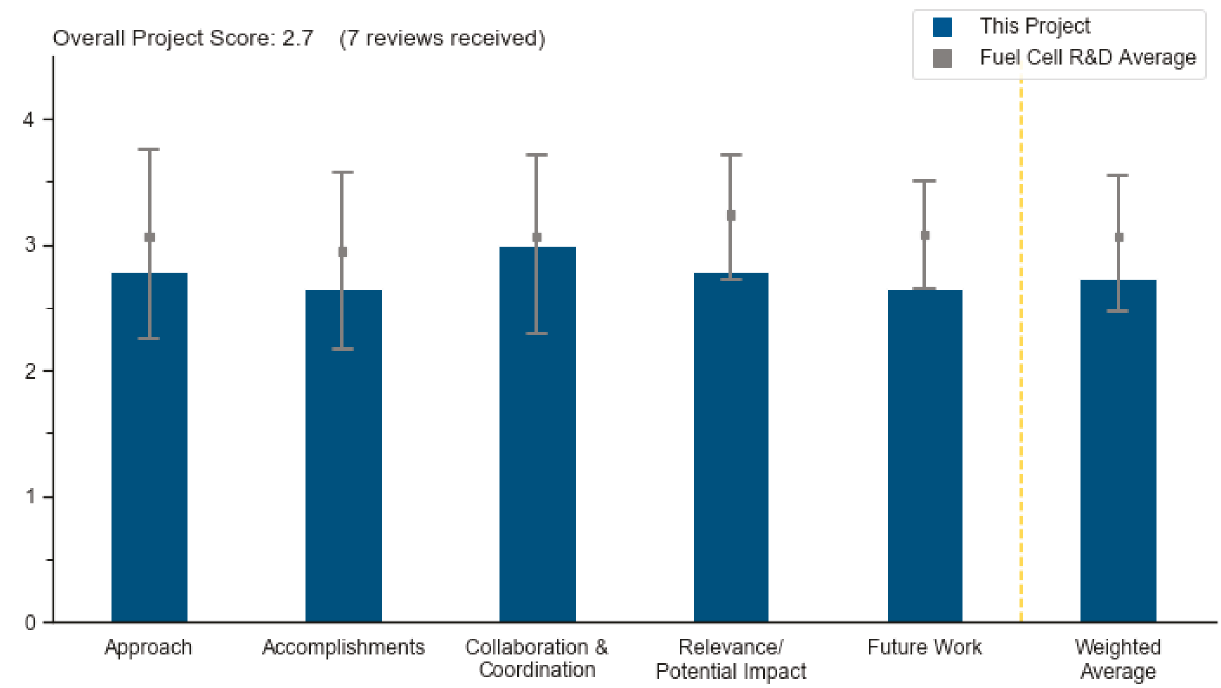
Project #FC-157: High-Performance Polymer Electrolyte Fuel Cell Electrode Structures

Mike Perry, United Technologies Research Center

Brief Summary of Project

The objective of this project is to improve the fundamental understanding of transport limitations in state-of-the-art membrane electrode assemblies (MEAs) for polymer electrolyte membrane fuel cells and use this knowledge to develop and demonstrate high-performance MEAs with ultralow catalyst loadings (ULCLs). Transport losses are a major barrier with ULCLs, but fundamental understanding of those losses is currently lacking. To gain better understanding of the nature of these losses in cathode catalyst layers, a detailed microstructure model of the cathode catalyst layer will be developed. This improved knowledge will then be utilized to develop improved MEAs that meet the U.S. Department of Energy's (DOE's) performance targets.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project scope is not clearly aligned with the barriers in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (MYRDDP); however, the project essentially addresses performance, cost, and durability, as inferred from other slides. Specifically, this project addresses the localized mass transport limitation of oxygen on the cathode side of the fuel cell, using modeling to inform catalyst layer development. The project approach is in direct alignment with MYRDDP targets of reducing mass transport limitation in low-catalyst-loaded electrodes and under low-humidity operation. This is accomplished through the understanding of transport phenomena. The approach of developing a detailed, geometric, microstructural model of the catalyst layer is a novel pathway and, compared to other projects, the focus on understanding is key. The project is validating models with real-world MEAs.

- The project's approach is to develop detailed geometric models of cathode catalyst layer (CCL) microstructures. The team will project and close the performance gap by using the model to design and build optimum electrode structures.
- As a model for addressing gas-phase transport losses, the project does well in determining which models consistently agree with experimental results observed for changes in platinum loading, ionomer-to-carbon ratio, and platinum mass fraction. The project then goes on to apply the appropriate models. Much of what the project has studied can be applied from an in-depth understanding of recent literature. However, it is not entirely obvious how the model is addressing condensed phases. There is some mention of how effectiveness factors and Thiele moduli change with water filling, but how water filling arises is not shown, and neither is how hydration of the catalyst layer and membrane is determined. The nanocolumnar catalyst is interesting, but there are many details missing, e.g., sputtering costs, reproducibility, batch size projections, and other information.
- This project uses a good mix of computational model development and validation with outside MEA data and their own. The model results have been used to make MEAs with lower transport resistances. It appears that this was brought up by reviewers last year, but it is hard to see the relevance or utility of the thin-film catalysts. The project would be more suited if it focused on carbon-supported, nanoparticle-based catalysts.
- The recently published hierarchal model helps with understanding the transport phenomena in the catalyst layer. The model advises that smaller agglomerates can improve performance. However, it is unclear how the team plans to control the agglomerate size.
- This project attempts to create a somewhat universal model to explain fuel cell behavior. The 2018 paper by Darling is an excellent paper, but it has some limitations, mainly due to its use of 21 variables. While some of the variables are easy to define—such as temperature, pressure, etc.—some are harder to define, such as ionomer-film thickness. The model seems to go in with the assumption that oxygen resistance is the most important factor, and then the model proceeds to prove its theory. While the model accounts for the density of primary particles and porosity, it does not account for pore size distribution. There have been some papers out showing that the pore size distribution of the catalyst layer is very important. Eikerling also emphasized porosity in his model. The authors do not try to match their model to a broad number of catalyst-coated membranes (CCMs). Another complexity is the gas diffusion media (GDM), which will clearly change the results. They use a United Technologies Corporation (UTC) gas management device, but no information is given. Without some more validation, it is hard to know whether the model is really useful beyond the researchers' laboratory.
- This project was not set up for success. The project promised to achieve DOE targets by first understanding electrode transport loss, then validating it, and then fixing it. However, the approaches for understanding the phenomenon are essentially the same as what others have done in the last nine years. Unsurprisingly, no particular learning was made. No specific plan for model validation was laid out. Therefore, this project will likely be a repeat of what others have already done. The project lead does not have access to the resources or expertise needed to prepare electrodes or MEAs to validate the model or to pursue the development of materials to achieve DOE targets.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project was delayed, and a no-cost extension is being implemented. In the meantime, the project has made progress toward the project goal. The team has met most of the project milestones and targets and is on track for others. The team should include dates with milestones, as its unclear how the no-cost extension shifts out the quarters. For example, it is unclear whether Quarter 6 (Q6) is delayed or on track, or when the go/no-go is. All tests are done in accordance with procedures outlined in the MYRDDP. There is a clearly outlined path for meeting the Q8 target.
- The team has made good progress in model development at different length scales. However, this has not yet translated into MEAs that meet the target metrics.
- The team made progress toward the project goal, but it is not clear if they asked the right question in the first place. They went into the study saying that oxygen transport resistance was the key parameter, and

they then proved it. A later talk by 3M showed that proton resistance in the ionomer has a big impact. Pore size distribution cannot be ignored.

- The recently published hierarchal model may oversimplify the diffusion in the catalyst layer. The model does consider the porosity and tortuosity to some extent (by dividing the bulk diffusivity by 4, it seems), but a catalyst layer with a similar porosity could have very different tortuosity and diffusivity. Maybe the incorporation with Lawrence Berkeley National Laboratory's (LBNL's) full-scale MEA model can better handle the mass transfer in the electrode.
- The model has been incorporated into the LBNL two-dimensional (2D) MEA simulation, but the modeling results shown depict radically low limiting currents that vary with particle size, which is hardly the reality with realistic fuel cells. For small cells with gas-phase transport, the model appears to predict performance losses well, accounting for three levels of oxygen resistance (nanoscale, agglomerate, and catalyst layer) as well as ohmic losses. The nanocolumnar catalyst still has low mass activity, which continues to raise questions as to whether this catalyst is a worthwhile part of the project. Substantial cell resistance needs to be removed, and a PtCo catalyst needs to be used to meet the Q8 targets.
- The project has not generated new experimental data to validate and test the critical parts of the model. The modeling approach has been established; its impact on the development of an optimum electrode structure is not clear. The statement that agglomerates smaller than 150 µm are needed is not particularly innovative. The suggested improvements (e.g., Pt-alloy catalyst, General Motors [GM] cell, thinner membrane, 950 equivalent weight) have no relevance to the optimized structures being generated through model predictions. GM and others have already reported results using these MEA features. The Q6 milestone (1 W/cm^2) has not yet been reached.
- The project is delayed. No new progress to the field has been made.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- The United Technologies Research Center (UTRC) team already has extensive collaborations with Ion Power, Inc. (Ion Power), the University of Arkansas at Little Rock (UALR), and several national laboratories, and the team is planning to work with Vanderbilt University (VU) and Los Alamos National Laboratory (LANL) on alternative CCL architecture.
- The team has made good use of partners and resources, including the Fuel Cell Consortium for Performance and Durability's (FC-PAD's) resources.
- The team expanded its collaboration with other members of FC-PAD.
- The project's sub-collaborations and FC-PAD collaborations are clearly defined, and a clear strategy exists for the team to work together to accomplish project goals. The project is leaning on the strengths of its FC-PAD partners. The UALR structures are interesting, but they appear more like a side project to obtain a different structure for the model as opposed to a direct effort in utilizing those structures in catalyst layers.
- The project's collaborations outside of FC-PAD include Ion Power, to deliver custom sub-MEA or MEA components, and UALR, to develop the nanocolumnar catalysts. Both have contributed to results, although the results need to be improved substantially to meet future targets. The model has been delivered to FC-PAD, particularly to the LBNL's 2D MEA model. Oak Ridge National Laboratory has assisted with transmission electron microscopy (TEM) characterization of the UALR catalysts. The project's collaborations could have been considerably enhanced by an automotive presence to guide the project toward the true modeling issues in the development of fuel cell systems.
- There is good collaboration with UALR and national laboratories. The contribution from LBNL's modeling work was not clearly presented.
- The project relies heavily on Ion Power to provide "innovative" electrodes for model validation. No progress has been made.

Question 4: Relevance/potential impact

This project was rated **2.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the MYRDDP.

- Detailed transport models at different length scales will have a significant impact on MEA architecture development and identify areas for potential improvement.
- The work being performed on this project clearly aligns with the needs expressed in the MYRDDP. The unique approach to developing and testing models to overcome oxygen transport limitations is relevant and has potentially very high impact in the field. What is less clear is the benefit of UALR's approach and its impacts.
- Most of the project aspects align with the DOE Hydrogen and Fuel Cells Program and DOE research, development, and demonstration objectives. It is unclear whether the durability test is a part of the project's tasks.
- Both LANL and UTRC have tested UALR's thin-film-catalyst-based MEAs, but the power density has not reached the 1 W/cm^2 target. The hierarchal model (with many assumptions) has been validated with two old datasets available in literature. On the basis of progress to date, the future contributions to novel catalyst and electrode development may be limited.
- Although understanding performance loss in low-Pt electrodes is crucial, model validation is difficult, and modeling alone cannot fix the problem.
- The project may not be able to deliver any true assistance to developers. Nearly all fuel cell developers have already found some way to treat oxygen transport resistances that is reasonably functional. The project does not take great lengths to address the biggest hurdles to development, which all have something to do with how hydration is managed in a cell. The balance between drying and wetting will affect how systems are designed. As the emphasis turns more toward medium-duty (MD) and heavy-duty (HD) trucks, a project focused on new catalysts and gas-phase transport may not be relevant for higher-platinum-loading systems that need high durability.
- It is not clear how this model could be of general use to help improve CCMs. If there is a belief of high oxygen resistance, the model does not explain how to fix it, nor does it explain the idea structure for low oxygen resistance. Agglomerate size is recognized as an important parameter, but it is not clear how this should be changed.

Question 5: Proposed future work

This project was rated **2.6** for effective and logical planning.

- Adapting and applying the developed model to others working on alternative CCL architectures adds to the impact of this project. It would be helpful to provide more details as to how the team plans to use modeling insight to make MEAs that meet DOE targets.
- Considering the state of the project, the future work needs to be more specific. There are remaining questions, including who will provide materials for model validation, what the metrics are, and what new approach in modeling is to be attempted. All of the noted topics have been heavily studied by others over the years.
- The future work reflects where this project needs to go. It would be nice to see more clearly the timelines and the revised dates based on the no-cost extension.
- Hopefully, the team can go into next year's work with an open mind and not just attribute results to oxygen resistance.
- The project will continue to improve the model based on nanocolumnar catalysts and gas-phase transport, and attempt to achieve a better match between model and experiment. It is questionable whether this will result in a real impact on developers. The work done on alternative CCL structures may be difficult to achieve in the time remaining for the project. It may be good to remove the thin-film catalysts from the project since these catalysts may still have problems with mass activity, batch size, cost of production, etc.
- The proposed plan will overcome some research barriers. It is unclear what improvement is expected on the models. Using nano computed tomography (nano-CT) at Argonne National Laboratory may not be able to provide too much help for this project because of the limited spatial resolution of the nano-CT (~25 nm). The approach mentioned in Padgett et al. seems more feasible ("Connecting Fuel Cell Catalyst

Nanostructure and Accessibility Using Quantitative Cryo-STEM Tomography," *Journal of The Electrochemical Society* 165, no. 3 [2018]: F173-180. doi:10.1149/2.0541803jes). The alternative CCL architectures (collaborating with LANL and VU) are not clearly presented.

- The proposed directions lack specificity. There are no clear-cut approaches or recommendations for developing a deeper understanding of the electrode structure or multiphase, multiscale transport processes.

Project strengths:

- The project participants are knowledgeable regarding all previous fuel cell models that address oxygen transport resistances. The models being used to address oxygen transport resistances are consistent with experimental results. FC-PAD and Ion Power are able to deliver results such as TEM, MEA components, and higher-level models.
- The project's strengths include the multi-length scale model that has been validated with multiple data sources and the application of the model to a range of CCL architectures.
- The project's strengths include its three journal publications. With FC-PAD support, the team is able to develop models, characterize microstructures, and measure cell performance.
- The project's focus on modeling first is unique and has high potential impact to help design electrodes and structures.
- The project has strong collaborations with industry, universities, and national laboratories. The multiscale models provide guidance on catalyst design and optimization.
- The project's attempt to build a physical model of a CCM is a strength.

Project weaknesses:

- The model seems to have a predetermined answer: oxygen transport resistance is most important. The project would do better to really push on the results with advanced GDM and ionomers and to try to look at the effects of pore size distribution.
- The project may not be in tune with the existing needs of the fuel cell development community. Some parts of the project feel like a catalyst development led by mathematical modelers. This is probably not the ideal means by which new catalysts are developed. The project has yet to demonstrate target performances at the MEA or catalyst level.
- There have been no novel contributions from the model to illustrate pathways for developing high-performance polymer electrolyte fuel cell electrode structures.
- The UALR structures are similar to nanostructured thin-film catalysts and do not add significant value here.
- The plan is not clear or specific. There is no momentum in the project.
- It is unclear how the thin-film catalysts developed here will have any sort of impact.

Recommendations for additions/deletions to project scope:

- The authors should check the literature again and read the work of Eikerling with an open mind. They might also look at results from state-of-the-art CCMs from companies such as W.L. Gore. The team should refer to "Manufacturing of Low Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning" (report number: DOE-GORE-18052). The team should also look at the Freudenberg GDM and the effects of relative humidity to help elucidate the effects of water management.
- The project should delete the catalyst development and add a focus on hydration and condensed phases. If there was some way to begin addressing durability, this would be better for the community. This appears to be outside of the scope of this project, but the goals associated with MD and HD trucks (e.g., 25,000-hour operation) appear to make durability a more pressing need than understanding oxygen resistances at low platinum loadings.
- The project should pursue a pathway to integrating the UALR structures into MEAs and consider the potential to match or contribute to models.
- UTRC should consider another round of brainstorming ideas.
- The project should stop the work on the thin-film catalysts.
- It is recommended that the project be discontinued.

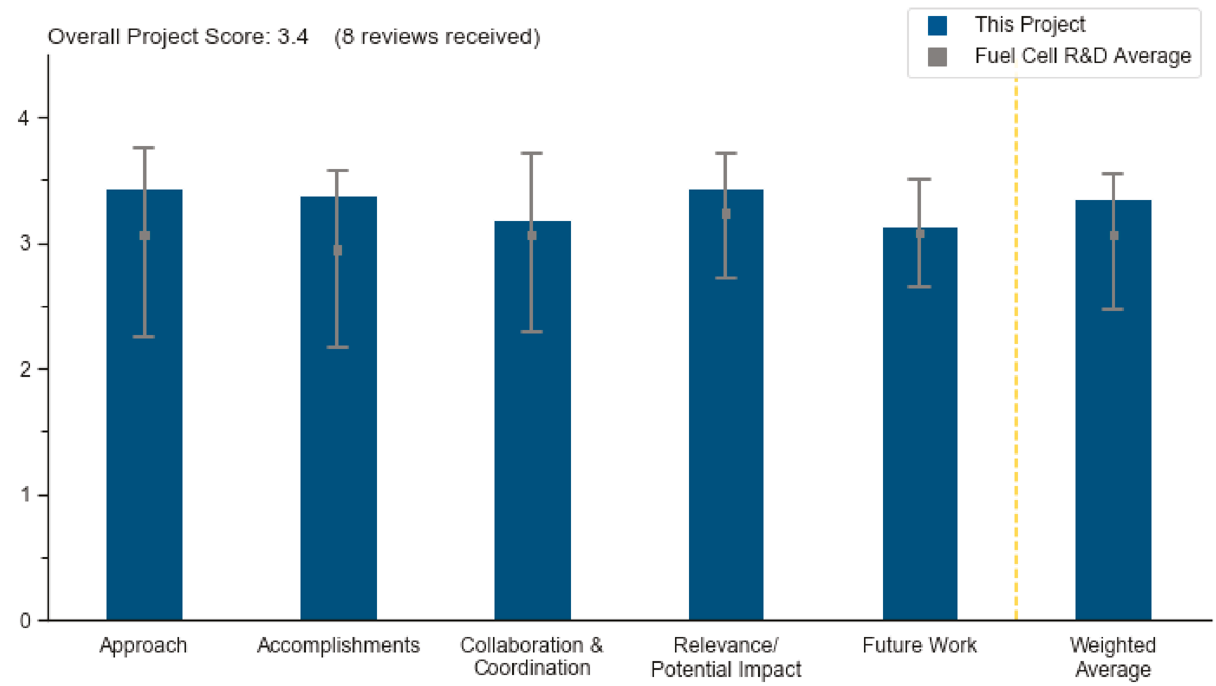
Project #FC-158: Fuel Cell Membrane Electrode Assemblies with Ultralow-Platinum Nanofiber Electrodes

Peter Pintauro, Vanderbilt University

Brief Summary of Project

Particle/polymer nanofiber mat electrodes are a promising alternative to conventional fuel cell electrode structures. This project seeks to better understand and further improve the performance and durability of low-platinum-loaded nanofiber mat fuel cell electrodes and membrane electrode assemblies (MEAs). Mat electrode MEAs with highly active oxygen reduction reaction catalysts for hydrogen–air fuel cells will be fabricated, characterized, and evaluated. The project will focus on nanofiber cathodes with commercial platinum–alloy catalysts and platinum–nickel octahedral catalysts containing various ionomer and blended polymer binders.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The objectives and barriers are well identified. The key issues of improving performance with low catalyst loading and at low relative humidity (RH) are being explicitly addressed. The proposed electrode mats will be easy to integrate with existing polymer electrolyte membrane (PEM) systems.
- This was a very nice presentation, and the project is on track to make some innovative catalyst-coated membranes (CCMs). The fibers seem to have high performance. While the fabrication approach is very good, the test conditions are questionable. One major problem with the work is the very high flow rates that are used in the test conditions for the CCMs. The project uses 80°C, 200 kPa (abs), 125 sccm H_2, and 500 sccm air for 5 cm^2 cells, while 4000 sccm H_2 and 8000 sccm air are used with all MEAs for cells with an active area of 10 cm^2. It is hard to understand the results under these very unconventional flow rates. The authors should use standard stoic rates of 1, maybe to a maximum of 2. The flow rate should vary with the

current. The Sigracet-29-BC gas diffusion layers are also obsolete. Running at 100% RH is also questionable.
- The project scope is not clearly aligned with the barriers in the Fuel Cell Technologies Office (FCTO) Multi-Year Research, Development, and Demonstration Plan (MYRDDP); however, the project essentially addresses performance, cost, and durability, as inferred from other slides. Specifically, this project addresses the localized mass transport limitation of oxygen on the cathode side of the fuel cell through the use of electrospun, fiber-based catalyst layer structures. The project approach is in direct alignment with the MYRDDP targets of reducing mass transport limitation in low catalyst-loaded electrodes and under low-humidity operation. This is accomplished through the understanding of structure–function relationships in the electrospun electrodes. The project team is also developing functionalized fibers for the electrospinning process that would help produce catalyst layer structures to improve mass transport. This should be compared to conventional electrodes made with the same polymers.
- This is a unique approach to generating catalyst electrodes. It is very flexible but also has the potential to be very insightful because of the different structures it creates. Economically, it is very hard to determine whether this is a valid approach. Peter Pintauro has spoken toward this in the past, stating that the approach will be valid if these can be made at low cost, but it bears repeating, especially if there is more evidence or if the team's thinking has matured. This is especially relevant as the larger-scale electrodes looked and behaved differently.
- This is a PEM fuel cell technology project looking at MEA fabrication using an electrospinning approach. The project has a large interactive component, and the contributions of various laboratories, showing interactions and the utilization of Fuel Cell Consortium for Performance and Durability (FC-PAD) laboratories. The electrospun electrodes are expected to improve performance at low RH conditions.
- The project's approach is novel and has impressive results in terms of power density.
- The project can still benefit from further systematic variation of compositions and process parameters, combined with FC-PAD's diagnostic and characterization tools, to correlate effects and enhance understanding of the underlying physics of the processes.
- The technical approach of the project is highly relevant to the FCTO mission. However, the focus seems to be on achieving only high activity and not high durability. It is not clear how the team plans to address durability requirements.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The authors have made excellent progress since last year. They seem to be on track to have a high-performance CCM. It is difficult to determine the true performance because of the unusual test conditions. The imaging of water was a really interesting experiment.
- The project's accomplishments are excellent, with good demonstration of power density and improvements in durability.
- The project has made progress toward the project goal. The team has met most of the project milestones and targets and is on track for others. The drive-cycle durability target was a miss, and the team should outline the path to resolve this. The milestone table makes it difficult to interpret when milestones are due; the past milestones over the course of the year leading up to the DOE Hydrogen and Fuel Cells Program (the Program) Annual Merit Review (AMR) are unclear. All tests are done in accordance with procedures outlined in the MYRDDP, although not all targets are met with one membrane, ionomer, or catalyst system. The Generation 2 (Gen 2) fibers using electrospinning show promise to achieve targets. The project is missing a clear understanding of the effects of the structure. There seem to be benefits such as in Co retention and low-humidity operation.
- There are outstanding results on the MEA performance side. The high performance at low RH shows that the approach works. The new materials are maintaining performance between high and low RH at high current densities. High performance is accompanied by good durability. The performance-versus-humidity data are missing comparison to typical baseline material at benchmark conditions. The measurements were shown at 80°C, 40% and 100% RH, and 200 kPa. Performance data are typically benchmarked to 80°C, 100% RH, and 150 kPa.

- There is good repeated performance and results on the performance, especially with the Co retention, though it is unclear why these electrodes should be better in this regard; this is certainly an area for further study. The project team should compare their results to the benchmarks more often or show the DOE targets in the presentation charts, which would make judging much easier. There are moderate results on the scaling portion, but undoubtedly, when the project team tunes the parameters, this will be achieved. The cost target and progress would have been good to see as well.
- There are interesting results at very low RH (40%), combined with neutron radiography results, which suggests water retention. The project still needs further development and progress to be state of the art at nominal RH.
- The targets relating to power output and durability have been met.
- The ionomer-to-carbon (I/C) ratios of the Gen 1 and Gen 2 MEAs are based on energy-dispersive X-ray spectroscopy (EDX) analysis, which has limitations on depth of penetration. The I/C ratios that were targeted for making MEAs are also not very clear.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The project team has made good use of FC-PAD, using many of the different characterization tools at the consortium's disposal. The team has Lawrence Berkeley National Laboratory down for "possible modeling of the electrodes." This should be engaged, as there is not a good understanding of why these work better. It is nice that the team has an industrial spinner to make sure that the process is scalable.
- The project is starting to see good results from collaborating with FC-PAD (e.g., imaging results from Oak Ridge National Laboratory [ORNL] and neutron radiographic water-mapping at the National Institute of Standards and Technology). The Nissan Technical Center of North America (NTCNA) baselines are improved but are still not clearly state of the art. Collaboration should be exploited to enhance the characterization of nanofiber electrode results. It is unclear whether the eSpin Technologies, Inc. (eSpin) work is complementary or mostly duplicative; the project could use more clarity on the respective roles.
- The neutron imaging work is excellent use of the FC-PAD laboratories. This project can really benefit from seeing the MEA water profiles since operating at low RH seems to be one of the primary advantages of this technology.
- There are very good collaborations, although the researchers would benefit from some more mainstream testing methods.
- There is clear exchange and collaboration between laboratories. There is apparent separation of tasks and expertise, with exchange of information between laboratories also apparent.
- The project lists good project partners with a scale-up partner, an industrial original equipment manufacturer partner, and FC-PAD laboratory partners; however, it is not clear what, if any, of the results were made with the partners' input or contribution. For example, the Nissan data shown on slide 10: it is unclear if that was with MEAs made at Nissan or simply tested at Nissan. It is also unclear why Nissan is testing with fixed flow polarization curves at a strange, high stoic. Many of the polarization curves are with a fixed flow that is excessively high, based on the required flow for proper stoichiometry. This can affect low-RH polarization curves dramatically.
- The NTCNA's participation seems to be very limited on the project with 75% of the work completed; it is not clear what the Center's contribution is, and there is a question of integration of the work. Further FC-PAD tasks are described under "Collaboration," but there is limited evidence for water distribution other than neutron imaging and scanning transmission electron microscopy (STEM) analysis of Co; perhaps this was done at ORNL, but it is unattributed on slides 7, 10, and 16. While mass and water transport in these novel structures seems to be critical, it is not clear when that work is to be performed and integrated, and this is not included in the future work slide.
- The work scope of eSpin is not clear. It is unclear whether the company is involved in any optimization of the nanofiber ink formulation for the manufacturing or is involved only in optimizing the manufacturing process parameters for the catalyst slurry provided by Vanderbilt University (VU).

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- MEAs with electrospun mats are showing remarkable performance improvements at low RH with low catalyst loadings. This is very relevant to DOE goals. Reducing catalyst costs in PEMs is a major objective, and this project directly addresses that.
- The project topics are right on target with the technology advancement and the Program goals. The project would result in decreased catalyst layer loading while upholding performance—and even improving it at low-RH operating conditions.
- High-performance, stable, low-platinum-group-metal-loaded, robust electrodes are key to programmatic success. Further progress is still needed in the high-power-density performance of the nanofiber electrodes, but it shows promise in stability and low-RH performance. High performance at low RH is also an enabler, given that target power density is tied to the Q/ΔT metric (i.e., driving higher temperature, which results in reduced RH). The project team is encouraged to further identify the reasons for this somewhat surprising low-RH performance that has been exhibited.
- The work being performed on this project clearly aligns with needs expressed in the MYRDDP; the project's approach to attack oxygen transport limitations using both ionomer and catalyst layer changes has the potential to meet DOE targets, in terms of performance and durability at low loading. While the practicality of the electrospinning process on a mass-market basis and MEA fabrication is not discussed, it should be evaluated.
- Based on the excellent performance results, the impact is substantial.
- Because this is a unique way to make MEAs that is showing great promise, understanding the design and manufacturing parameters is critical for large-scale adoption and for understanding the cost implications. The responses to the comments from AMR 2018 are not sufficient. As additional data with more slurry properties are available and new binders are investigated, it should become easier to use design-of-experiment concepts to systematically understand the parameters and to help optimize the process variables.
- Though the project's performance has been impressive to date, it is not clear what tweaks the team has left for further improvements in light of DOE goals. It would be interesting to see the project use the better 3M ionomers or the better catalyst that General Motors and 3M have been using in conjunction with these structures. The project will always have some impact just because it is different; this system will need to be better understood and modeled in order to understand why the team is seeing performance gains.
- If the authors' work can be scaled, etc., it may become an important approach. It is not clear how it would scale to a roll-to-roll process.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The proposed future work covers the logical continuation of the project and addresses the questions that have arisen during the project. One could not have predicted that Gen 2 MEAs at either electrode would give high power at low RH, but it is definitely a question worth investigating.
- The project shows the benefit of the fiber format for the electrode; some imaging was done to show the water profile in the cell. More modeling or analysis work should be done to determine the mechanism for a fiber format of the catalyst layer showing improvement. This mechanistic understanding will likely lead the research team to even more improvements.
- There is no dispute with the proposed future work, aside from the need to normalize test conditions with DOE standard methods.
- Overall, this is a very sound project plan moving toward the completion of the work.
- It would be beneficial to see more systematic parameter and process variation, combined with FC-PAD diagnostics, to further identify the mechanistic impacts of nanofibers on performance, RH dependence, voltage stability, etc. Voltage loss breakdowns should also be performed to elucidate the low-RH

performance and measure potential mass transfer effects; for example, the high I/C ratio of the "core-shell" morphology may negatively impact local oxygen resistance.
- The team is right to want to try new ionomers of lower equivalent weight and new catalysts. The team should have done more work to fundamentally understand why these structures are better; modeling with Lawrence Berkeley National Laboratory would help in this case. There is no mention of future scalability studies or economic analysis, which should be done or, if it is not an issue, at least that should be reiterated; however, this seems like more steps than what the best processing methods are using today, especially if the project team is casting in the salt form.
- The project's future work mainly focuses on reaching performance targets, but there is little focus on integrating fundamental understanding and the use of FC-PAD capabilities to understand what is happening in these structures and help accelerate the development. It does not seem to make sense that the project team should continue (or include) conventional catalyst layer development with the functionalized ionomers for electrospinning.
- The only recommendation is for the project team to focus on one catalyst for mat electrodes made at eSpin until the optimization variables are understood.

Project strengths:

- The team is very experienced with electrospinning ion-conductive polymers. Electrospinning enables the production of nanoscale architectures with several features that are inherently beneficial in fuel cell electrodes (e.g., porosity, connectivity, etc.). Engaging with an industrial partner early in the project will help convince others of the potential impact of the results on a large scale.
- The project's strengths are in the principal investigator's (PI's) slurry development and in the industry partner for manufacturing mat electrodes. More focus on ionomers and design for manufacturing would help industrialize this method of making MEAs.
- Electrospinning produces novel catalyst layer structures that seem to have the potential to make an impact toward project targets.
- The unique structures being generated with tunable parameters should make for an excellent tool for understanding performance. This is a good use of the FC-PAD team.
- The PI has a strong background in nanofiber technology. FC-PAD's characterization capability is a key attribute that has been utilized to greater extent in the second year.
- The project has excellent performance results on a novel approach to catalyst layer design.
- The project has an innovative approach to making CCMs and seems to be getting high-performance results.
- The project has a sound approach and a good team and working strategy.

Project weaknesses:

- There are not many weaknesses. The project shows good progress overall.
- The project teams have the capability to fully characterize the performance (e.g., R-O_2 local, mass transport, electrochemical-surface-area loss, specific activity), but they have not yet used that capability sufficiently.
- The transfer of the electrospinning process from VU to eSpin appears to be a problem since the eSpin mats lack the durability of the VU mats. This is probably an issue with scale-up, but it begs the question of whether the mat-spinning process can be achieved on a useful scale.
- More could be obtained from the project with better project management and collaboration with sub-partners and FC-PAD. The conventional electrodes with electrospun polymers should be deemphasized after having initially demonstrated no benefit.
- The project's teaming could be improved. Polarization curves should be run at constant stoic rather than constant flow.
- The project's unusual test conditions (i.e., the very high reactant flow rates) make the data hard to understand in comparison with standard CCMs.
- There is a lack of economic analysis. The project's approach will take more steps than have been contemplated today. Though the baseline materials being used are relevant, it would be good to see more variation.

Recommendations for additions/deletions to project scope:

- The researchers should consider talking to a manufacturer about how to use the VU process in a practical system. This will prevent the project from falling into the “valley of death.” The national laboratories are not a transition sponsor. Perhaps the small company American Fuel Cell (AFC) might be willing to talk to the team (although AFC might have been bought out by Plug Power).
- A comparison of mats made with Pt catalysts on different carbon supports could shed light on the MEA performance. It would be beneficial to see some additional focus on the durability of the mat electrodes.
- The project team should add more characterization and modeling to understand the performance differences between these systems and cast systems. The expected cost in comparison to existing methods should be shown.
- There are questions on the role of eSpin. It would also be good to see more voltage-loss breakdown analysis. More systematic parametric variation is recommended to elucidate the mechanisms and benefits of nanofiber electrodes.
- The project team should make some effort in modeling and understanding the mechanisms of improvements in catalyst layer performance based on the fiber format.
- The conventional electrodes with electrospun polymers should be deemphasized.

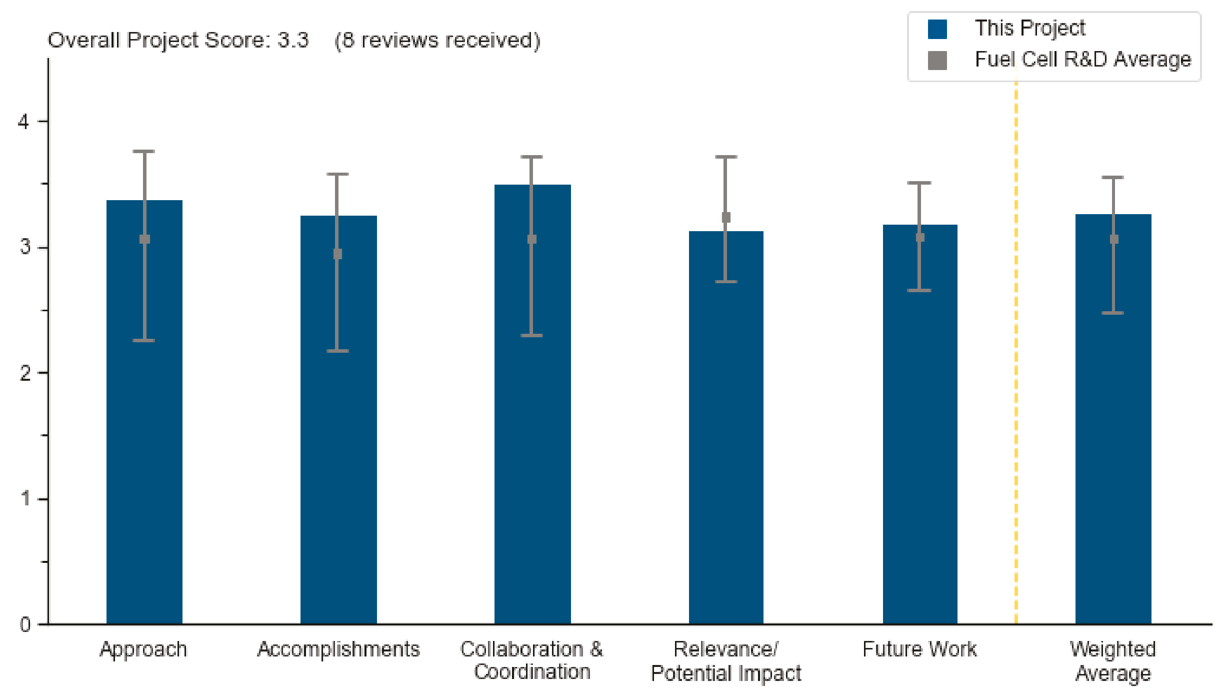
Project #FC-160: ElectroCat (Electrocatalysis Consortium)

Deborah Myers, Argonne National Laboratory, and Piotr Zelenay, Los Alamos National Laboratory

Brief Summary of Project

ElectroCat (the Electrocatalysis Consortium) was created as part of the Energy Materials Network in February 2016. The goal of the consortium is to accelerate the deployment of fuel cell systems by eliminating the use of platinum-group-metal (PGM) catalysts. ElectroCat and its member laboratories—Argonne National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, and Oak Ridge National Laboratory—will develop and implement PGM-free catalysts and electrodes by streamlining access to unique synthesis and characterization tools across national laboratories, developing missing strategic capabilities, and curating a public database of information.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project covers large, sprawling work, with multiple parties and activities. Nevertheless, it is surprisingly focused on the two key points of PGM-free catalysts: activity enhancement and durability extension. This is the type of effort needed to truly understand this class of catalysts and is the most appropriate for the advanced resources and personnel of the national laboratories. There is a nice combination of theory, analysis, and experimental and synthetic work.
- The project aims to develop advanced PGM-free catalysts and electrodes aimed at enabling significant cost reductions for fuel cell electric vehicles. To date, the project approach appears to focus primarily on increasing performance via catalyst activity and electrode transport; this work is excellent. While achieving performance is ultimately necessary, much more focus needs to be placed on durability in the immediate term.

- The project's approach is to develop and implement PGM-free catalysts and electrodes by streamlining access to unique synthesis and characterization tools across national laboratories, developing missing strategic capabilities, and curating a public database of information. This project has very strong leaders from four national laboratories, each with proven capabilities and expertise in some of the key technologies that are critically important for the success of this project. At this stage of the project, additional expertise is required on the catalyst layer and on degradation.
- The science content of this project is world-leading. The researchers are clearly very receptive to feedback from the community, which keeps them in touch with reality.
- The overall project approach appears strong. Progress is clearly being made on improving catalytic activity. One suggestion is that additional modeling of the electrode could be used. The electrodes are thick, and there may be some polarization associated with ionic conduction, triple-phase boundaries, etc., not just intrinsic catalyst activity. If this might be the case, some dedicated experiments and modeling could help clarify the issues, especially when looking at getting to the ultimate performance targets (which may require even thicker electrodes). Another suggestion is that durability under practical operating conditions has clear potential to be a showstopper for this class of catalysts. While performance is improving, durability is paramount to ultimate success. Additional work on durability, and articulating whether this class of catalysts may ever have sufficient durability, is encouraged. Scavengers can help (although they reduce activity), but it appears this effect is more or less short-lived.
- The project approach is well thought out and well structured and is designed to systematically answer the key questions in the development of PGM-free catalysts. The combination of the high throughput, characterization, automated learning, and performance evaluation work is an effective approach to developing relationships and advancing the performance and understanding of catalysts and catalyst layers. More modeling work would be useful to guide the work on electrode structure. Atomic and mesoscale models are being used to guide the catalytic behavior and active-site understanding. The durability work has increased with some good progress. However, some of the suppositions require further confirmation. It appears that the team is depending mostly on electrospun electrodes to provide improved mass transport and high-current-density performance. However, no indication was provided on feasibility or the rationale behind those expectations.
- The approach of working on material discovery and tool development at the same time is really good. There are many unknowns for PGM-free catalysts, including new tools needed to improve performance or even new material discovery by understanding the current materials.
- Much investment has been put into this one material for some time. It is clear that it is of no practical use without magnitudes of improvement in stability. The focus should be only two areas: determining the degradation mechanism and whether it can be prevented. Any other area is a waste of funding.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The accomplishments and progress are excellent and truly a testament to the capabilities of the national laboratory facilities and researchers in characterization and materials development. Of particular relevance were the identification of a correlation between the atomically dispersed (AD)Fe and the oxygen reduction reaction (ORR) activity (as seen on slide 14), the high-throughput materials fabrication and utilization of machine learning (slides 23–25), the accelerated stress test (AST)-induced loss breakdown (slide 28), and perhaps most importantly, a roadmap to achieving the required performance (slide 36). To date, the progress made toward addressing durability appears to be modest, consisting primarily of assessments of decay rate versus operating conditions (e.g., potential, cycling under air versus N_2) and the impact of a radical scavenger, which are important initial steps. It appears that the durability of the catalysts assessed is in the order of tens of hours.
- The work is structured via well-defined milestones that are on track or have been exceeded. Overall, there has been excellent progress on improved fuel cell performance over the past 10 years. Over the report period, improved performance was achieved both in the kinetic region, via catalyst understanding and synthesis approaches, and in the mass transport region, via electrode structure. The reported performance of 36 mA/cm^2 is highest, not the average. The goal was still exceeded, but the project should be quoting the

average, with error bars. The work on electrode structure is still relatively limited, although some interesting results are being achieved. The ionomer layer studies are interesting, showing better performance with decreasing hydrophilicity (high equivalent weight, lower ionomer percentage) nearer to the microporous layer is expected to result in improvements in water management and increased utilization. The use of the high-throughput approach should provide useful insights. There still does not appear to be much use of model correlations or a model-driven approach in this area, although the future work does mention that the project will be using models. There was some reasonable progress on understanding durability issues and mechanisms, the mitigation of shelf-life issues, and the use of cerium to address peroxide degradation mechanisms. Cycling in air versus nitrogen highlights the importance of using a range of realistic conditions to explore degradation mechanisms and impacts. The cerium work can be further explored to confirm mechanisms involved. There was a nice analysis on the improvements needed to achieve power density targets, with a path laid out to achieve them. However, the feasibility of achieving these steps is not explicitly stated. They will certainly be very challenging. The high-throughput approach should provide valuable trends that can then be examined and understood with model approaches. However, error bars should be shown on the plots. The progress on the data hub is not shown; the milestone status indicates this work is in progress.

- Significant progress has been made in tool development. Nuclear resonance vibrational spectroscopy (NRVS) with NO as the surface probe for detecting surface Fe sites is very helpful in conjunction with Mossbauer analysis for active sites. The project team has also put efforts into understanding the effect of carbon source and dopant on Fe in order to gain some insights; however, so far this project is lacking in material discovery. The same polyaniline (PANI)-type catalyst has been used to show good performance in meeting milestones. An improved version of PANI is adequate for proceeding, but it limits other material discovery. Hopefully, the team can show a few more catalyst candidates that meet both performance and durability targets. The layered electrode structure results are promising, and with some more optimization and lower catalyst loading, perhaps MEA performance can be further improved.
- The hypothesis for the most likely failure mechanism for the loss of catalyst activity is well supported (i.e., the formation of the hydroperoxyl radical). The improvement of the highest levels of activity was only mediated by the need for an additional 12x improvement in order to make this class more feasible for implementation. Additional focus on the interactions implicit between electrode structure design and ionomer may help bring about greater activity.
- The project team has made good progress in a challenging area.
- This project team has shown and continues to show progress in each of the four key areas of development: catalyst development, electrode and MEA development, high-throughput fabrication, and modeling. However, the rate of progress in the areas of catalyst-layer structural optimization and performance stability has decreased compared to previous report periods, putting the project's goals at risk. The area of Fe migration remains a fundamental concern. Fe that reaches the membrane is known to severely limit the membrane's durability because of the Fenton reaction. Since this project introduces Fe into the catalyst, it must define a solution path. The authors also need to resolve the cause and mitigation of the new results found during AST. The fact is that there are large losses in the kinetic region when cycling in air, but the Fe-reversible redox couple remains relatively unchanged. This seems to suggest a counterintuitive, possibly new, decay mechanism.
- The performance milestone was achieved. Catalyst durability is clearly being looked at.
- Most of the project's effort was devoted to milking out the most initial activity from a very unstable material. This will have no practical use. More work should be done on understanding the degradation mechanism and whether it can be prevented.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The work of the national laboratories in the consortium appears to be well coordinated. The other funding opportunity announcement partners should also provide effective overall collaboration, with a variety of techniques and approaches used to improve the PGM-free results.

- Collaboration among the four national laboratory team players is really good and evident from the results. The collaboration with many partners outside of ElectroCat is also very encouraging.
- It was particularly pleasing to see a group of researchers starting with very fundamental catalyst discovery transition all the way to fuel cell testing.
- Collaboration across all of the national laboratories appears well coordinated, extensive, and effective.
- Interactions, both "within" and "outside" the consortium, are very good, extensive, and strong. It is unclear how the fruits of this effort will transition to commercial adoption later, and whether feedback from commercial entities has been codified enough to know what is an acceptable commercial or lifetime target (independent of DOE targets). In other words, the project team needs to define a minimum viable product (MVP), with industry input. The product should be defined for first-entry markets and not necessarily transport.
- There is good collaboration, although it is quite limited to selected project members. There is also good use of the national laboratories' advanced and extensive capabilities.
- It appears coordination is being done well.

Question 4: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The success with PGM-free catalysts supports DOE's goal of acceptable cost for high-volume automotive applications of hydrogen fuel cells. Baked into this goal is lifetime durability, which also addresses relevance and impact. As a methodology that aids the fuel cell community, the inclusion of machine learning and high-throughput catalyst development has additional relevance but may not be as goal-oriented as the key performance indicators.
- This work can definitely have an impact on DOE's long-term goal of fuel cell commercialization with cost reduction, but it is still far from where it needs to be. DOE has spent millions of dollars on PGM-based catalysts, so one hopes the Department will continue to support PGM-free catalyst development as well—for a long enough time to give this team an opportunity to meet the ultimate targets.
- Durability and cost are the primary challenges to fuel cell commercialization and must be met concurrently. The PGM catalyst is projected to be the most expensive single contribution to the cost of the fuel cell stack. Eliminating PGMs while maintaining the current level of specific power, power density, peak energy efficiency, and durability will significantly accelerate the deployment of fuel cell systems.
- Much progress has been achieved in PGM-free catalysts; however, the eventual applicability to high-current-density and high-power-density durable applications is still much in doubt. With the improvements obtained, it is likely that these catalysts will find areas of application, thus increasing the relevance of the work.
- The project is clearly pursuing the reduction of PGM loading for ORR, which is directly on the pathway to achieving the polymer electrolyte membrane fuel cell (PEMFC) cost goal. In addition to doing good science, the project appears focused on the performance objectives.
- While excellent progress is being made toward developing improved activity catalysts and electrodes with improved performance, these materials have a low probability of meeting any relevance toward reducing fuel cell system costs unless the durability is substantially improved (not by tens but by thousands of hours). It is unclear whether the non-PGM catalysts based on atomically dispersed metals can be sufficiently stable because of demetallation and active-site degradation. Additionally, it is also unclear, and perhaps unlikely, that these materials will be able to meet support durability; it is not known whether start/stop degradation will occur.
- Eliminating PGMs does not necessarily mean lower cost. Because the cost of all the other components combined is large, the cathode catalyst with the highest activity, power, and durability will give the most cost-effective fuel cell stack. The current material is Fe, which is not compatible with PEMFCs, as it has very low stability or usable activity.
- From the presentations and discussion after, it is difficult to see what cost benefit these catalysts could provide. This is not a failing of the project, as the team is still developing the catalyst, so solid cost numbers are not expected. With the additional processing and increased thickness of the electrode, it is not likely that this electrode system would be significantly lower in cost than a conventional electrode. This is

opinion only, and those who are more familiar with the project will likely be able to provide a more considered comment. It would be beneficial to include a rough estimate of what savings could be achieved for an electrode if the project is successful.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- Durability is the number one consideration on the list, which is a good sign, given the importance of this metric to the overall effort for developing PGM-free catalysts.
- The project team has a clear plan for improving performance and has already demonstrated good progress.
- There is a comprehensive summary of proposed future work focus on slide 36. This slide details the relative expected impact for improvements in the power train of the MEA (e.g., activity, mass transport, resistance, etc.). The project should address lifetime with inhibitors.
- The proposed future work is as expected; durability needs some serious consideration while the project team continues improving the performance. The use of developed tools should lead to new material discovery to meet the ultimate targets. Some focus on data hub and machine learning is encouraged, but that should not distract from the main focus of PGM-free catalyst development. Based on these preliminary results, layered electrode structure would need more attention in future work.
- Achieving the power density improvements will be very challenging. The team is depending on electrospinning for mass transport and some ionomer approaches. However, achieving 12x activity is undoubtedly the most challenging and may not be achievable. There was little mention about other approaches to electrode design, although the appendix shows some reasonable approaches around using the combinatorial cell. The multiscale modeling efforts mentioned should be pursued to guide the electrode development.
- The project's future work aims at improving the performance and durability of the PGM-free catalysts, directly in line with the key needs. However, it is unclear what fraction of effort will be devoted toward durability, the largest barrier to date and where most development is needed. Only one of the four bullets on slide 38 addresses durability, and only a few of the quarterly progress measures and milestones on slides 5–8 address durability.
- Short-term durability has identified some potentially significant issues. Decreases in catalyst activity of 50% and 70% suggest that fundamental changes to the basic catalyst may be necessary to produce a stable catalyst. If this catalyst cannot be stabilized, alternative processes need to be identified. The potential risk with Fe is high, and so a solution path is needed.
- The project should focus on degradation.

Project strengths:

- The project's strengths include the outstanding teamwork among many members and organizations; the excellent state-of-the-art analytical methods being used to support or eliminate hypotheses; and the various talents and expertise being harnessed for real improvement of state-of-the-art PGM-free catalyst activity, the understanding of limitations for active site density, and potential failure mechanisms.
- The project has a very capable team to accomplish its tasks. The principal investigators (PIs) are leading these efforts from the front. New tools have been developed that can assist in material discovery in coming years. The collaboration with partners outside ElectroCat is also great.
- The project is extraordinarily effective at utilizing the excellent national laboratory capabilities (including facilities and expertise) to rapidly improve the activity and performance of PGM-free catalysts and electrodes.
- There are very systematic, comprehensive, and aligned efforts toward improving catalyst activity, durability, and stability. Extensive characterization and catalyst-level modeling has been incorporated, and the project has a strong team.
- This project group is very experienced, as shown by their previous work. The PIs and their partners are capable of successfully managing this project.
- The technical knowledge and the quality of the science in this project is world-leading.

- There is a good balance of focus on performance targets and scientific investigation. Improvements in performance have been shown.

Project weaknesses:

- The same catalyst, or version of that catalyst (PANI), has been used to meet the targets. The project needs to look into new and different catalysts as well. The same MEA is not used to show the ORR activity and mass transport in air targets. A higher-loading MEA (~6 mg/cm^2) was used to meet the ORR target and lower loading for other MEA performances. It is expected that all targets should be met with the same MEA, or at least with similar loadings. Finally, the durability is very poor and needs to be improved without sacrificing performance.
- Durability concerns have increased during this report period. Alternatives that are more stable need to be defined. The fundamental mechanism responsibility for the losses in the kinetic region need to be identified. Alternative catalyst-layer structures need to be defined and evaluated, and the stability of the hydrophobicity of this layer needs to be a primary parameter. Developing a solution path to verify that Fe will not leach out of the catalyst layer over time, at all operating conditions, is required.
- The project needs a definition of an MVP that is at an intermediate performance between automotive goals and other, more near-term applications. The project team should also start the transition to air tests. It is acknowledged that air data was posted in the presentation, but now that catalyst activity is sufficient to actually consume enough oxygen to start mass transport limitations, the development of thick three-dimensional electrodes poses significant challenges that mean that earlier efforts are needed.
- This is not a weakness of the project per se, because it looks like there is not currently a metric that is not being met, but overall, more metrics and an emphasis on durability, even at this stage of performance, seem important. Going for performance first and then thinking about stability should be avoided. Performance and stability need to be pursued in parallel. However, it is understood that this is still early for developing PGM-free catalysts, and the team does appear to recognize this.
- This is perhaps not a weakness of this project, but in general, there is an over-emphasis on capital cost and performance within all DOE projects. This is not a bad approach at this stage, as cheaper fuel cells would be great, but a greater emphasis on lifetime expectancy would be appreciated. If PEMFCs cost roughly what they do now but had an 80,000 hour+ lifetime, that would open up additional markets for hydrogen as an energy carrier and would be highly disruptive. This project team should apply themselves to a long-life, reasonably low-performance fuel cell for stationary power. Perhaps this is not possible in this project and may require additional membrane experts, but it would be a good use of the approach and expertise used in this project.
- Approaches to electrode structure could be better developed.
- The project's focus should be on degradation.
- The project is not placing enough emphasis on improving durability.

Recommendations for additions/deletions to project scope:

- The project should strongly consider de-emphasizing activity and performance development and dramatically increasing focus on developing durable materials. It is clear that the activity and performance may reach commercially acceptable levels, but the durability demonstrated (at tens of hours) is very far from Pt-based materials. It is also unclear what the cost savings of a PGM-free MEA will be, relative to a PGM-based MEA. As Pt contents continue to decrease with state-of-the-art PGM-containing MEAs, the need for PGM-free may be decreased. Current reported results by General Motors and Los Alamos National Laboratory (Spendelow) show feasibility of <0.10 g/kW (albeit also without meeting requisite durability). This translates to 9 g of Pt, or about $300 at current Pt prices. The other costs associated with the catalyst and electrode are likely to be similar for PGM-free. Analysis should be conducted for where the "break-even" point is for PGM-free compared with PGM, e.g., what level of performance and durability are required to match the cost of current commercial or laboratory technology.
- The project team should prioritize degradation work. Eliminating other non-value-adding work can save much funding.
- The project needs to focus more on durability and, perhaps, some more on electrode modeling, especially if catalyst loadings rise and electrodes get thicker.

- There needs to be more focus on material discovery and improving durability.
- A recommended addition would be electrode structure modeling.

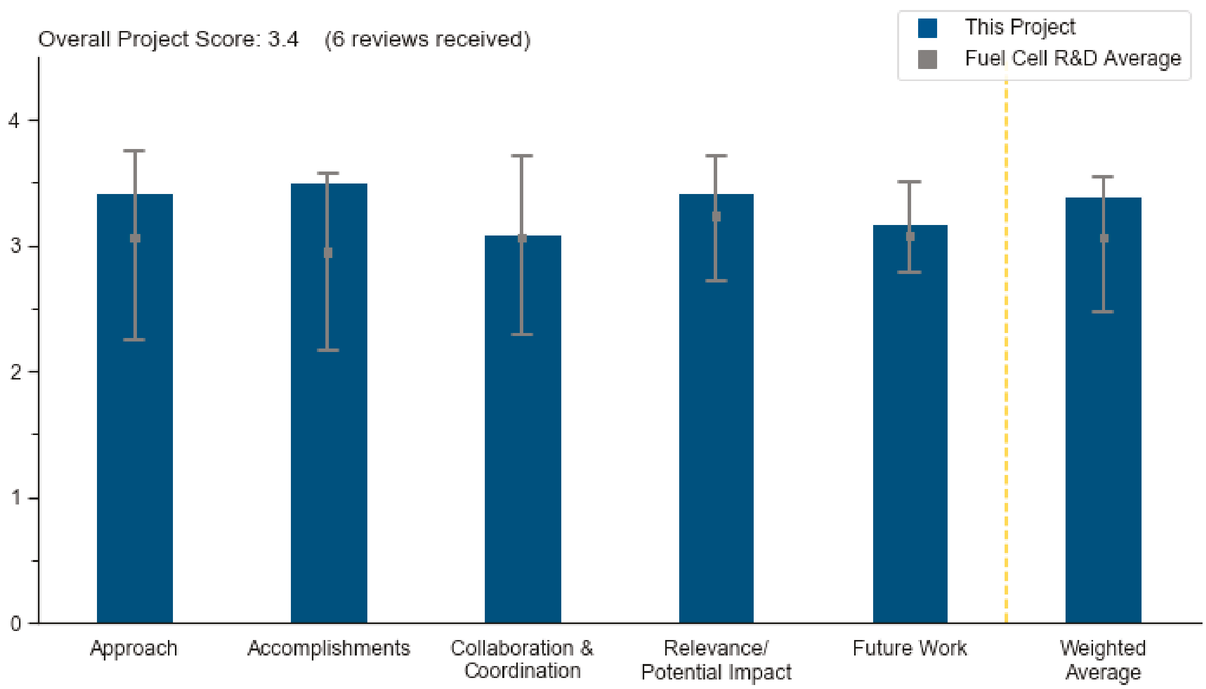
Project #FC-161: Advanced Electrocatalysts through Crystallographic Enhancement

Jacob Spendelow, Los Alamos National Laboratory

Brief Summary of Project

Los Alamos National Laboratory (LANL) seeks to design active and durable oxygen reduction reaction (ORR) catalysts based on fully ordered intermetallic alloys on highly graphitized nitrogen-doped carbon supports and demonstrate them in high-performance membrane electrode assemblies (MEAs). Synthetic work is guided by computational ORR kinetic studies, and each round of synthetic development is further guided by feedback from MEA testing and characterization studies.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project approach is excellent, pursuing the development of highly active and stable intermetallic catalysts on supports with improved durability. The project appears to use modeling, materials fabrication approaches, and materials characterization effectively to drive the technology forward.
- The project put forth several techniques to achieve the ordered intermetallic catalysts and appears to have down-selected to the scalable LANL synthesis. The project combines synthesis, theory, and electrode integration for a comprehensive effort. There is also an interesting avenue of research in using the University of Buffalo's (UB's) platinum-group-metal (PGM)-free-type materials as a support.
- Stabilizing PtM-alloy catalysts is a good approach. However, one reviewer asked why the team limited itself to transition elements for the M_1M_2Pt system. It should also be made clear why the team chose Vulcan carbon for the PtM synthesis, and if there is a plan to explore high-surface-area carbon with a similar approach. The team should also elucidate why they use N-doped carbon supports and state whether

other types of carbon will be used. These are fundamental questions that the national laboratory teams should address.
- The project approach is good, with different synthesis methods guided and supported by modeling, testing, and characterization and well-defined plans for scale-up and MEA validation. It is not clear whether there is a thermodynamic basis for the use of intermetallics. It is also unclear whether there are any phase diagrams used in the design of ternaries.
- The approach targets many of the barriers in catalyst development. The approach is very similar to currently funded and previously funded projects.
- The approach being pursued on the project is feasible and logical.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Impressive accomplishments have been achieved. It is promising to see that the ordered structure remains after the catalyst accelerated stress test (AST) in MEAs. The $L1_0$-PtCo catalyst is also showing significantly reduced loss of Co content. Most of the targets have been met with this catalyst. The work with the hydrogel supports is very promising and shows very good activity and stability. Optimization of the electrode integration is needed and may be completed by the structure of these supports.
- The team has made exceptional progress in developing highly active and durable intermetallic catalysts. One catalyst has met several DOE targets, including mass activity and electrocatalytic (cyclic) durability. The hydrogel supports look promising for support durability with Pt catalyst.
- The team has achieved excellent accomplishments toward highly active PtM alloys. More work needs to be done in durability and in transferring this performance into an MEA and obtaining the same high activity, but this is a good step in that direction.
- The project appears positioned to achieve the DOE 2020 targets for catalyst performance in a single material, which is an outstanding accomplishment.
- Progress has been made with the new PtCo catalysts, some of which meet the DOE performance targets. The reduced Co leaching is promising.
- The presentation slides mentioned that particle size remains mostly unchanged after 30,000 cycles. However, a larger image that includes various particles is necessary to see if there is any Pt-Co agglomeration due to particle sintering and Ostwald ripening processes under 0.6–0.95 V cycling conditions. The conclusion should at least be supported by particle size distribution or X-ray diffraction fit. It is not clear if the Mn hydrogel is a new support or is derived from the polyaniline as N-doped carbon support with Mn. In any case, "Mn hydrogel support" can be oxidized to higher valency during 1.0–1.5 V potential cycling or during normal operating conditions. Leached Mn can affect the membrane and act as a Fenton-like reagent.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- The project has good collaboration; the partners' contribution to the project is clearly demonstrated.
- The collaboration between LANL and IRD Fuel Cells and the collaboration between LANL and UB are both clear and effective. One area for improvement would be explaining exactly how the results from the University of Pennsylvania (Penn) and Brown University (Brown) fed into the materials prepared by LANL. It was also not clear if the best catalysts were prepared at LANL, Brown, or Penn or if the results at Brown and Penn even fed into the work at LANL.
- The project has very good collaboration; however, the contribution from partners is not clear in the presentation. There are three entities preparing catalysts using various techniques, but the presentation is not clear as to which technique is considered successful. The project ends in September 2019, and there may not be sufficient time for MEA scale-up production and catalyst or MEA validation by EWII Fuel Cells (EWII). EWII's involvement in years 1 and 2 is unclear from the presentation.

- There are multiple catalyst development partners in this team. It is not clear what the focus was for each of those partners or how they contributed to the overall project. Future MEA fabrication and scale-up methods need to be better elucidated.
- While the roles of each organization were well described on slide 21, it is unclear how much of the catalyst development work was done at LANL versus Brown or Penn.
- It is unclear what the current roles of Brown, Penn, and EWII are in the project.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project's scope and goals align with the DOE Hydrogen and Fuel Cells Program's technical objectives, and the team has the potential to help make progress toward research, development, and demonstration targets for performance in low-loaded catalyst layers.
- This approach shows much promise for developing highly ordered PtM alloys with good activity, and the approach has the potential to meet DOE cost targets.
- The team is directly addressing key barriers for commercialization, catalyst activity, and durability.
- The potential impact is very high for achieving PGM-loading and durability goals.
- The approach is very similar to currently funded and previously funded projects, and therefore a similar outcome is expected.
- Based on the MEA results, this project appears to be achieving DOE's intended goals for this funding opportunity announcement. One slight criticism is that LANL's method was stated to be scalable, but the details of the processing were not provided. Traditionally, preparing these alloys in small nanoparticles is challenging, so it is not clear what LANL is doing differently if the team is not using a protective coating, as stated in the question-and-answer session. If the method used is not scalable, the technology would obviously not have the intended impact. The final months of the project will examine scale-up, so it is likely that that question will be answered soon.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed tasks are in line with the current accomplishments and overall project goals.
- The future work appears to be logical and is likely to be successful.
- The proposed work looks very good. The scale-up of the down-selected $L1_0$-CoPt catalyst seems appropriate. Work needs to be done to select the most appropriate support. Perhaps the principal investigator might consider a more conventional high-surface support instead of Vulcan, if he has not already. The hydrogel support requires significant optimization and scale-up.
- The proposed future work is logical, based on the project's current status and the remaining gaps to the project's targets. Some additional effort should be placed on support durability with the advanced catalysts on hydrogel supports.
- The proposed work is a logical continuation of the presented effort. AST and accelerated durability test protocols are normally recommended in 25–50 cm^2 MEAs. Without knowing the catalyst preparation process used, it might be difficult to obtain gram quantities with good quality control for the final deliverable.
- The proposed work is very generic and does not elaborate on how the team plans to increase the high-current performance of N-doped supports. This would be needed to understand the source of the lower performance at high current density first. To guide them further in their optimization work, the researchers should plan to study ionomer–transition-metal interactions within MEAs in detail.

Project strengths:

- The team has been exceptionally effective at developing highly active catalysts with improved durability and demonstrating a good balance of fundamental and practical materials development, modeling, and characterization.
- The MEA results and progress on this project made Jacob Spendelow's 2019 Hydrogen and Fuel Cells Program Awards Fuel Cell R&D award well deserved.
- The team has strong partners in catalyst synthesis and support development. The role of the industry partner for the MEA scale-up is not clear.
- The strength of this project is the high activity and the stable catalyst that maintains its intermetallic structure through the catalyst AST.
- The catalyst–support combination study is interesting. The team has made progress toward MEA validation and demonstration of scale-up.
- The team has made very good progress on addressing most barriers.

Project weaknesses:

- The project has few weaknesses. One is perhaps the electrode integration, but this seems to be a focus of the future work.
- Scalability could be a concern, depending on the catalyst synthesis procedure that is down-selected.
- More understanding on certain findings would be good. For example, it is not clear what is preventing Co from leaching, whether there is an effect of the non-PGM particle size, or how the hydrogel support helps with performance.
- Along with maintaining mass activity, the team also needs to address the maintenance of specific surface area. Where shown, the specific surface area losses were significant. Meeting durability in MEAs will also require having stable surface area to avoid performance loss due to the increased local oxygen transport losses that are anticipated to occur.
- The project is focused on only transition metals to provide ordered structure, even for M_1M_2Pt alloys. It is suggested that the team explore the possibility of other metals to provide stability to the ordered PtM structure. The focus on support development should be minimized until significant progress is made in the understanding of this catalyst's durability, primarily regarding the catalyst–support interactions.
- The scalability of the process is unclear because the exact synthesis approach for the best materials was not revealed.

Recommendations for additions/deletions to project scope:

- This team seems to be addressing some critical aspects of alloy catalysts. It would be good to see additional scope devoted to understanding the role of other metals (other than transition metals) in enhancing the durability of M_1M_2Pt catalysts. The team seems to be missing a partner who can help in understanding durability. The interaction of this team with the Fuel Cell Consortium for Performance and Durability (FC-PAD) is not clear, and once the project researchers have reproducible MEAs from their industry partner, they should consider teaming with FC-PAD to understand durability.
- The project team should consider assessing the intermetallic catalysts for Pt and Co dissolution kinetics in coupled rotating disk electrode testing/inductively coupled plasma mass spectrometry (ICP-MS) testing at Argonne National Laboratory (Vojislav Stamenkovic) to determine whether Pt dissolution is improved relative to Pt random alloys.
- It would be good to see comparisons to commercial PtCo catalysts.

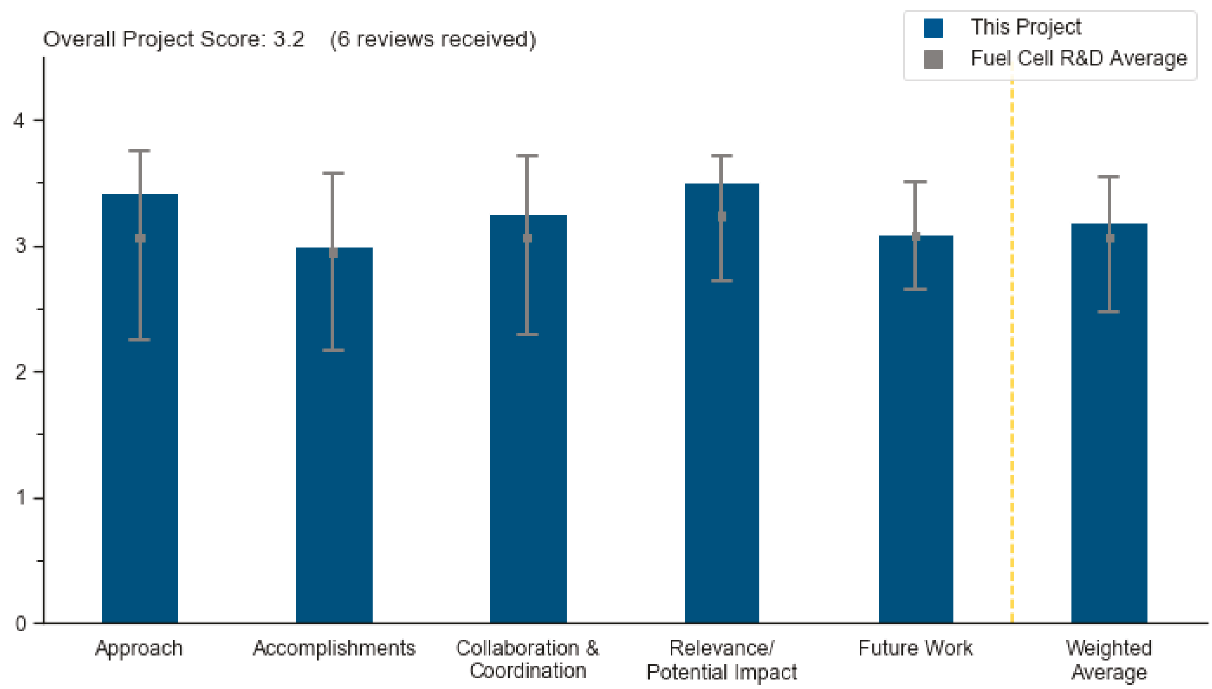
Project #FC-162: Vapor Deposition Process for Engineering of Dispersed Polymer Electrolyte Membrane Fuel Cell Oxygen Reduction Reaction Pt/NbOx/C Catalysts

Jim Waldecker, Ford Motor Company

Brief Summary of Project

The objective of this project is to develop, integrate, and validate a new cathode catalyst material by developing and optimizing a vacuum powder coating physical vapor deposition (PVD) process. Project tasks include (1) developing a new cathode catalyst powder made of titanium, niobium oxide, and carbon; (2) improving the PVD process for manufacturing the catalyst powder; (3) scaling up the PVD process cost-effectively; and (4) integrating the developed cathode catalyst powder into established fuel cell manufacturing processes.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach to develop and validate a new Pt-based Pt/NbO_x/C cathode catalyst by developing and optimizing a vacuum powder coating PVD is valuable and novel. It does deserve attention and support since such a methodology has not been thoroughly examined. The project is supposed to address all relevant steps in the development of new materials, such as electrochemical evaluations of the catalyst for high durability, power density, and mass activity. In addition, the effort is aimed at developing the manufacturing process by demonstrating scalability and cost-effectiveness.
- Improving the durability of carbon-supported platinum group metals (PGMs) is critically important for the fuel cell industry. The proposed approach of achieving it through the synergistic interaction of platinum and carbon with NbO_x compounds is feasible and integrated with other activities in the field.
- This continues to be a more original project on low-PGM oxygen reduction reaction (ORR) electrocatalysis than most of the run-of-the-mill efforts that have for decades focused (often successfully) on Pt alloys, core–shell structures, etc. The same applies to the selection of vapor deposition as a method of catalyst

synthesis. However, by being more original than most, this project is also more risky. Given the existing fundamental science challenges, the project has made a move in the right direction by revising the scope to have greater emphasis on materials characterization and durability, including the nature of interactions in PVD Pt/NbO_x/C catalyst and durability comparisons between Pt/NbO_x/C and Pt/C reference catalysts.

- The project approach is logical and directed at barriers of cost, durability, and performance. The project has appropriately adjusted its approach to include higher NbO_x content, which should be more likely to demonstrate the effects of metal–support interactions and potential for improved durability.
- Utilizing niobium oxide to stabilize the Pt/C catalyst is a novel approach. The addition of NbO_x has a significant effect on the support stability and catalyst durability.
- The approach has improved from last year in terms of including more direct measurements of the Pt–Nb interactions, thus including some science in the project. One of the important aspects that can come out of this project is understanding the degree to which Pt and metal oxide interactions occur and how much they can change and/or stabilize the active catalyst particles. It is unclear what the advantage is of having catalysts made by both Oak Ridge National Laboratory (ORNL) and Exothermics, Inc. (Exothermics). It is not clear, with the catalysts made to date, why large-scale batches of catalyst are needed in this project.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made tremendous progress since the 2018 Annual Merit Review. The principal investigator (PI) explained the interaction of NbO_x with Pt catalyst and its role in stabilizing the catalyst using X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) techniques.
- The PI presented excellent progress toward project objectives. Milestones that were not critical for the DOE mission were re-evaluated, while critical milestones were completed.
- The accomplishments and progress are clearly presented and show promise that the approach of this effort would lead toward novel catalysts with improved durability. Nevertheless, while the losses in mass activities for various samples are satisfactory, voltage losses for the majority of samples are still substantial. The system of choice demonstrates promise for the future work by performance that was measured in 5 cm^2 single-cell tests with the Exothermics 180920 catalyst. These results show that the sample meets the second go/no-go mass activity target, with the beginning-of-life (BOL) mass activity of 389 A/gPt and end-of-test (EOT) mass activity of 290 A/gPt. Considering that the focus of budget period 2 was on improving durability with increased NbO_x content, the project demonstrated progress, even though other technical targets need to be addressed as well.
- The project has met the year 2 milestone for determining Pt–NbO_x interactions. The project has met the milestone of <40% loss in mass activity and <100 mV loss at 0.8 A/cm^2 in the electrocatalyst durability cycle. The project is behind on reaching the performance milestone of >500 mV at conditions meeting the heat rejection target with a loading of <0.125 mgPt/cm^2 and P 150 kPa or less. The project is behind schedule for meeting durability in support corrosion tests. The reasons for the low maximum power performance are not yet understood. Additional diagnostics should be performed, including loss breakdown to determine pressure-dependent and independent mass transfer resistances, high-frequency resistance, and H+ transport resistances.
- The XAS and electronic interactions are informative for this project and other projects. It appears that there is a lack of Pt–Nb interactions; however, there is a suggested interaction between Pt and O from NbO_x. This data set is important for understanding why there is not a direct Pt–Nb interaction and why the Nb XAS signal does not change with Nb content. It is unclear why the BOL mass activity of 389 A/gPt was reduced to 290 at EOT. It could be particle growth or loss of bonding with the NbO_x. These are important questions that should be answered going forward. There does not seem to be a good correlation between the electrochemical active area (ECA) and mass activity loss. Not many data were shown to understand whether this is due to conditioning or an unrelated effect. The project should show more than ECAs and polarization curve performance. Data such as particle size distribution and change in distribution with mass activity should be shown. An explanation of the cause behind the mass activity loss is needed. The ECA on slide 15 does not seem correct (58.68 reduced to 5.43, meaning a 90% loss). There is either a ~10% ECA loss (if it should be 54.3 m2/g) or a ~90% ECA loss (if it should be 5.43); neither correlate well to the mass

activity loss of 25%. It is curious that the project PI does not bother to do any quick rotating disk electrode (RDE) cycling measurements to evaluate the catalyst durability, when for so long the PI insisted that RDE measurements needed to be done for everything.

- An increased emphasis on fundamental science, while commendable, has not provided clear answers to questions about the ORR mechanism on $Pt/NbO_x/C$ catalysts. That being said, the XAS studies at Northeastern University (NU) have afforded some interesting insights but, as is typical for such studies, few firm conclusions. A more complete picture of interactions between the three components in this complex catalyst system (including carbon support) would be desirable, helping with the design of future $Pt/NbO_x/C$ catalysts with higher activity (including the high current range) and durability (over a wide range of NbO_x content).

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- This project has an outstanding collaboration involving three industries, two universities, and a federally funded research and development center. The contribution from each partnering entity can be seen throughout the presentation.
- The collaboration is well executed, and the partners are well coordinated.
- This is a very strong team with complementary capabilities. Problems with EWii Fuel Cells, LLC (EWii) testing (i.e., electrode conditioning) indicate possible miscommunication between partner organizations. Collaboration with external partners who have interest in materials of the type under development in this project and the synthesis approach being used could help overcome at least some challenges.
- Collaborations appear to be working, for the most part. There appear to be substantial differences in observed performance between the partners. The reasons for the differences need to be determined, and comparable performance needs to be measured for the same materials by the different partners. Interactions with collaborators outside of the project (the Fuel Cell Consortium for Performance and Durability [FC-PAD], for example) are not apparent.
- The team collaborated between partners and with members of FC-PAD.
- The NU measurements appear to be the science behind this project. It is unclear what the advantage is of having catalysts made by both ORNL and by Exothermics. It is not clear why, with the catalysts made to date, large-scale batches of catalyst are needed in this project. EWii seems to be present to make scaled-up membrane electrode assemblies (MEAs), but the catalyst does not seem to have progressed enough to date.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project focuses on high-performing and more durable catalysts, as well as a reproducible and scalable manufacturing process. For that reason, the relevance and impact to DOE goals could be significant if the project is successful.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program (the Program) and DOE research, development, and demonstration (RD&D) objectives; the project has the potential to advance progress toward DOE RD&D goals and objectives.
- The project focuses on developing a $Pt/NbO_x/C$ catalyst for high durability, high power density, and mass activity to meet the DOE 2020 technical targets for electrocatalysts and catalyst supports.
- The work is relevant and could have impacts on cost, durability, and performance. The work could provide an alternative catalyst preparation route that is amenable to mass production. The metal–support interactions could be expected to lead to improved durability.
- More durable, higher-mass active catalysts are important for the commercialization of fuel cells. This project correctly addresses a major cost and durability issue with fuel cells.

- The project is very relevant to the Program's objectives and, by using a different approach, promises improvements in performance of nanodispersed Pt catalysts, especially in terms of durability. However, the tendency for Pt agglomeration needs to be overcome.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The proposed future work focuses well on the remaining challenges and is aligned with the remaining 40% of the project timeframe.
- The proposed future work will lead to further understanding of this new class of catalyst material.
- The proposed future work is well aligned with project goals and DOE technical targets.
- The proposed work is logical and well justified. Ultimately, by the end of the project, it would be beneficial to have some kind of a judgment call on the viability of this class of ORR catalysts. Existing discrepancies between the performance of small-scale samples from ORNL and large-scale samples from Exothermics should be understood and eliminated.
- The proposed future work is logical and directed toward meeting the upcoming go/no-go decision point and determining loss breakdowns. Additional work to try to correlate properties with microstructure would be beneficial (for example, how H+ losses or pressure-independent mass transport resistances correlate with NbO_x or Pt content or connectivity).
- The continued XAS studies are good; they could be expanded more. The cost estimates will probably not be very relevant until a promising catalyst is produced. The durability measurements are important, as improved durability is a major objective.

Project strengths:

- The project has demonstrated the Pt/NbO_x catalysts without added resistance from the PVD catalysts. The surface analysis (i.e., XAS) from this project is important for understanding the particle interactions and what value these types of interactions will have in terms of stabilizing and/or changing the electronic state of Pt.
- Substantial progress has been made in materials composition reproducibility. There was a significant increase in batch size. The project is completing critical milestones on MEA performance and durability.
- The project has an original approach, well-executed collaborations, promising performance, and durable and novel materials.
- The project has demonstrated good activity for Pt catalysts (as opposed to Pt alloy), which should show good durability.
- The originality of the approach, promising improvements to catalyst durability, is the biggest strength of this project.
- The project has shown excellent collaborations and tremendous research progress.

Project weaknesses:

- The project has looked at only a few ionomer-to-carbon ratios and what are relatively low NbO_x contents. The current electrodes that were made suggest that the project has a problem with high currents. The catalysts do not appear to be showing better durability to catalyst cycling, which is a major (or the major) objective of this project: more durable catalysts. If the project is not showing better durability, then the project needs to show higher mass activity, but it is not even looking at active particles like PtCo, so it will not compete with those types of catalysts.
- The PVD process appears to be less controllable than was predicted at the outset of the project. Particle size distribution and other parameters do not appear to be as easy to manage as was originally thought. Based on the RDE results, MEA performance has been poorer than expected.
- MEA evaluations in 50 cm^2 are needed, as are improved power performance and optimization of the catalyst composition.
- The shift of the project scope toward fundamentals has not yet provided the level of understanding needed to design better Pt/NbO_x/C catalysts in the future.

Recommendations for additions/deletions to project scope:

- It is unclear what value the cost analysis adds if the catalyst cannot show improved durability and/or mass activity. The project should concentrate on showing the improvement in performance before spending time figuring out how much more expensive these catalysts will be compared to traditional catalysts. The science from the XAS measurements should be expanded to other interactions, if possible, so that the community can know whether the proposed metal oxides have potential. Metal oxide supports have been proposed for a long time, with little real promise to date; the XAS can help evaluate this potential. The project should measure catalyst properties such as particle size distribution and understand the causes behind the loss in mass activity, which could be particle growth or loss of bonding with the NbO_x. These are important questions that should be answered going forward.
- The project should focus on better understanding the higher mass activity obtained by the Pt/NbOx/C catalyst compared to state-of-the-art Pt/C catalysts.
- The still-high voltage loss at 0.8 A/cm^2 and the large scatter of the durability test data are of concern and should be addressed.
- Evaluations should be done in 50 cm^2 MEAs.
- The project should facilitate MEA fabrication and testing activity.
- There are no recommendations for additions or deletions.

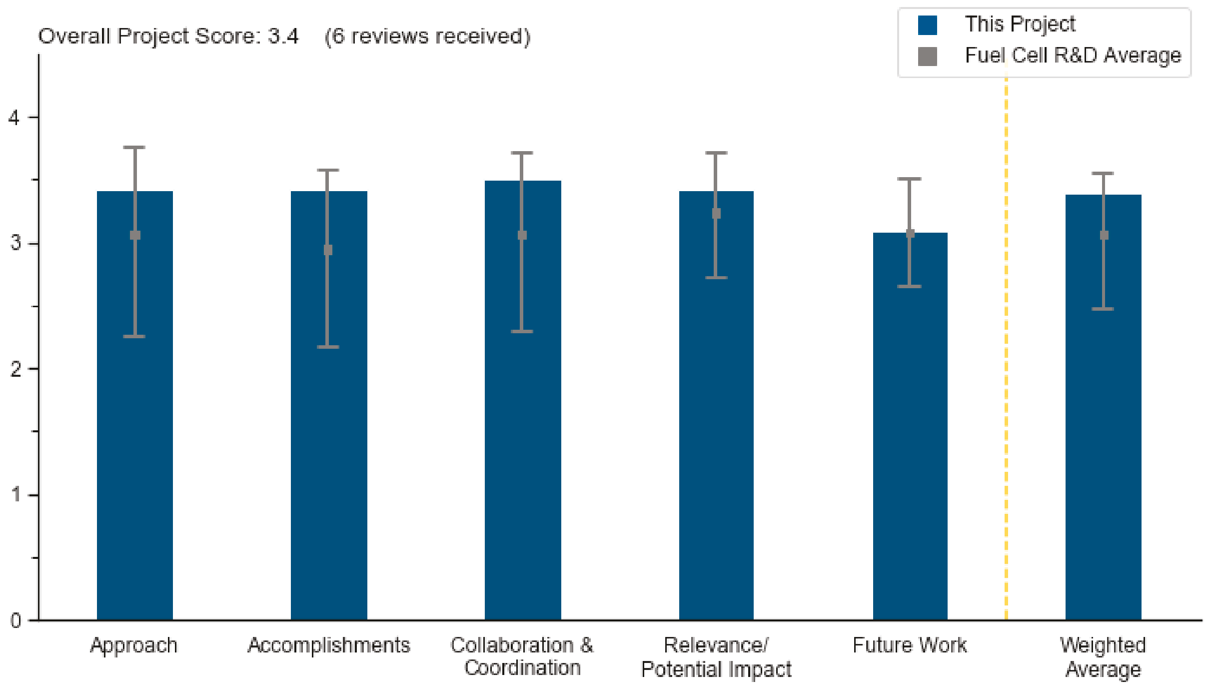
Project #FC-163: Fuel Cell Systems Analysis

Brian James, Strategic Analysis, Inc.

Brief Summary of Project

This project seeks to estimate current and future costs (for years 2020 and 2025) of automotive, bus, and truck fuel cell systems at high manufacturing rates. Analysis projects the impact of technology improvements on system cost, identifies low-cost pathways to achieve U.S. Department of Energy (DOE) automotive fuel cell cost goals, benchmarks fuel cell systems against production vehicle power systems, and identifies fuel cell system cost drivers to help facilitate Fuel Cell Technologies Office (FCTO) programmatic decisions.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has a very good approach to assessing current and projected costs (in 2020 and 2025) of automotive, bus, and truck fuel cell systems at high manufacturing rates, using the design for manufacture and assembly (DMFA) analysis combined with the questionnaire sent out to system developers. This year, the choice is to put aside the light-duty vehicles (LDVs) in order to concentrate the efforts on medium-duty vehicles (MDVs) and heavy-duty vehicle (HDV) trucks, which is an excellent strategic choice to accompany the imminent development of fuel cell trucks. The report on cost will be released in September 2019. The project also identifies low-cost pathways and presents very interesting side studies quantifying the impact of durability on cost and completing the ways of improving durability.
- The approach taken by Strategic Analysis, Inc. (SA) is almost always appropriate and good. SA performs an essential service in quantifying costs for the community that would otherwise not be available. The pivot toward HDVs is a great addition. Some of the choices employed need further analysis, but they are off to a strong start. The areas beyond HDVs are of slightly less interest and are less impactful. A project like this has a hard time directly affecting DOE targets.

- The approach is valid and helps in overcoming the listed barriers. Insight on the operational costs (e.g., fuel, maintenance, consumables, etc.) and stack replacement costs (given the knowledge on the degradation performance) would be valuable. An interesting result would be the dollar-per-mile rate compared to another conventional solution with an internal combustion engine or a different powertrain.
- The DFMA method for cost estimation is appropriate. The continuously close interaction with component suppliers and system developers is key to fairly accurate cost estimations. Updating the LDV model biannually now while focusing on MDVs and HDVs makes sense.
- While not directly working on technologies that could reduce barriers, the project's cost analysis plays a necessary role in assessing the DOE Hydrogen and Fuel Cells Program's (the Program's) progress toward overall goals.
- The approach to the work is comprehensive in looking beyond component cost reduction and also including recycling and manufacturing techniques.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Great accomplishments have been globally presented again this year. This progress will help DOE achieve its goals by tracking how technology changes increase or decrease cost. However, switching from metallic to flexible graphite bipolar plates (BPPs) remains questionable. Ballard Power Systems, Inc.'s (Ballard's) arguments have been well presented, but it would have been interesting to have the feedback from other industry partners, in particular from Nikola Motor Company (Nikola). The already demonstrated lifetime in buses and the reduced cost projections have been underlined. However, the preliminary cost results indicate that BPPs are not considered as part of the major cost difference between LDVs and MDVs/HDVs. However, using flexible graphite BPPs will lead to decreased mass and volume stack densities. Quantified impacts may be compared with corresponding DOE targets. Even if the Toyota Mirai is currently using Ti materials for BPPs, Ti should not be used as a reference material in the quantified cost impact of durability measures. All the other original equipment manufacturers (OEMs) are developing coated stainless steel. The integration of two-dimensional manufacturing is very relevant and may be regularly updated in the future. Analysis of end-of-life vehicle recycling and disposal cost is of high interest.
- The work done on HDVs is a critical emerging need. To date, the work is built around the light-duty framework and a focus on capital cost, which is insufficient for the heavy-duty market, where total cost of ownership (TCO) is more important. The team recognizes this and has done a good job of putting the first study in place so that it can be built upon and refined. The flexible BPP work was somewhat surprising, as it was cheaper and more durable without any shown performance losses. The question that immediately comes to mind is why this approach would not displace metals in light-duty application. The end-of-life recycling and disposal cost was interesting, but perhaps less impactful.
- The project has defined objectives on MDV and HDV trucks. Achievements are aligned with the project objectives with reporting on cost. Results are due in September 2019. This choice is also of immediate interest to DOE on fuel cell truck development. Therefore, the accomplishments and progress of the project are excellent in the direction of DOE objectives as well.
- The accomplishments demonstrate success in moving the focus and analyses from LDV to MDV/HDV technologies and markets. This has further aligned the project with DOE objectives. Ballard has been identified as the sole supplier that can achieve the required performance and cost targets. This could create a future situation that drives higher cost owing to market rather than technical factors. Alternatives should be identified.
- The project shows advancement with respect to 2018 milestones and, most importantly, achievements that indicate the feasibility of DOE targets.
- The project continues to stay current with the inclusion of MDV/HDV cost analysis and cost assessment of developing technologies.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The project has a close collaboration with the National Renewable Energy Laboratory and Argonne National Laboratory (ANL) for acquiring knowledge, data, and review of the assumptions and results. Other collaborations with Ballard, 3M, and Precors Technologies have been set. Therefore, the project has a very good approach for seeking information and feedback by setting up relevant collaborations, which also allows the team to be up to date on new developments to integrate into the cost model. However, this year, it could be relevant to collaborate with HDV truck developers (Nikola, for instance), as the effort is concentrated there. These partners could bring very interesting guidance on objectives and priorities and give a relevant review of the assumptions, etc. In addition, these kind of collaborations will help with the choice of system and hybridization architectures. Specifications should come first from the system and then from the components.
- SA is doing an excellent job of collaborating, mainly with the ANL systems analysis project but also by expanding with many component and system developers, suppliers, and end users. This interaction gives confidence in the results. However, neither material nor system configuration selection should rely on only one partner.
- The project has a few funded partners to fill in specific gaps but does a great job of leveraging the community, particularly since the team is investigating areas that are often highly proprietary. Outside of having direct OEM insight, it is likely the best option.
- Strong collaboration is demonstrated with the project partners, and the project has utilized other industry expertise to inform the approach. While the presentation refers to a list of ~30 industry participants, this list is not included in the backup material.
- Close interaction with the ANL systems analysis project is key and effective. The project has an extensive list of collaborations as required for project effectiveness.
- There is very good collaboration and networking within the project.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is very relevant to supporting the Program and to advancing progress toward its goals and the FCTO Multi-Year Research, Development, and Demonstration Plan (MYRDDP). The project provides up-to-date cost assessment by integrating very recent technology achievements and is very reactive and flexible to DOE interests, thereby allowing DOE to have very efficient follow-up on costs. The focus on MDVs/HDVs this year is an instance of this flexibility. The project is also helping progress toward MYRDDP objectives by assessing ways to reduce cost to achieve DOE objectives. The project also provides guidance on where future focus (and funding) should be directed. The project has very interesting side studies, such as its study of the impact of recycling on cost and its investigation of end-of-life recycling. The project should also open a study on the second life of a fuel cell as a means of lowering cost and expanding durability. The business model could have interesting results. The project will make great gains in efficiency if it associates with OEMs that can provide a final system vision as the input while keeping the excellent current collaborations.
- Both the relevance and potential impact of this project are strengthened by the addition of MDV and HDV topics and the studies beyond the baseline that analyze multiple cost drivers and pathways. The potential impact of the project is strong with the inclusion of direct input and feedback from the MDV and HDV developers. The shift of focus from LDVs and buses will also allow the project to inform future DOE programs and objectives in the near term.
- This project provides a powerful tool for forecasting the costs for fuel cell systems and allows for systematic updates based on achievements of other projects or of industry interviews. This really contributes to identifying fuel cell system cost drivers to help DOE to refine and update its targets.

- Quantifying cost is critical to demonstrating that DOE targets have been met. In particular, the HDV analysis will be critical in helping establish targets once the TCO issues are better understood.
- The project plays a necessary role to DOE in providing a status update on the key cost metric. Thus it is of more use to the Program and managers than to having direct impact on the technology. However, it has indirect value in identifying promising technology enablers (or, just as important, areas and proposals of limited potential benefit).
- The project is critical to understand the feasibility of DOE targets and guiding future funding opportunity announcements.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- Incorporating durability into cost modeling is a very good choice, as are sensitivity analyses for HDVs. There should be a stronger focus on the TCO for HDVs, rather than the laundry list of lower-priority issues listed in the proposed work section (e.g., fluorine recovery, perfluorosulfonic acid synthesis, platinum-group-metal [PGM]-free synthesis).
- The proposed future work represents a comprehensive and ambitious set of analyses. This list should be prioritized with a plan to execute in order of priority, to better address the disclaimer that "any proposed future work is subject to change based on funding levels." It will be informative to further understand if LDV manufacturing can be leveraged for MDVs/HDVs.
- The proposed future work is in line with project objectives. The identified remaining challenges and barriers have been well identified. However, not all of them are considered in the proposed future work, some of which in particular can be considered as crucial for MDV/HDV development.
- The project has played an important role in assessing the potential cost impact benefit of DOE fuel cell projects, but often only when the projects have reached a more mature stage. It would be worthwhile to provide earlier preliminary analysis to help guide and assess the potential benefits of projects' approaches and proposed work.
- The proposed future work is aligned with the current achievements. It lacks ambition toward longer-term goals. Some questions about different investigations exist, for instance, as to whether PGM-free catalysts are realistic for MDV and HDV trucks. Concerning the application, it is not clear where the priorities are in terms of materials or what the sound compromise is between material price and durability.
- Future work should include a more detailed analysis of operating costs. Also, an assessment of the second-life potential of fuel cell stacks could be another interesting contribution of the project.

Project strengths:

- The project has an excellent approach to providing current and future cost projections, integrating the latest technology achievements. The project is very active in setting up relevant collaborations, either to feed and update the model or to have guidance and review on the assumptions and results, which will increase the robustness of the results.
- There is excellent experience in DFMA and cost analysis, with excellent collaboration with the ANL systems modeling work. The project has employed a stable calculation methodology over the years and continuously incorporates feedback from industry and works closely with industry.
- The project demonstrates strong collaboration with broad expertise. This allows the project to conduct studies with impacts beyond the baseline cost; for example, the addition of recycling and disposal cost analysis is very valuable for the developers as both a cost and environmental consideration.
- There is a strong basis for this work. The project has a great approach as well as transparency on its approach and data. The results fill a significant gap that would otherwise be a mystery to the community.
- The team's strengths include its extensive fuel cell cost analysis history, expertise in cost assessment, and list of collaborations.
- The project benefits substantially from the contribution of its industrial partners. The cost projects are extremely valuable.

Project weaknesses:

- In the past, a weakness would have been “access to state-of-the-art materials,” but that has been effectively addressed with the Fuel Cell Consortium for Performance and Durability partner projects and strengthened collaboration with the ANL systems analysis project.
- The cost analysis is partially relying on the results of performance and durability modeling from the ANL project. As these results are based on single-cell testing with no validation of the model at stack and system levels, this appears to be the main project weakness.
- Given the collaborations with industrial partners, it would be valuable to understand when the reported production volumes will be met. Moreover, longer-term perspectives (after 2025) might be explored. The expected projection uncertainties should be included in the charts.
- The project should diversify the stack and system suppliers to have less bias on the results. Although there is work done on systems, the project lacks a system vision and guidance. It needs also to update priorities to application needs.
- The proposed future work is ambitious and should be expressly prioritized according to how it best aligns with DOE objectives.
- The project is perhaps taking on too many different topics rather than maintaining a sharper focus.

Recommendations for additions/deletions to project scope:

- The questionnaire is a very good point. It should go further toward actual collaboration with developers. With trucks, for instance, there is a need to update the vision and constraints for truck applications. It is not very relevant for trucks to have Pt-free loading, and it may be that the compromise is more on durability. The powertrain architecture should be extended to the range extender, as this could define the developers’ choice to upgrade to fuel cell MDVs and HDVs. If the scenario of a second life for fuel cells is integrated with different applications, an impact on lowering cost and extending durability will be seen. In that case, the durability will be assessed on the whole life cycle of the product. The project team should (as much as possible) diversify stack and system suppliers, including internationals, to have less bias on the cost projections. It could be relevant to assess the impact of operation modes such as start-up and shutdown in terms of “penalty” on durability and cost, as this is part of the real operation of a system. Similarly, as part of real operation, recovery phenomena should be also included (in terms of a “bonus” for durability and cost). The same goes to the break-in and characterizations, which are part of the real operation. Again, collaboration with end users for input on that point could lead to very efficient assumptions.
- MDV/HDV development is currently of high interest, and the project should therefore intensify its investigation by considering the following:
    - Investigating the TCO and not only the fuel cell system cost means taking into account capital expenses and operating expenses, as a huge amount of hydrogen is consumed and system efficiency appears more critical than for LDVs.
    - Potential synergies between the LDV and MDV/HDV components and production plants should be investigated, as should how far, in terms of cost projections, MDV/HDV systems could benefit from LDV developments.
    - There should be a sensitivity analysis on the level of hybridization between the fuel cell and battery on the MDV/HDV TCO.
- Ideally, the focus would be sharper on HDVs in the short term. There should be a stronger focus on TCO for HDVs (meaning the tradeoffs in cost, performance, operating strategy, and durability, perhaps getting more input from the ANL HDV modeling efforts). At this time, it is not clear what the most cost-effective way is to run these systems that have very different tradeoffs from LDVs, and this team has the ability to help make an impact in this area.
- It would be interesting to understand whether the cost of Pt is expected to substantially influence the cost of the system in the mid-future. Given the expected rise in production volume, it would be good to know how platinum costs will change.
- There should be more focus on early cost assessment of other DOE project proposals to better assist in approach directions.
- The project team should explain why the identified system solutions are not currently in models and what additional barriers need to be overcome.

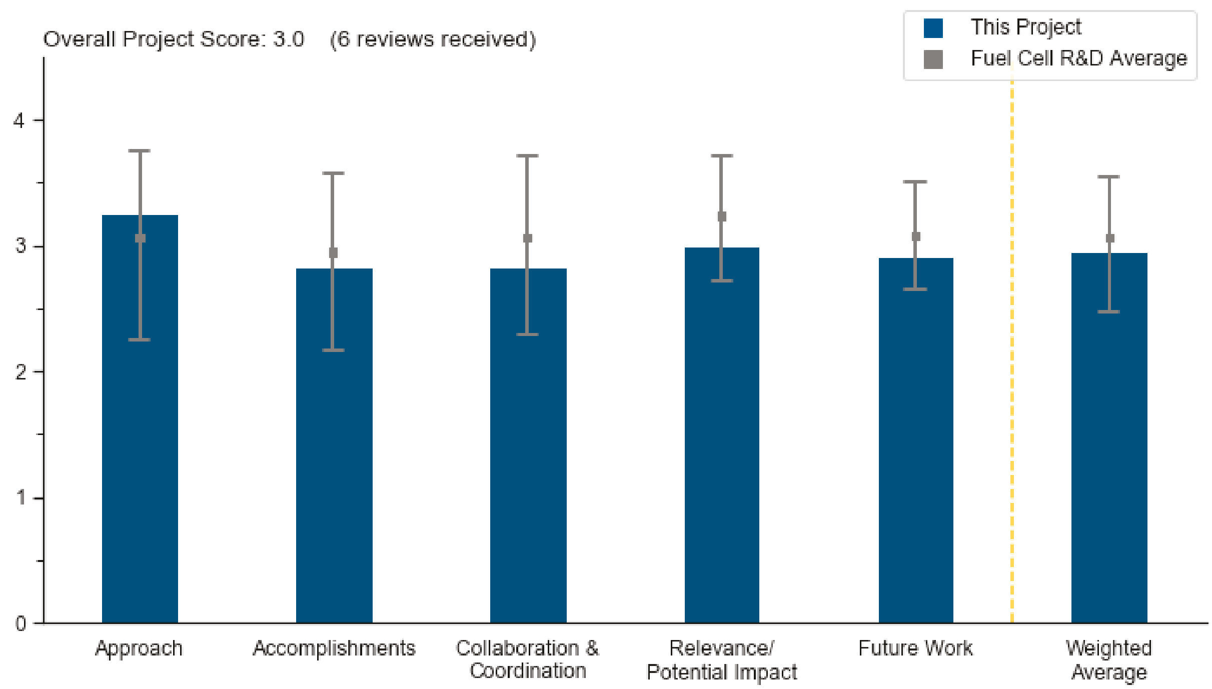
Project #FC-170: ElectroCat: Durable Manganese-Based Platinum-Group-Metal-Free Catalysts for Polymer Electrolyte Membrane Fuel Cells

Hui Xu, Giner, Inc.

Brief Summary of Project:

The project objective is to develop a Mn-based platinum-group-metal-free (PGM-free) catalyst and membrane electrode assembly (MEA) as a replacement for current PGM catalysts. The developed catalyst and MEA will have lower cost/cost volatility, improved corrosion performance, improved de-metalation performance, and reduced membrane degradation compared to the baseline. The developed catalyst and MEA will be tested on a development fuel cell stack.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project is sharply focused on overcoming critical barriers in the development of PGM-free catalysts for polymer electrolyte membrane fuel cells (PEMFCs). The team combines experimental measurements and theoretical computations to search for better catalysts.
- This project is focused on developing durable, Mn-based, PGM-free catalysts by implementing chemical synthesis in aqueous environments. This would substantially lower the cost of production, with a proposed increase in performance.
- The approach covers necessary development areas such as the study and optimization of the catalyst synthesis and corresponding density functional theory (DFT) modeling, as well as optimization of the electrode.
- The project effectively balances new materials development, characterization, and modeling to advance toward the project's objectives.

- The team appears to be focused on the milestones and pursuing the right approaches (experimental and computational) to further understanding and improve the performance of project materials and MEAs.
- The approach seemed promising, but the execution seems less so. The synthesis and electrode seem to be progressing, but the DFT and diagnostics do not. Also, the assumption that these catalysts do not hurt the membrane has not been proven.

Question 2: Accomplishments and progress

This project was rated **2.8** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Significant progress has been made in material synthesis, as demonstrated by the polyhedron structure for the Mn-N-C catalysts developed in aqueous solution. Moreover, the particle size can be controlled by tuning the concentration of metal salts; particles did not agglomerate, hence preserving morphology after high-temperature treatment. These parameters allow insight into the structure–function correlations of Mn-based PGM-free catalysts. It was found that large particles tend to form optimal electrode pore structure. Another important result, obtained by X-ray diffraction (XRD), shows that the Mn does not affect the crystalline structure of zeolitic imidazolate framework-8 (ZIF-8), and Mn-oxide was not detected. Catalytic performance in RDE testing indicated that half-wave potential reached 0.82 V. After electrochemical evaluations, atomically dispersed and N-coordinated Mn sites, along with porous and partially graphitic carbon, are preserved in the Mn-N-C catalysts, indicating promising durability. A higher degree of graphitization relative to Fe-N-C catalysts may explain the enhanced durability. In terms of MEA performance, there is significant improvement from last year; however, this is still substantially lower when compared to the state-of-the-art (SOA) Fe-based catalysts. All of these achievements are well aligned toward DOE technical targets.
- The team has demonstrated excellent progress toward project objectives through clear and measurable performance indicators (such as activities of catalysts and fuel cell performance). The team has made important contributions to overcoming some critical barriers.
- The project has made good progress toward improving the performance (four-fold) and activity (five-fold). The catalyst's durability in rotating disk electrode (RDE) testing is excellent, but it has not been demonstrated in the MEA.
- The apparent progress in electrode performance is substantial, and there are some catalyst synthesis trends to back it up. However, the quality and consistency of the results are scattered. "Breakthroughs" abound without explanation, and unsupported conclusions have been drawn. Some examples include the N-content by Raman spectroscopy that was claimed but is not an accepted trend.
- It looks like the team did achieve the year 1 goal for activity in an MEA at 0.9 V (10 mA/cm^2), although just barely. The figures showing the impact of things like particle size, ionomers, catalyst synthesis route, etc. are helpful for seeing the range of approaches that the team is pursuing to make improvements. It would be helpful to see a clear statement about the conditions for which it seems it will be possible to hit the targets (i.e., what particle size, what active site density, etc.). The presentation does not appear to have much information on degradation. It appears degradation was not a milestone yet, so this is reasonable, but it would be helpful to see baseline data on durability and degradation.
- The performance gap with the SOA Fe-based catalyst is still significant, as the stability is not superior. The team presented progress of 4 mV less of voltage loss in RDE testing when compared to 2018; this is not convincing because of the lack of batch statistical data.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- The collaborations between team members are well coordinated, and productive outcomes have been demonstrated.
- The team is well coordinated, and the roles of the participants are clearly defined.

- The collaboration with Giner, Inc. (Giner), SUNY State University of New York at Buffalo (UB), and ElectroCat is good. The project is involved with the University of Pittsburgh, but the actual interaction is unclear; the collaboration with General Motors is also unclear.
- The interactions among the groups in the project appear good. It is somewhat hard to tell if interactions with the wider DOE laboratories are taking place or whether that is important for this team to succeed.
- The team of collaborators is well established; however, it is unclear how the data at Giner and UB compared with each other, especially in tasks where there is duplication of test effort, such as in Task 3.
- While the roles of each collaborator are well described on slide 26 and are logical, it is unclear what specific contributions each organization made.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project aligns well with the objectives of the DOE Hydrogen and Fuel Cells Program and DOE research, development, and demonstration (RD&D). If successfully conducted, the project will have the potential to advance progress significantly toward DOE RD&D goals and objectives by dramatically reducing the cost of catalysts for PEMFCs. The development of low-cost catalysts is vital to the broader commercialization of PEMFCs.
- If successful, this project may have significant impact on DOE's PGM-free strategy.
- PGM-free catalysts are a major goal, and the best so far are Fe-based, so Mn is a better approach.
- This team is clearly addressing the goal of developing PGM-free oxygen reduction reaction catalysts and electrodes.
- While the project is making good progress toward advancing activity and performance, durability has only been minimally addressed. If the durability of the Mn-based PGM-free catalyst is similar to many other PGM-free catalysts (i.e., low in MEA testing), it is unclear how relevant this class of materials will be toward addressing key commercialization barriers.
- The potential impact of this project is still uncertain owing to the lack of progress in the catalyst's performance and stability.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The project is continuing to advance the catalyst activity and appears to be rightly emphasizing durability.
- The priorities in the proposed future work appear to be good. It is good that studying durability, improving performance, and working on MEAs are all priorities.
- The proposed future work is well aligned with project goals and DOE technical targets.
- The proposed future work focuses on overcoming the remaining technical barriers. The tasks are well thought out and scientifically sound.
- The project should increase its focus on understanding and improving the stability of the proposed formulations, specifically in quantifying the dissolved and oxidized content, in addition to achieving performance targets.
- The general approach makes sense, but the details are lacking. One main issue is that the connection between size and electrode structure is contradictory; on slide 24, the claims around ionomer penetration and coverage do not make sense for a small particle.

Project strengths:

- The project's strengths include its well-defined systems and systematic approach. There is a high level of control of physicochemical parameters that is leading to improved understanding of catalyst performance and is providing guidance for the future work. This is a well-executed team effort with clearly defined achievements.

- The key concept of the project is well conceived, excellent progress has been made so far, and the future work is focusing on the remaining challenges. The results have the potential to reduce the cost of catalysts dramatically for PEMFCs.
- The project's strengths include its alternative approach to the Fe-based catalysts. The team did achieve the year 1 performance goal, and it looks like there is a reasonable balance between performance improvement and scientific work.
- The new approach to non-PGM catalysts appears to be effective. The project has made excellent progress in one year.
- The project has a complex approach to understanding the impact of synthesis conditions on performance.
- The project is showing promising catalyst and electrode improvement.

Project weaknesses:

- It is not clear whether the project is on track to hit its year 2 performance goal. No MEA durability has been shown yet, although it looks like this is not yet a milestone. The team should consider whether the DFT modeling is proving helpful for the synthesis and durability efforts.
- The project has presented many misreported, inconsistent, and "optimistic" conclusions. It also has unclear differentiation from other projects, except for the Mn approach. The DFT contribution is also lacking.
- The claim of improved stability is not supported by any sufficient datasets. There is a lack of statistical data from the catalyst batches and no inductively coupled plasma data on the main leaching elements.
- The project's weaknesses include the poor performance demonstrated in MEA testing. It is hard to envision that any of the PGM-free systems would be able to meet expectations in real systems.
- As of yet, the project has not placed sufficient emphasis on addressing durability.

Recommendations for additions/deletions to project scope:

- The project team should include statistical data on multiple batches and quantify the formulation's stability to acid wash. The team should also address transport losses with high content of an ionomer more specifically related to the MEA structure.
- The project team should add membrane stability testing to confirm that Mn-N-C catalysts do not degrade the electrode. The researchers should also use consistent testing to ensure that their conclusions make sense.
- Extensive durability studies are needed.

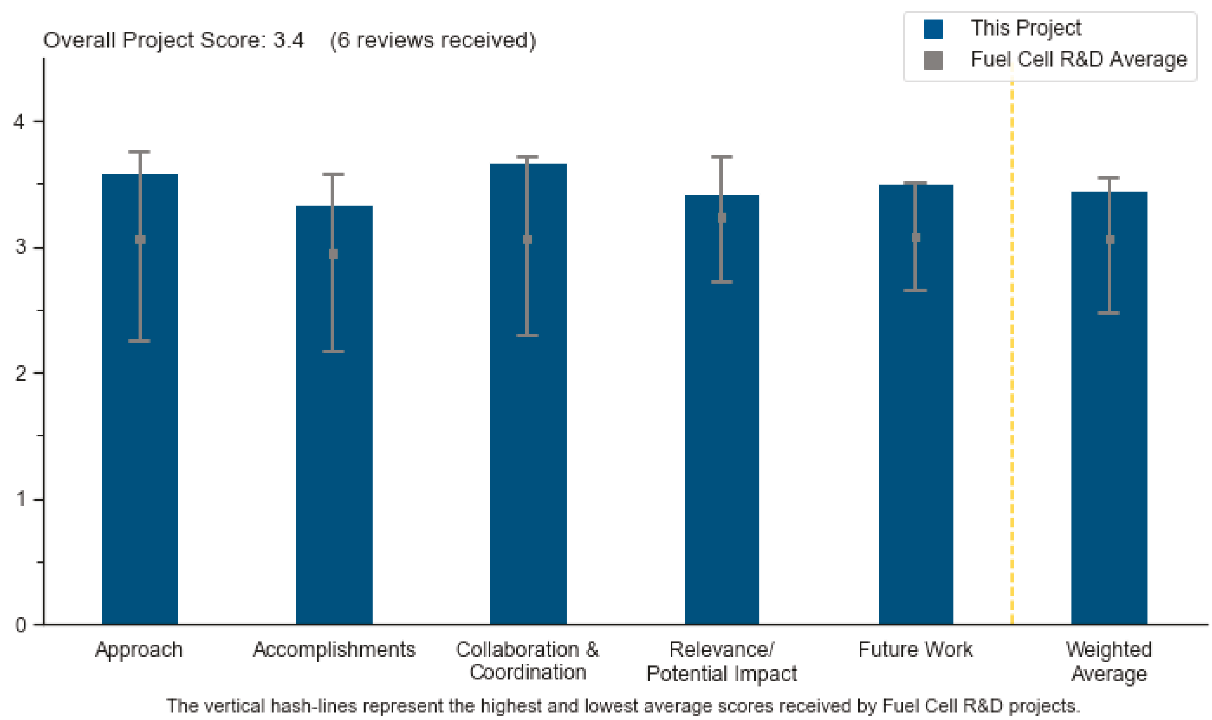
Project #FC-171: ElectroCat: Advanced Platinum-Group-Metal-Free Cathode Engineering for High Power Density and Durability

Shawn Litster, Carnegie Mellon University

Brief Summary of Project

This project is developing platinum-group-metal-free (PGM-free) oxygen reduction reaction catalysts for polymer electrolyte membrane fuel cell cathodes. The team is undertaking a thorough approach that combines advanced, atomically dispersed metal–organic-framework (MOF)-derived Fe-N-C catalysts, PGM-free specific cathode architectures, and advanced ionomers. This project seeks to (1) enable high-power density and improve durability with new cathode structures designed specifically for PGM-free catalysts; (2) increase PGM-free catalyst activity and stability through novel synthesis approaches, including using a simplified, low-cost method; (3) mitigate PGM-free cathode flooding for fast oxygen transport across thick electrodes; and (4) integrate advanced ionomers into the electrode structure for optimal performance and durability.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project effectively combines catalyst synthesis, membrane electrode assembly (MEA) testing, electrode engineering, advanced microstructural characterization, and modeling to demonstrate improvements in PGM-free MEA performance, along with improved understanding of transport and reaction phenomena and structure–function relationships.
- Overall, the approach appears excellent. The use of modeling and numerous experimental techniques is sharply focused on meeting the project goals. The approaches appear appropriate and well organized.
- The project's approach is impressive.
- The project is well organized and covers all the major elements of the catalyst and electrode in a direct, highly focused scientific approach. It would be beneficial to see the group focus on not only the

macroscopic view of the electrode but also a more physical, chemical, and analytical approach for the catalysts. It is suggested that the team look at Mössbauer spectroscopy as a tool for understanding the Fe electronic structure and the impact on electrocatalysis. It would also be good to see the group re-investigate the older, well-known, non-ionomer-based (polytetrafluoroethylene [PTFE]) electrode layer compositions (or hybrid versions) rather than just the current conventional approach.

- The model-based design approach is sound, and it has produced excellent results. It would be good to see less emphasis placed on catalyst activity and more placed on understanding material issues and transport limitations in the electrode.
- The project's approach is to use a state-of-the-art (SOA) catalyst, demonstrate performance, and then scale up the catalyst fabrication process and develop and demonstrate catalyst layers and MEAs that meet performance. An SOA PGM-free catalyst was received and used to demonstrate performance. Good progress has been made at the fundamental level as measured using a rotating disk electrode (RDE), but MEA performance is poor, and stability at the MEA level is very poor. The data suggest issues with both the cathode catalyst layer and the catalyst-layer gas diffusion layer (GDL)–GDL interface. The project needs to optimize these components and their interaction.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Compared to the milestones, it appears this project is ahead of schedule. It also looks like some interesting analysis is being done on the durability question, which may lead to strategies to improve durability (i.e., changing carbon phases). There is excellent use of modeling and various types of electrochemical measurements, as well as additional characterization techniques.
- The project is making outstanding progress. Significant accomplishments were made in the past year in improving catalyst and electrode performance. The project is breaking new ground in high MEA performance and is meeting and exceeding its goals. Durability is still a major concern, especially since a large part of the performance improvement appears to be due to the use of higher operating temperature, which could accelerate degradation. The project should be reporting on all MEA performance metrics using the same MEA construction. It appears that the researchers are using different membrane thicknesses and catalyst loadings to optimize MEA performance separately for the high-current and low-current targets; this practice may be common in the field, but it should be discouraged since it makes results less relevant to the real world.
- The results have generated significant progress and therefore have contributed to furthering the advancement toward achieving the goals. The key now is to better understand the implications of the results and refine the model, as well as the experimental plan. As progress is made, the initial challenges change. The efforts required to address the challenges are also in need of refinement. It would be helpful to see how such challenges change over the lifetime of the project. The team could maybe use a spider chart to track progress and include the primary metrics, such as conductivity, catalyst activity, degradation, durability, performance, and even some form of a water management metric.
- The team has made good progress toward its milestones. Moving forward, it is recommended that increased focus be put on the high-current-density, transport-limited regime and less focus be put on catalyst activity.
- This project has met the initial half wave potential goal of 0.87 V versus reversible hydrogen electrode as measured by RDE, but the power produced is well behind that shown by other developers. Roughly 40% of the project has been completed, but only about 25% of the budget was used. This suggests that additional resources are needed to accelerate development to improve the cathode catalyst layer and GDL. High high-frequency resistance (HFR), very high accumulated water-induced mass transport losses, and 30% performance loss in less than 40 hours will each require significant effort to resolve. The authors report reversible and irreversible losses. However, their data show the decay rate after recovering the recoverable losses is much higher than the earlier decay rates, so the reversible losses are not really reversible.
- The electrode development is impressive, as is the catalyst work. It is unclear how much progress is occurring in catalysts, with the overlap with other projects.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- Fantastic collaboration appears to be the key to this project's success. Outstanding catalysts developed by the University at Buffalo group have contributed greatly to the good results.
- There is good collaboration apparent with all partners, including the Electrocatalysis Consortium (ElectroCat) and others.
- Key personnel need to reach out to teams that are further along in the development of this type of catalyst, such as ElectroCat, Energy Materials Network (EMN), and consortium members, including national laboratories. The proposal clearly and completely defines the roles and contributions of each team member, and the final team, facilities, and equipment required to complete this project are fully in place, ready and available. This project has full commitment from senior management and the corporate officers of its partners.
- The team has strong collaborations among university, industry, and national laboratory partners.
- The project appears well organized, and the team members appear integrated.
- It is not clear how fuel cell initiative changes at 3M will impact the company's involvement in the project. It is not clear that Giner, Inc., is the right partner for synthesis scale-up. This should involve a chemical company.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This is probably the most promising PGM-free project, with exception of the Fe effect on membranes.
- PGM-free catalysts are critically important for commercializing fuel cells. Fe-doped MOFs have shown significant progress, and additional performance and stability improvements are required. Focusing on reducing HFR, water management, and other mass transport issues, as well as reducing decay, will provide significant benefits for this technology.
- The project is quite relevant, as a successful outcome of all the non-precious-metal development efforts, including this one, will likely make the technology more attractive cost-wise, as well as reduce dependence on platinum sourcing from outside the United States. A successful project will also help redefine the cost and performance mode for all fuel cell applications and provide guidance. It is not clear yet that non-PGM fuel cells will be significantly less costly, because if the current–voltage behavior is lower than that of platinum-based systems, additional membrane surface area may be needed. In other words, membrane costs may increase, as may additional internal cell hardware, to make up for the lower performance of the non-PGM catalysts.
- The project has strong potential impact, as transport limitations are a significant loss for high-loading PGM-free catalysts at high power densities. The focus should continue to be on the nature of these losses.
- The project is clearly focused on DOE goals. Limited durability at this point does raise the question of whether these materials are serious contenders to meet the durability targets, but this project will help answer that question.
- Within the context of PGM-free research, this project is highly relevant and is already having a large impact on the field. However, the relevance of PGM-free catalysts to the industry is still questionable. With the development of extremely low-PGM-loaded MEAs in recent years, PGM cost is no longer the major obstacle that it once was. Furthermore, the durability of the catalysts developed in this project is still far too low to be relevant in transportation or most other applications.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The proposed work is consistent with the development plan and should provide additional insight.
- The future work is solid and well planned. The increased focus on durability is a good idea.
- The project's proposed future work is excellent.
- The goals seem informed by current results and project targets.
- In their future work, the researchers need to reach out to teams that are further along in the development of this type of catalyst, such as ElectroCat, EMN, and consortium members, including national laboratories. The approach and plans should be provided.
- Model-driven design should be more emphasized, with model and theory results leading to improved treatment and understanding of performance and stability. At this point, the description of future efforts is general and could be more precise.

Project strengths:

- The project plan is addressing the right metrics, and the team is doing a good job at focusing on using relevant external testing methods. The team is very good and has a handle on looking at the key variables so as to further the development of the model and PGM-free catalysts.
- This project group is very experienced in working on the scale-up of laboratory processes and in MEA development and fabrication.
- The team has strong background in catalyst synthesis, characterization, and scale-up.
- Overall, the project looks well organized and is making progress toward hitting the technical targets.
- The project's greatest strength is its excellent collaboration with a strong team.
- The project has great methodology and execution.

Project weaknesses:

- It would not be called a weakness, but it would be good to see the team expand beyond the current conventional wisdom regarding electrode composition and structure. The project needs a chemical company at some point to address the synthesis and scale-up of the catalyst.
- A reduced role of modeling is detected in the near future, which reduces the potential for impact.
- The project has a reliance on Fe-based materials and an unclear catalyst focus.
- This project needs to add resources to accelerate the rate of development.

Recommendations for additions/deletions to project scope:

- The following are suggestions for the project. (1) The project should include the evaluation of the Fe-based catalysts using Mössbauer spectroscopy. The impact is on gaining an understanding of the differences in the catalyst. (2) The project should develop a hybrid hydrophobic–hydrophilic electrode composition by determining whether adding some hydrophobic character will address performance. The impact is on water management behavior in the electrode. Alternatively, the team should concentrate the ionomer at the membrane–catalyst interface. (3) The researchers should look at the PTFE content of the microlayer as well. They should even consider removing it and looking at a higher-PTFE GDL character.
- The project should maintain a model-based design approach by continuing modeling activities. The team should compare performance accomplishments to model predictions.
- It may make sense to include other catalysts from other projects.
- There should be more focus on durability.

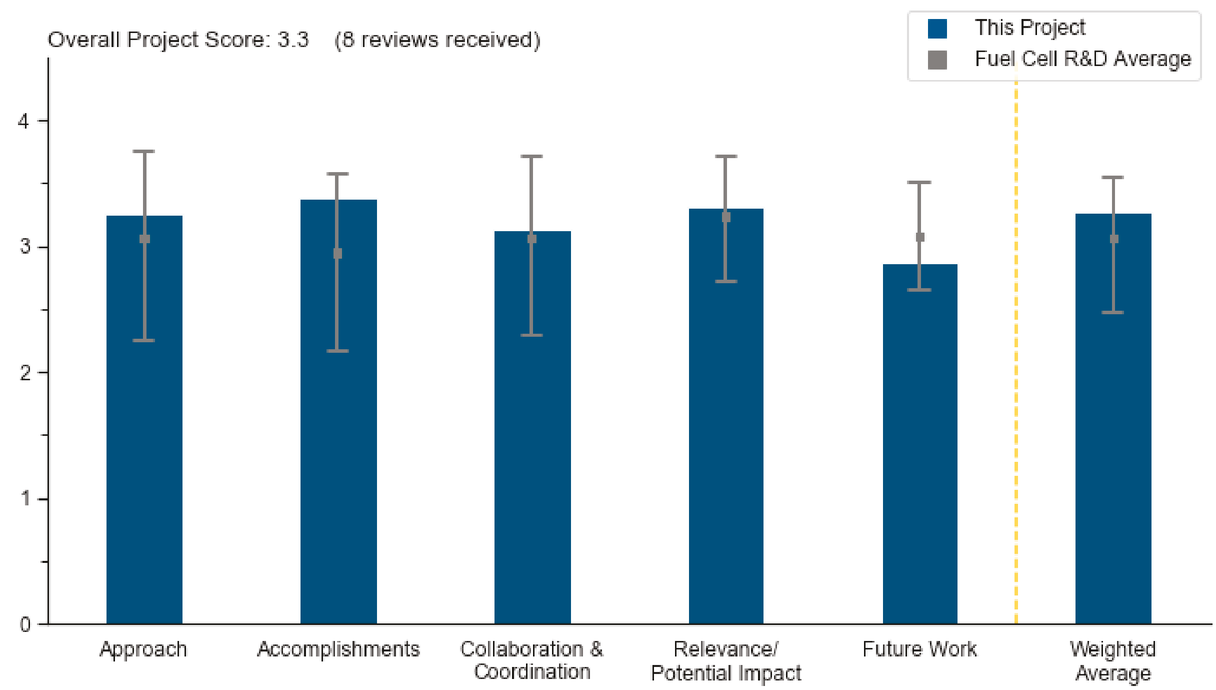
Project #FC-172: ElectroCat: Highly Active and Durable Platinum-Group-Metal-Free Oxygen Reduction Reaction Electrocatalysts through the Synergy of Active Sites

Yuyan Shao, Pacific Northwest National Laboratory

Brief Summary of Project

The project objective is to improve the activity and durability of platinum-group-metal-free (PGM-free) oxygen reduction reaction (ORR) catalysts through dual active sites for enhanced oxygen reduction and hydrogen peroxide (H_2O_2) decomposition. Materials and synthesis innovations include (1) dual active sites for ORR and H_2O_2 and (2) thermal shock activation for high activity through increased active site density. The developed catalysts will lower cost, reduce H_2O_2 formation by 50%, maintain the activity level, and double the durability compared to baseline platinum catalysts.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Use of the dual active sites is a unique and effective approach that can address activity and stability simultaneously.
- The radical scavenger approach is good, and the results are promising. The team needs to further improve membrane electrode assembly (MEA) performance.
- The goal of the project is very clear: increasing the durability of PGM-free catalysts in polymer electrolyte membrane fuel cells (PEMFCs) by reducing the H_2O_2 yield. Although it is inconclusive whether H_2O_2 is the major reason for the poor durability of PGM-free catalysts, recent studies have suggested so. The approach to address this issue is also very clear: creating dual sites with FeNC and MOx that reduce H_2O_2 via the 2X2 mechanism. The results are promising, showing that mixing FeNC with certain metal oxides does increase stability and reduce H_2O_2 yield in rotating disk electrodes (RDEs) and increase the durability

of PEMFCs. Overall, this approach appears to work. What is missing in the logic chain is direct evidence showing that the improved durability in PEMFCs is indeed related to the reduced H_2O_2 yield identified in RDEs. There is also no comparison between the MEAs with or without oxides subject to long-term PEMFC operation. The thermal shock synthesis was not sufficiently justified.

- Peroxide formation likely contributes to the degradation of PGM-free catalysts, and this project seeks to reduce the effects of peroxide formation through the addition of ceria. This project appears to be more focused on reducing degradation in comparison with other work being done on PGM-free catalysts, which is needed. However, it is not clear that ceria decomposes peroxide byproducts significantly faster than the peroxides destroy the active sites. It is strongly recommended that the project team design experiments or perform modeling to determine the extent to which this approach will work. Approaches that prevent peroxide formation may be required to meet the durability requirements for commercial adoption.
- The approach overall appears good. Various types of synthesis are taking place and being translated into MEA performance testing. While the goals are being met, it is a little hard to understand the strategy behind the work for the coming year other than trying out a variety of new synthesis approaches. It would be helpful to see quantitative gaps, and how the proposed approach would be able to meet those gaps. It is not clear that the approach to improving durability will work. The work shows improved durability, but it is still far from the ultimate targets, and simply trying new scavenger compositions is unlikely to address the challenges. It may make sense to try to approach the durability in a more fundamental way to help create ideas that would get closer to achieving the ultimate targets.
- The overall approach is good, and the team seems to be on the right track to address durability issues arising from peroxide radicals. However, the effect of the peroxide radical on catalyst degradation (i.e., CO_2 emissions) and membrane degradation in an MEA is not well elucidated. The team should focus on understanding these effects via a clear design of experiment and the support of good analytical tests. The effects of loading and the tolerance to peroxide radicals due to catalyst loading are also not very clear. Slide 7 shows a good comparison between FeNC and FeNC–NCeOx system durability, but it is difficult to compare the effect of loading, as it was not provided for the FeNC system.
- The project's approach is to use rational design to develop durable, highly active, PGM-free ORR electrocatalysts. The project is also developing dual active sites for ORR and H_2O_2 : MNx and radical scavenger. The thermal shock process has been tested and shown to be ineffective for the removal of Zn. NTaTiOx has shown promise. Modifications are needed to address these processes. Priority should be given to identifying and verifying a workable process.
- Other reviewers may disagree, but the focus on catalytic activity is misplaced. The focus should be on building dual-catalyst functionality and evaluating the effect of this technique on the performance, stability, and chemical environment of the cell. To that end, it is time to drop the thermal shock approach, as it has not contributed significantly to these goals. Also, as a national laboratory is conducting the project, the nature of the "direct loading" approach should be fully revealed.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made significant progress and achievements. The activity already met the final target, and the performance met year 2 milestones. In addition, the durability improved dramatically. The validation of the method of mixing FeNC with metal oxides suggests that peroxide is likely the major cause for the poor durability of FeNC.
- Mass activity reached 35 mA/cm^2 at 0.9 V (H_2/O_2), for which the DOE target is 44 mA/cm^2, and achieved 138 mA/cm^2 at 0.8 V (H_2/air). Both of these are the best in the field.
- The project has made significant progress since the last DOE Hydrogen and Fuel Cells Program (the Program) Annual Merit Review, with more promising fuel cell data. The current density of 30 mA/cm^2 in an H_2/O_2 cell represents a result similar to that of the state-of-the-art. However, at low potential, the polarization current density is still low.
- Relative to the milestones, it appears that progress is excellent. The bigger challenge is around durability, which has not really shown up in the milestones to date.

- The team has made excellent progress in achieving reduced CO_2 emissions in the presence of the scavenger. There has been more limited progress in thermal shock synthesis.
- The project is achieving targets with respect to activity and is showing improvements in durability. Relative to the other ElectroCat projects, these are good results. There is some question of whether the dual-site catalyst is really more stable or only appears more stable because it starts at lower performance (the degradation graph was "normalized"). It would be helpful to show the non-normalized data.
- The project's progress toward overall goals is promising. However, some of the fundamentals are not covered sufficiently. For example, slide 15 does not show the differences between the various thermal shock samples. It is not clear what parameter was changed between samples 1 and 4 that led to either improved or poor RDE performance. Significant improvements that result from any process variables should be accompanied by sound scientific explanations, which are lacking in the presentation slides. No qualitative explanation has been offered to explain the effect of thermal shock.
- This project is underachieving and underspending. Additional resources need to be applied to development tasks. RDE performance on Pt is low, and using that Pt performance gives a claimed delta for Pt performance that is artificially high. There has been significant progress at the RDE level, but there is a long way to go, and the iR-free performance at the MEA level is low. In addition, both the high-frequency resistance and decay are very high. The fundamental causes for these losses are not understood.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- The team is strong and appropriate to what was proposed for implementation. The collaborations with national laboratories are great. The whole collaboration nicely covers all the necessary aspects, including synthesis, characterizations, modeling, RDE, and MEA evaluations, and these aspects were well integrated. The thermal shock method is new and works in one case. The detection of CO_2 is a good method. X-ray absorption spectroscopy (XAS) is also very informative in detecting the Fe species. However, there is no direct evidence, either microscopic or spectroscopic, for the close proximity of the FeNC site and the metal oxide sites. High-resolution transmission electron microscopy (HRTEM) and XAS may do it.
- This is a good, complementary team. For the next presentation, it is suggested that the project team specify each institute's efforts and achievements.
- The project has good collaboration among multi-institutions.
- The project's coordination appears adequate.
- The presentation could have made clearer what the contributions of Washington University and Ballard Power Systems, Inc. (Ballard) were to the presented results. There is a good integration of ElectroCat resources.
- Pacific Northwest National Laboratory and Washington University appear to be collaborating well. The motivation for the thermal shock approach was not clear, and those results seem to be a separate side project. The motivation for pursuing this approach needs to be described.
- The project's key personnel are qualified, as demonstrated by the completion of previous projects and by their publications on work in this and related fields. The team, facilities, and equipment required to complete this project are not fully applied. This project has the full commitment of senior management and corporate officers of partners.
- The collaboration between organizations is not very clear. It does not seem like some of the expertise that lays within this project team has been efficiently utilized. For example, no explanation has been offered for the improvements observed in hydrogen–air performance with cycling. Moreover, the principal investigator (PI) suggested that the team had not performed the polarization curve tests until equilibrium was reached. This clearly suggests that the expertise of collaborators such as Ballard has not been fully utilized to understand this phenomenon. It seems like these tests were not performed at Ballard.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- If this project were successful, there would be potentially very high impact on durability for both PGM and non-PGM catalysts. Detailed understanding is key, however, and the perspective of original equipment manufacturers, who have undoubtedly considered such approaches, will be essential.
- The project shows progress toward improving the activity and durability of PGM-free catalysts. The potential for a breakthrough result that completely solves the degradation issues with these materials seems unlikely, although the approach may contribute to the solution.
- PGM-free catalysts are critical for PEMFCs because the cost and dependence on foreign precious metal can be resolved by a PGM-free catalyst.
- The team is focused on Fuel Cell Technologies Office goals.
- The work has advanced the development of PGM-free catalysts, but the performance needs significant further development.
- Reducing PGM loading is critically important to the successful commercialization of PEMFCs. The potential for this conceptual approach to be successful has not been demonstrated.
- It is not clear if this project is targeting new highly active catalysts or targeting a subset of non-PGM catalysts and working to improve their durability. With many of the slides lacking fundamental explanations for observed improvements or decreases in performance, it is difficult to judge potential impact.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- This project's most important contribution to the Program's goals and objectives would be to provide a clear way to improve the durability of PGM-free FeNC catalysts, which would implicate the original causes of the poor durability of FeNC catalysts. The poor durability of FeNC is basically the most important issue and the toughest barrier impeding the commercialization of FeNC catalysts. Mixing oxides mildly reduced the ORR activity of FeNC, but the reason behind this is not given. A counterbalance between activity and durability may be important for the advancement of PGM-free catalysts.
- The catalyst performance has made significant improvement. However, the more stable catalyst has lower MEA or fuel cell performance. Therefore, a new idea on how to improve both stability and performance needs to be addressed.
- The proposed future work should seek to build understanding of these catalytic systems. During optimization, the team should consider both the fractional and absolute loading of the scavenger, as well as the influence of "direct loading" on electrocatalytic activity. Optimization should also include the energy and coulombic efficiency of oxygen reduction since scavenging may represent a loss of electrons. Thermal shock should be de-emphasized since it does not appear promising.
- It is suggested that the project team focus on the MEA ink formulation, which will provide a better understanding of the factors determining performance. The team is encouraged to work on MEA structure characterization to build the property–structure–performance relationship needed to guide MEA development.
- The project's future work needs to focus more on verification of the process that produces a catalyst with the required performance and durability. In addition, MEA scale-up and catalyst layer structural issues are formidable and will require significant additional development attention.
- Better dispersion of ceria is a logical approach, but the team does not appear to have an understanding as to whether this approach will be enough. Modeling and analysis of the degradation mechanism would be a beneficial addition to this project. As the team seems to have strong characterization capabilities, using those to understand degradation mechanisms would help in this field.
- The future work, as outlined on slide 24, is not clear or precise. For example, the optimization parameters that would be targeted to improve performance or durability are not clearly justified with supporting evidence in the content of the slides. It is recommended that the project team refocus on their specific areas

of strength, which seem to be in catalyst synthesis. It would be beneficial to see more catalyst systems investigated using a similar approach to the one taken so far (i.e., creating dual active sites to mitigate radicals).

- The future work appears rather exploratory and is not based on clear hypotheses generated from a fundamental understanding or a quantitative gap analysis. It should be determined whether pursuing scavengers containing Ta will introduce cost challenges and what the criteria will be for selecting scavengers. Overall, the proposed work seems lacking in detail.

Project strengths:

- The overall strength of this project lies in the great performance of the catalysts in terms of both activity and durability, as well as in the validity of the proposed strategy. The reported activity of FeNC is comparable to the state-of-the-art, while durability was dramatically improved, a big deal in the PGM-free field. The proposed strategy is very straightforward and targeted: mixing FeNC and metal oxides. This makes the logic flow and the big picture of this project very clear. Characterizations, including the CO_2 detection and XAS, are very relevant, informative, and insightful.
- This project group is experienced in working in this field, and the project has chosen partners that have been proven capable of successfully completing this type of research.
- The project's strengths include its unique approach of using dual active sites and the complementary team on catalyst synthesis, MEA, and characterization.
- Relative to other work on PGM-free catalysts, this project appears to be focused more on reducing degradation, which is needed more than increasing performance.
- The team has made strong progress with promising results and good impact on durability and decomposition.
- The project has a good idea and has made good progress.
- The project is hitting the performance milestones.
- The strengths of this team are seen in their catalyst synthesis approaches. Although the team has very good partners in Washington University and Ballard, those partners do not seem to have been utilized well for electrode or MEA design and testing. For this project to be successful, the PI would need to engage those partners effectively.

Project weaknesses:

- The primary project weakness seems to be that the overall objectives and targets are not well defined. The team has a good industry partner that can provide guidance and direction to target in order to improve the technology readiness level of this technology.
- To meet development goals, this project needs to apply resources to increase the rate of progress. The processes and procedures needed to verify catalyst layer performance and stability over time at all operating conditions are expected to overwhelm the current level of resources.
- The project needs a more fundamental understanding of the mechanism of dual active sites. It is critical to understand how much H_2O_2 the scavenger can handle, namely, what the scavenger's capacity to stabilize the catalyst might be, as well as whether it would be consumed in the course of fuel cell operation.
- Direct evidence for the adjacent dual sites is missing. It is unclear what kinds of oxides are good choices and can effectively reduce H_2O_2. While the dual-site system works, its potential has not yet been fulfilled. While thermal shocking works for one case, the oxide NTaTiOx is rather unusual, which projects cost concerns.
- The project could use a deeper focus on hypotheses that drive fundamental understanding to make improvements. It is not clear that the durability is on track, although it does not appear to be in the milestones yet.
- More careful performance evaluation is needed. ElectroCat should do this.
- It is not clear whether ceria decomposes peroxide byproducts significantly faster than the peroxides destroy the active sites. The potential for a breakthrough result that completely solves the degradation issues with these materials seems unlikely if only a dual-site approach is pursued. The motivation for the thermal shock approach was not clear, and those results seem to be a separate side project.

- This is not the most transparent project, as some of the new technology is hidden. Relatively little scientific understanding can be gleaned without full disclosure.

Recommendations for additions/deletions to project scope:

- The project team should design and perform experiments or modeling to determine the relative rates of peroxide decomposition on ceria versus carbon corrosion. The team's wide array of characterization techniques should be used to better understand the degradation mechanisms. The team should also show the non-normalized degradation data to prove that the approach is working.
- The team should fulfill the potential of the dual-site system by systematically varying the type of metal oxides, the molar ratio of FeNC and oxide, the catalyst loading, etc. The team needs to understand why some oxides work and some do not, and the project should directly image the adjacent FeNC and oxide sites.
- The team is encouraged to look into the capacity of the scavenger, namely, the mechanism of the scavenger that deals with H_2O_2 and how long it can last in the course of fuel cell operation.
- The project scope may need to be redefined so that the team focuses on its areas of strength, which seem to be catalyst synthesis.
- The thermal shock approach should be rolled back since its ability to contribute to the project is questionable. At this point, catalyst development should focus solely on the effect of the scavenger on performance and durability.

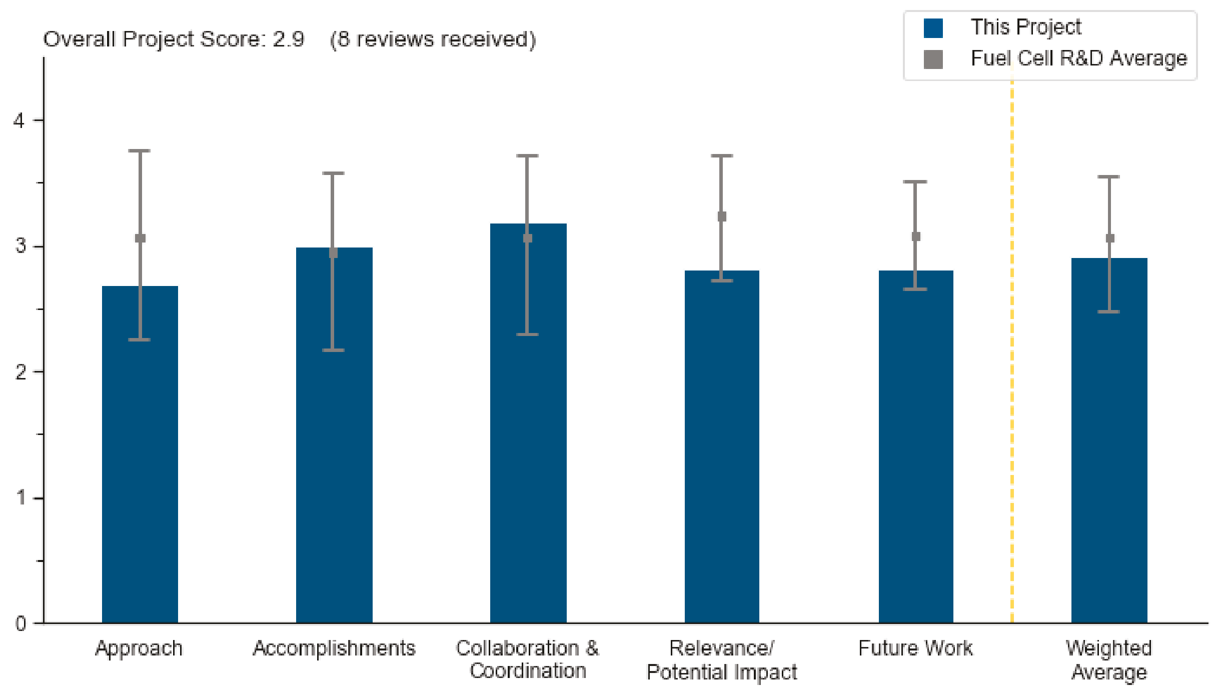
Project #FC-173: ElectroCat: Platinum-Group-Metal-Free Engineered Framework Nanostructure Catalysts

Prabhu Ganesan, Greenway Energy, LLC

Brief Summary of Project

The project objective is to develop durable, highly active electrocatalysts for the oxygen reduction reaction (ORR) through a unique, bottom-up, rational design to enable a better understanding of the platinum-group-metal-free (PGM-free) active sites and improve activity. Fiscal year (FY) 2019 objectives include (1) catalyst development based on high-surface-area polymers, (2) membrane electrode assembly (MEA) optimization and fuel cell testing, and (3) achievement of 25 mA/cm^2 in a H_2–O_2 fuel cell test at 80°C and 100 kPa.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **2.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The plan to improve catalyst activity was presented and is feasible. The team also appears to have an understanding of the primary issue with low MEA performance. The area that is most lacking from the approach is the identification of durability barriers and a strategy for addressing durability. The team's strong modeling could be applied toward helping understand degradation mechanisms. Even if the team cannot match "world-record" PGM-free performance, providing insight into degradation mechanisms would be beneficial. The team is encouraged to focus on non-Fe catalysts to improve durability.
- The project's approach is to develop durable, highly active, PGM-free oxygen reduction electrocatalysts using rational design. The project is structured to focus on hydrogen and oxygen performance using fully humidified reactants. The performance goals for hydrogen and oxygen were met, but the decay is very high, with 60% loss in four cycles. The development progress and spending are on schedule, and milestones have been met for the hydrogen–oxygen effort. The fact that the development efforts have been

almost exclusively on hydrogen–oxygen tests to date is a significant concern. The ultimate requirement is a hydrogen–air MEA.

- The polyporphyrin approach represents a good direction. The synthesis support from Northwestern University (NU) is also very good. The catalyst performance progress is slow.
- There is an adequate combination of synthesis, half-cell testing, MEA testing, and computational analysis. It is hard to see how this will improve upon already existing PGM-free catalyst materials.
- The objective of this experiment and modeling project is to develop durable, highly active, PGM-free oxygen reduction catalysts for hydrogen and air fuel cells using a rational design approach. The project began on September 1, 2017, and is scheduled to end on December 31, 2020, so it is about 50% completed. The principal investigator (PI) has developed catalysts based on high-surface-area polymers that are pyrolyzed. Experimental results were shown of poly-phenylporphyrin and a zeolitic-imidazolate-framework-based (ZIF-based) Fe/MN catalyst with unusually large particles (200–300 nm) and low metal loading (0.08–0.35 at%). On the other hand, the surface area of this catalyst after pyrolysis was very high, at 1263 m^2/g. The project examined the composition and morphology of these Fe-based catalysts using electron energy-loss spectroscopy (EELS) and x-ray absorption near edge structure (XANES). There was also a modeling component to the project. The team demonstrated active site and reaction pathway modeling for Fe-porphyrin and FeN_4 in graphene, but it was not clear how the modeling work is giving the PI new insights for improved catalyst performance. There was also some fuel cell testing of poly-phenylporphyrin. While the FY 2018 target for fuel cell activity was met, catalyst stability and durability remain issues. High degradation rates were observed at a voltage hold of 0.4 V, with less degradation during a potential hold at 0.7 V. It is not clear how or whether the durability will be improved. Modifications were made to the polyporphyrin synthesis to improve fuel cell performance, but details were not given at the Hydrogen and Fuel Cells Program (the Program) Annual Merit Review (AMR). It appears that part of the low-fuel-cell-power problem is due to a poorly designed cathode with the PI's PGM-free catalyst. It is recommended that the PI devote more time to proper fuel cell MEA preparation.
- It was difficult to see what actual approach is being used for what problem in FY 2019. On slide 4, four red dotted boxes were used to highlight (1) synthesized porphyrinic polymers, (2) added heteroatom and peripheral functionalities, (3) a proposed model for active sites, and (4) the optimized MEA for optimized catalysts. It is unclear whether all of these are for increasing surface area, for increasing the density of active sites or activity per site, for improving durability, or for identifying the key issues. Apparently, the team is trying to answer many challenging questions. However, the approach seems not clearly described.
- Some project targets are set, and progress is being made, for example, with the 900 mV iR-free oxygen performance. However, some other significant targets have had 0% progress, with the project 40% complete. For example, no progress has been made with the more realistic power density target set for air operation at 800 mV cell voltage, with a current density target of >150 mA/cm^2 on air; not even one chart of air performance was shown. The last point is about durability: no target has even been set for the project.
- Much investment has been put into this one material for some time. It is clear that it is of no practical use without magnitudes of improvement in stability. The focus should have been put in only two areas: determining the degradation mechanism and whether it can be prevented. Any other area is a waste of funding.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team has made progress toward meeting the 2020 performance target for MEAs operating on oxygen.
- In FY 2019, the project team met the MEA activity target of 30 mA/cm^2 at 900 mV iR-free cell voltage. The rotating disk electrode test result was improved from 2.03 to 2.78 mA/cm^2 at 800 mV, exceeding the 2019 target of 2.0 mA/cm^2. This is significant progress. However, the performance enhancement factor was not clearly identified, and durability needs to be improved.
- While the catalyst requires additional development efforts for operating on hydrogen–oxygen, the additional known issues that involve the cathode catalyst layer suggest that early testing on hydrogen–air should be a major part of development, even at this early stage. Mass transport and even some portions of kinetic losses are known to be significantly more severe when operating on air. An early understanding of

the fundamental mechanisms associated with operating on air should be used to guide the catalyst development. The ultimate requirement for the catalyst wettability may impose requirements on the catalyst fabrication process.

- The PI has made good progress regarding the activity of his PGM-free catalysts. Durability tests were performed this past year, as suggested by a 2018 AMR reviewer, but the results were not good. There was a significant drop in current density during a 5 hour 0.4 V hold, with less current loss over a long period of time when the potential was fixed at 0.7 V. This means that the durability issue was quantified via direct fuel cell performance data, but it has not yet been corrected.
- The team is making progress toward improving activity and appears to be meeting the project targets in that regard. However, highly active catalysts that rapidly degrade are not useful for any applications of interest to DOE. More progress and focus are needed to address degradation.
- Good progress has been made for the current density target at 0.9 V. However, the team is strongly encouraged to focus on developing the precursor conversion to reap the benefit of the precursor.
- The project's activity targets have been met. The durability of the material at potentials where H_2-O_2 is evolved is limiting.
- The project has made good progress from this point last year. It would be good to see more results on durability.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The final team, facilities, and equipment required to complete this project are in place, ready, and available. The team's personnel are qualified, as demonstrated by the successful completion of previous projects and publications. This project has full commitment from senior management and corporate officers of partners. Ample facilities are available to support and complete this work.
- The collaboration and partnership with Savannah River National Laboratory (SRNL) and ElectroCat appear quite strong. It is not clear whether Ballard Power Systems (Ballard) has contributed significantly to the project. NU provided characterization. Overall, the project appears to be a collaborative effort.
- The results were obtained from collaborative efforts. The lack of contribution from Ballard (who is a no-cost partner) is understandable at this stage. Studies using modeling may aim more at the materials on trend to guide the search for suitable heteroatoms.
- A wide variety of partners is on the project, from small businesses (including the lead) to national laboratories, universities, and a leader in polymer electrolyte membrane fuel cells (PEMFCs) (Ballard). However, no data were contributed from Ballard, whose role is the "evaluation of promising electrocatalysts."
- This project has very good multilaboratory collaboration. The presentation showed that the project has leveraged the works from many laboratories, including ElectroCat. However, it is not clear whether the lead institution has made a major impact.
- This is a focused and capable team.
- The collaboration is adequate.
- The collaboration and coordination of the various team members were somewhat weak and not clearly described in the AMR slides. The modeling work and results seem separate from the catalyst development efforts. The modeling results indicate a specific improvement in ORR kinetics (e.g., a new reaction pathway for FeN_4 on graphene). This will be important only if the PI can see and/or monitor the reaction pathway. Otherwise, he will not know whether such a new pathway exists. Similarly, it is unclear how the PI will modify the catalyst synthesis to create additional open Fe axial sites, as suggested on slide 12. The specific accomplishments of the NU researchers were not clearly identified; slide 6 indicated that they prepared a poly-azoporphyrin catalyst, but the properties and activity of this catalyst were not discussed. It is not clear how California State University, Northridge, has contributed to the project or whether there are plans for Ballard to perform experiments in year 3. Al Anderson and Edward Holby seem to be doing modeling work, but it is unclear whether these two researchers are working together or separately.

Question 4: Relevance/potential impact

This project was rated **2.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- There is a need to develop high-activity, PGM-free oxygen reduction catalysts for hydrogen–air fuel cells.
- Reducing PGM loading is critically important to the successful commercialization of PEMFCs.
- The project objective is relevant to the long-term goal of eliminating the use of PGMs for a large impact on cost reduction. It is still unclear that significant advances can be made toward this goal, as the durability results add more challenges. Ultralow-PGM catalysts, with non-PGM active sites on support, may be more promising.
- The project shows progress toward improving the activity of PGM-free catalysts. The approach for addressing degradation issues was not presented. To be useful for any DOE-relevant applications, orders of magnitude of improvement are needed in the durability of PGM-free catalysts. The team's modeling and approach for preparing catalysts could be directed toward exploring degradation mechanisms and generating ideas for addressing durability, but it is unclear whether the project will attempt this.
- DOE has a subset of targets and goals for PGM-free catalysts, and this project has hit one of those targets; however, it still appears to be far off from the others. To make a meaningful contribution to the overall goal of the Program, much progress still needs to happen.
- Non-PGM catalysts have significant promise for future fuel cell integration. However, it is hard to see what this project will add to the already existing knowledge and materials for non-PGM catalysts.
- Eliminating PGMs does not necessarily mean lower cost. Because the cost of all other components combined is large, the cathode catalyst with the highest activity, power, and durability will make for the most cost-effective fuel cell stack. The current material is Fe, which is not compatible with PEMFCs. There is very low stability and usable activity.
- The PGM-free catalyst performance from this project needs to catch up quickly with the results from other projects.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The proposed future work appears to be adequate to meet the specified targets.
- It is not clear what the lead organization will contribute in regard to the future work. Polyporphyrin still represents a promising direction. The team should give more focus to MEA performance optimization at both high-V and high-I regions.
- To be fair, the presentation ran long, and the future plans were not presented in detail. The plan for improving MEA performance was logical. A plan should be added for addressing durability that combines modeling and the many parameters that the team can control with catalyst synthesis. Even if the team cannot solve degradation, presenting a better understanding of degradation would move this field forward.
- For future work, the PI proposes to explore new catalysts (i.e., different porphyrin links and the use of different transition metal centers). It is not clear how this work will improve catalyst durability, which is the number one issue with the PI's catalysts right now. Early on, during year 3 of this project, the PI should down-select one or two catalysts for MEA optimization and fuel cell testing, with durability as the focus. The modeling work should be de-emphasized unless the PI can show how it is directing or steering research work.
- The proposed future work appears to be more of the same. A durability target appears to be missing in the work. The approach should have a durability go/no-go decision point; if the material were fundamentally flawed with respect to durability, then future work on the material would be questionable.
- Future work on this project needs to devote significantly more effort to fabricating and testing MEAs on hydrogen–air.
- It would be good to see more work on durability.
- The proposed future work is mainly a continuation of multiple tasks. It is unclear how the electrochemically active surface areas were determined. Studies using modeling could screen metals as possible active centers.

Project strengths:

- The team is making progress toward improving activity and appears to be meeting the project targets in that regard. The collaboration and partnership with SRNL and ElectroCat appear quite strong. The modeling results were insightful.
- The PI has made highly active catalysts. The end-of-project catalyst activity target (30 mA/cm^2 at 900 $mV_{IR\text{-}free}$) has been met. This is the primary strength of the project.
- This project group is capable of conducting the research and development on PGM-free catalysts. Scaling up and verifying the stability of hydrogen–air is likely to present significant challenges.
- The project team has met performance targets and demonstrated the need to address catalyst durability at high current densities.
- The project addresses a challenging subject. The team is well qualified to carry out the proposed tasks.
- The novel PGM-free material is making progress on oxygen power density.
- There is very good collaboration in this project.
- This is a focused team.

Project weaknesses:

- The durability of the PI's catalyst is poor. The project team did not present a path forward for rectifying the durability problem. The PI discussed only "modification" of the catalyst, with no details. Cathodes with the PI's catalyst in a fuel cell MEA performed poorly. It is not clear how the results of the modeling work will be translated into new catalyst design. For example, it is not clear how new catalyst designs in year 3 will target open Fe axial sites, as per slide 12.
- The direct link between the computational work and the synthesis and experimental work is not very clear. Material durability is a critical weakness that could be difficult to fix.
- Testing MEAs on hydrogen–air should be given priority.
- There did not appear to be sufficient focus on understanding and addressing catalyst degradation.
- More work should be put toward the weaknesses of durability and air power density.
- The project has not led with strongly innovative ideas so far, which may take time and more experience.
- There has been slow progress.

Recommendations for additions/deletions to project scope:

- The team's strong modeling and the flexibility of the catalyst synthesis approach should be applied more to help understand degradation mechanisms. The team should consider non-Fe metals, such as Co or Mn, to avoid membrane degradation. Even if the catalysts are atomically dispersed, the Fe is likely released through degradation.
- It is recommended that the PI devote more time to (1) optimizing electrode and MEA fabrication, (2) testing the catalyst in a fuel cell under different temperature, relative humidity, and gas flow conditions, and (3) improving the durability of catalysts in fuel cells. The project team needs to collaborate better and coordinate tasks more effectively. There should be better utilization of talents in year 3, and the PI should better explain the contributions of each team member in next year's AMR presentation.
- It would be beneficial to see more durability work.
- The project needs a go/no-go decision point for durability.
- The team should propose strategies for improving durability.
- The cause of activity decay should be studied.

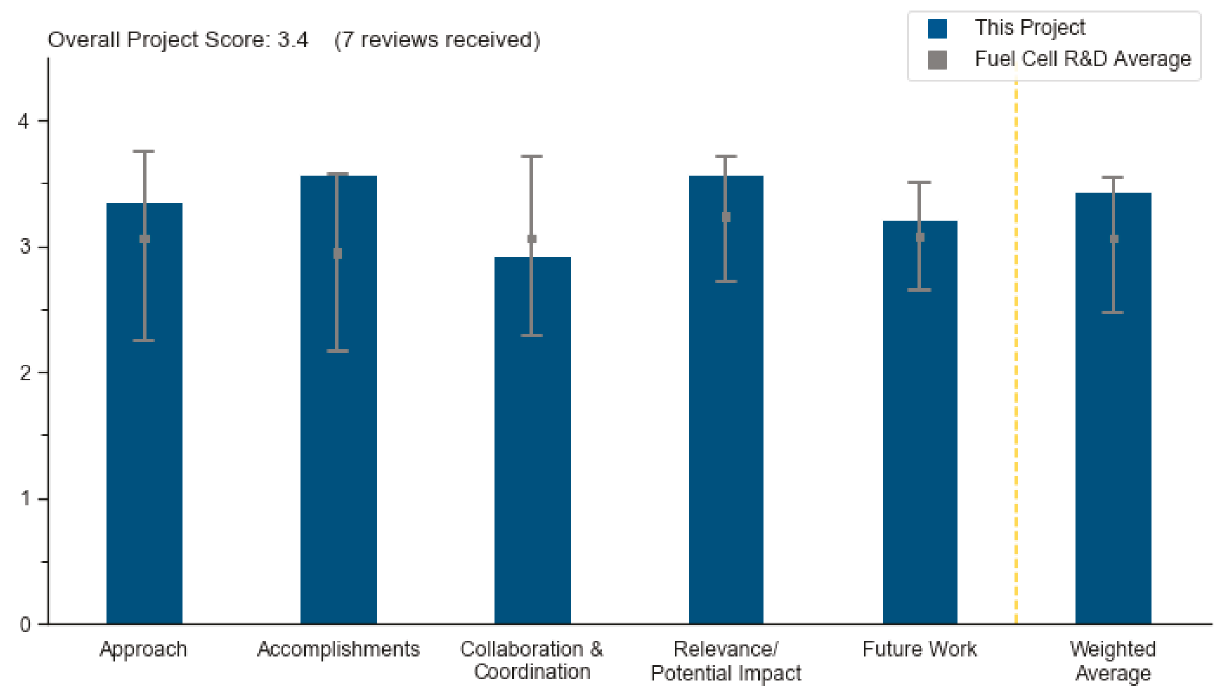
Project #FC-174: Highly Efficient and Durable Cathode Catalyst with Ultralow Platinum Loading through Synergetic Platinum-/Platinum-Group-Metal-Free Catalytic Interaction

Di-Jia Liu, Argonne National Laboratory

Brief Summary of Project

The project objective is to develop ultralow-platinum@platinum-group-metal-free (PGM-free) nanofiber cathode catalysts that achieve all U.S. Department of Energy (DOE) fuel cell catalyst/membrane electrode assembly (MEA) performance metrics, particularly in the high-current/power-density region. The approach reduces platinum usage through synergistic interaction between ultralow-platinum and PGM-free sites by improving catalyst activity and durability/transport by using a porous nanofibrous network catalyst support instead of a conventional carbon support.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project approach is focused on development of an ultralow-Pt-loading cathode catalyst that can achieve DOE targets at high current densities. This unique approach is very well thought out, with well-defined direction to move forward.
- Targeting the durability and mass/charge transport barrier through utilizing a porous nanofibrous network allows for high specific surface area. Using metal–organic-framework (MOF)-based synthesis that allows for use of industrial processes provides flexibility and scalability to the material.
- This project demonstrates a promising approach combining a PGM-free catalyst support produced by electrospinning and ultra-low loadings of Pt-Co catalyst.

- This low-Pt approach with the synergetic PGM-free site is a very effective way to meet all the DOE targets on an MEA level.
- The idea of using PGM-free supports to create an ultralow-Pt electrode is worthwhile, especially in the context of an ordered support such as a MOF, which would be expected to distribute Pt uniformly. The use of electrospinning to generate a more hierarchical electrode is interesting, but it would also be good to see evidence of why mass and charge transfers were expected to be enhanced. Enhancements for surface area and corrosion resistance are more obvious. Since PGM-free supports are known to generate hydrogen peroxide, it would have been good to have seen how this could be addressed in the initial approach to the project. It should have been understood at the beginning that this would need to be mitigated.
- The approach is somewhat duplicative of multiple approaches: high-surface-area materials, in situ Pt-Co alloy formation, etc. The project approach is very much similar to what Popov has done. Further, actual details on the approach are unclear and were not clarified during the question-and-answer (Q&A) session. However, project results are promising.
- This work seems diffuse with multiple non-overlapping goals. A focus on the synergistic catalyst effects is recommended.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- To date, overall accomplishments have been excellent. In-depth material analysis and testing clearly helps evolve an understanding of what the material is doing and how it behaves under various conditions. This is essential to advancing and progressing to a more mature and finished product that can be transitioned into functional fuel cell stack hardware.
- The project results are unbelievably good. For example, polarization curves on slide 17 are nearly perfectly straight in air, which is something even original equipment manufacturers (OEMs) cannot achieve.
- The results on a single selected MEA met all the DOE targets. The project accomplishments are excellent.
- The approach has yielded exceptionally high mass activity with low loading through a synergistic effect between the support and catalyst. The power density is still lower than desired. Given the very low loading, there could be a modest increase to reach power density targets while still having a very low MEA PGM content.
- The team has made good progress toward milestones and has generated interesting insight into catalyst mechanisms.
- The project has clearly shown the ability to achieve extremely high mass activities, and the polarizations are beginning to achieve 1000 mW/cm^2 under the heat rejection limit (0.675 V). Durability to 30 K electrocatalyst cycles has also been shown for both nanofiber and non-nanofiber electrodes. However, the nanofiber electrodes are having difficulty meeting high power density. The Q&A session revealed that there may still be some robustness issues related to peroxide generation at high temperature and low relative humidity. Electrodes have not yet been tested at low temperatures. No support corrosion accelerated stress test (AST) data were shown this year.
- The project met all 2025 DOE targets in terms of catalyst and MEA performance.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- Collaboration on this level of work is acceptable and seems highly coordinated. Additional collaboration partners who are interested in moving the technology to the next level would be ideal.
- There seems to be a good collaboration with Purdue University on modeling the interactions between the catalyst and support. It is important that the project partner with an OEM for optimization of the MEA for power density.
- The team has incorporated collaboration with university partners, particularly in modeling.
- There is a well-coordinated effort between experimental and modeling teams.

- It appears that Purdue University helped on the modeling that indicated that hydrogen peroxide should theoretically be reduced by nearby Pt, but very little evidence exists of other outside collaborations. The information presented does not clearly show where there are collaborations with the Fuel Cell Consortium for Performance and Durability (FC-PAD), nor what the impact was.
- Validation of performance from the industry sector would be wonderful.
- Project collaboration is not clear.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project offers a novel, very promising, and scalable approach for making an ultralow-Pt/PGM-free catalyst that already meets all 2025 DOE goals in terms of performance. The project has potential to advance polymer electrolyte membrane fuel cell technology.
- This project is quite relevant to the DOE strategy of using low-Pt or PGM-free catalysts. The demonstration from the results shows the potential impact on getting a high-performance MEA with low Pt loading.
- The project work performed, and results shown, indicate a clear and impactful potential contribution to the industry. It could be quite a huge step if the material can be manufactured in a more cost-effective manner than traditional fuel cell stacks while maintaining performance.
- The development of a high-activity, durable catalyst is central to the mission of the DOE Hydrogen and Fuel Cells Program. This project features catalysts that are able to achieve high activity and durability. Support corrosion metrics and status appear to be missing from the target table. Robustness metrics are missing from the target table.
- The project has potential for significant impact. The proposed approach requires a technical assessment to evaluate cost. However, this would be beyond the scope of the presently funded work.
- This project can potentially have high impact if the proposed mechanism of synergy can be proven.
- The targets of performance and costs are highlighted.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- Testing the material at high temperature is a highly relevant and important next step to improving overall fuel cell performance. Each step in the proposed plan is logical and will provide useful information.
- The future plan is well balanced between catalyst development, integration into MEAs with different types of membranes, and MEA independent validation.
- The future work slide consists of six bullet points, two of which are mystifying: the use of high-temperature membranes and thin membranes. This seems to be a tangent, considering that not all the work with the catalyst is complete. The project scope should focus on the catalyst; if the membrane directly affects the catalyst, then membrane work could be justified, but that does not appear to be the case. Unlike a company such as 3M or Plug Power, Argonne National Laboratory has not and should not be in the business of developing MEAs. Rebalancing the platinum from anode to cathode is a fair future task, as well as further optimizing the catalyst layers. Addressing robustness to peroxide formation in dry conditions and observing performance at low temperature and wet conditions should probably be emphasized more in the future work than it is.
- The future work plan can be improved by focus on mechanistic understanding and reduced consideration of MEA issues.
- There are too many avenues of future work proposed. Key efforts would be the optimization of cathode loading for power density and PGM content as well as the National Renewable Energy Laboratory testing.
- The future work should focus on validating the performance in H_2–air MEAs.
- Degradation product studies are needed to confirm stability.

Project strengths:

- The project team demonstrates excellent material and catalyst analysis. Multiple different approaches were analyzed and compared against a state-of-the-art material. There is a clear and logical proposed path forward.
- The project proposes a unique approach to make catalyst and support in a one-pot synthesis. Flexibility of the synthesis allows one to control support porosity and also catalyst activity and durability at the same time. Modeling is used as a tool for understanding synergetic interactions between the catalyst and support.
- The team has made an excellent start on potentially exciting scientific contributions. The following are project strengths: (1) the project met the DOE targets on the H_2–air fuel cell stack, (2), the project discovered synergetic effects on the Pt_3Co and CoN_4 PGM-free site, and (3) the laboratory met DOE targets with ultralow Pt loading using a MOF frame.
- The project has demonstrated a catalyst capable of extremely high mass activity. The project has shown durability with respect to the electrocatalyst AST within a fuel cell. The project began with a novel and ordered concept: the integration of platinum into a PGM-free catalyst that has its own activity, as well as a set structure.
- The project strength is the combination of Pt and PGM-free catalyst supports to achieve high mass activity with reasonable power density.
- The project team demonstrates good performance.

Project weaknesses:

- The project still needs to address robustness to a wide array of automotive conditions, including dry conditions and wet. The project sorely lacks collaboration, especially with industrial partners. Generation of hydrogen peroxide under certain conditions could become a showstopper under realistic automotive conditions.
- Project claims are overstated. The project approach combined several approaches that have limitations but does not address them. Benchmarking is suspect.
- The following are project weaknesses: (1) cobalt nanoparticle dissolution could degrade the Nafion™ film, (2) the understanding of this synergistic effect must be clearer, and (3) H_2–air high current performance is still poor.
- The weakness of the proposed synthetic approach is the limited ability to control the amount of cobalt nanoparticles that leach and degrade fuel cell performance.
- A current weakness is the below-target power density.
- The work plan for this project is too diffuse and should be more focused.
- An interested transition party would round out the project as complete.

Recommendations for additions/deletions to project scope:

- Future work associated with novel membranes should be deleted. Industrial partnerships should be added to understand robustness needs and issues that arise under realistic mobile application operation. Material should be added to slides related to the batch size and scale of manufacturing achieved to date.
- Electrode stability by FC-PAD is needed to confirm the issues others reported with this approach (membrane degradation, Co and Pt leaching, and migration).
- The proposed mechanism should involve copious generation of desorbed peroxide. Rotating ring disk measurements are strongly encouraged.
- Additions to project scope would be validating the low Pt loading and the high performance through collaboration with automotive OEMs.
- The project should evaluate the effect of cobalt leaching from cobalt nanoparticles on fuel cell performance.

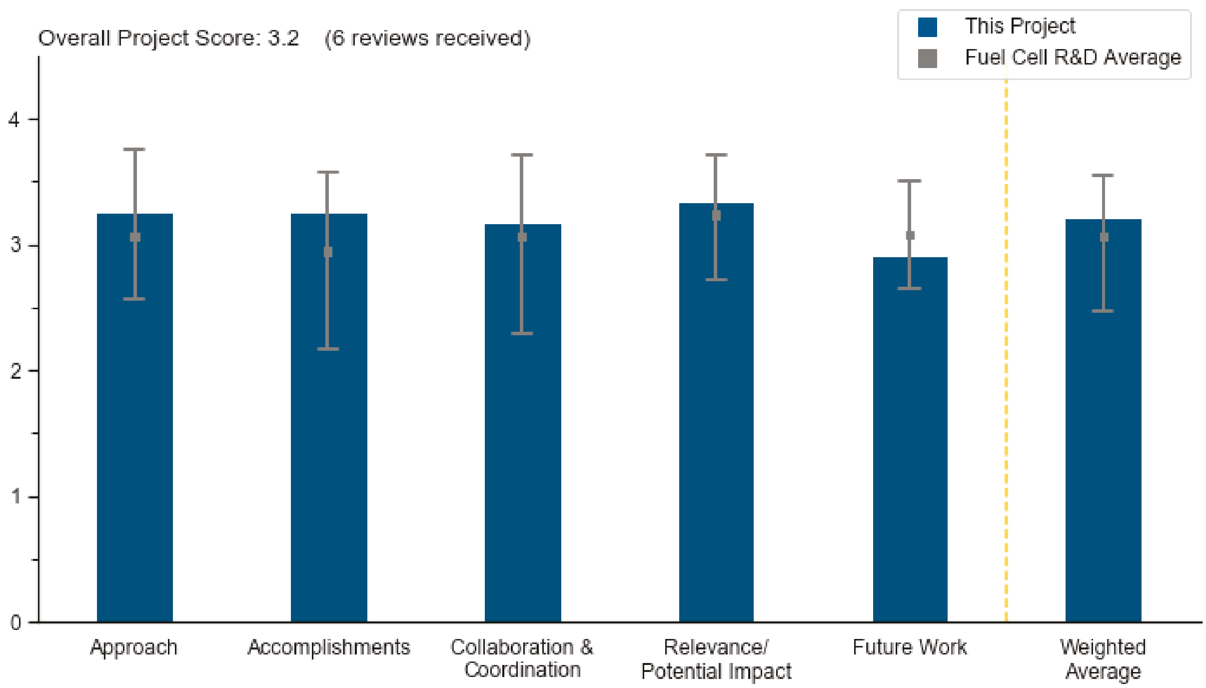
Project #FC-178: Lab Call Fiscal Year 2018 (Membrane): Spirocyclic Anion Exchange Membranes for Improved Performance and Durability

Bryan Pivovar, National Renewable Energy Laboratory

Brief Summary of Project

Alkaline exchange membranes continue to be challenged with cation degradation at high temperature and pH conditions. State-of-the-art trimethyl ammonium cations exhibit limited durability under fuel cell operating conditions. Research has indicated that cations with a spirocyclic structure have improved durability. The project is incorporating spirocyclic ammonium cations into alkaline exchange membranes to improve membrane durability. The project addresses the barriers of cost, performance, and durability by aiming to (1) synthesize novel spirocyclic ionomers to membranes and ionomers in alkaline membrane fuel cells (AMFCs), and (2) optimize performance to meet the U.S. Department of Energy's AMFC targets.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project is positioned well to leverage related projects at the National Renewable Energy Laboratory (NREL). There is little chance that the synthesis will not work as planned, and the new spirocyclic materials can be tested using the same protocols used for other anion exchange membrane (AEM) projects. The objectives and barriers are clearly defined.
- The team is extremely competent and experienced. The fundamental approach is excellent. The development of tasks and sequence of work is clearly well thought out and well executed.
- The project's approach is to identify and produce spirocyclic, ammonium-cation-based AEMs that show increased stability in alkaline environments. The project is running parallel tracks: one to characterize membranes and perform accelerated aging, and the other to develop membrane electrode assemblies (MEAs) and test fuel cell performance.

- The current project is based on previous work done on multiblock copolymers of polydiallylpiperidinium segments in a polysulfone backbone, with the goal of scaling the synthetic procedure for the production of AEMs for long-time testing.
- This project is focused on evaluating polymer chemistries based on cations that have proven to have high stability. Unfortunately, the backbone design includes ether linkages that have been proven to be weak points for degradation and appear to be degrading as expected, based on color change and brittleness after hydroxide soak compared to the perfluoro (PF) AEM membranes. However, the team provided a good justification in that such polymers allow for the evaluation of electrode ionomer adsorption in different ways than other polymers; this should be the focus moving forward.
- Spirocycles may open up a new path for the development of a durable AEM. It appears, however, that the selected chemistry (i.e., the backbone) may not give the expected results; it has poor durability at higher ion exchange capacities (IECs).

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The development of advanced AEMs is of crucial strategic importance in reducing the cost of fuel cell systems and meeting overall DOE goals for decarbonization and reduced U.S. dependence on fossil fuels. This group of spirocyclic anionic polymers is an important candidate in the portfolio and should be explored. The project has done an excellent job looking into these materials and characterizing their performance.
- The project has developed spirocyclic membranes with three different IECs. The team has measured greater peak power than existing Generation 2 PF AEMs with IEC 1.7, and the project nearly matched long-term stability with IEC 1.3. It would be great for the team to demonstrate longer life with IEC 1.7 power performance. The team also tested an MEA with low platinum group metals (PGMs) that meets performance goals.
- The spirocyclic materials have been made and tested, and the fuel cell performance meets the stated goals. The durability is highly questionable, and the inverse relationship between stability and IEC limits the power output because of the use of less conductive membranes. The possibility of using the spirocyclic polymers as electrode ionomers is an interesting idea, based on the initial results.
- Year 1 focused on the synthesis and evaluation of the polymer chemistry and evaluation of the MEAs. Given that it was follow-up work from the post-doc's chemistry work in graduate school, it was expected that most of the synthesis would have been done already, and in-depth MEA results evaluating the role of the different cations would have been the focus. However, this project can still be successful if this electrode work is the dedicated focus in year 2.
- A major milestone on MEA performance (0.6 V at 600 mA/cm^2 on hydrogen–air) was met, and another milestone was partially met on the durability target. However, after 500 hours of testing, the proposed spyrocyclic AEM with satisfactory initial area-specific resistance (ASR) demonstrated substantial loss of IEC and conductivity and became easily breakable. The mechanical properties have to be substantially improved.
- The first-quarter (Q1) milestone was not met; it was met at 500 hours instead of 1000 hours. The project team is testing some membranes at a relatively low temperature. Good peak power density (1.48 W/cm^2) was shown with AEMs of poor durability. When using the only reasonably stable membrane, the power dropped to 0.85 W/cm^2 at the same testing conditions. The proposed ionomer appears not to solve the problems laid out by DOE.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- Given the low scope of the project funding, it is difficult to expect much external collaboration. However, the principal investigator (PI) has wisely and excellently integrated the polymer into existing AEM efforts in order to benchmark against other polymers. This should continue.
- Though there is no direct collaboration, this project effectively leverages the AEM efforts of the Advanced Research Projects Agency-Energy (ARPA-E), the Membrane Working Group, and HydroGEN Advanced Water Splitting Materials.
- This is an NREL-only project, and outside partners are not needed at this early stage. NREL is well positioned to work with relevant partners when the time is appropriate.
- This is an NREL-only project, but there is good leveraging of existing related efforts at NREL.
- This is an NREL-only project, but there have been interactions with other institutions.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The development of advanced AEMs is of crucial strategic importance to reducing the cost of fuel cell systems and meeting overall DOE goals for decarbonization and reduced U.S. dependence on fossil fuels. This group of spirocyclic anionic polymers is an important candidate in the portfolio and should be explored.
- The project is designed to directly address DOE milestones for AMFCs. The proposed spirocyclic polymers offer a realistic opportunity to improve AMFC performance and durability.
- Spirocyclic AEMs show good promise and merit further development. There is great return on investment for this project.
- The project is highly relevant to DOE goals in the development of AMFCs that do not contain PGMs; the potential impact may be high.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program and DOE research, development, and demonstration objectives, but the proposed ionomer chemistry will not work well.
- The polymer is useful in that it uses a different cation from most other membranes, but there probably would be more direct ways of evaluating this phenomenon, and the polymer itself has poorer stability than the PI's other PF AEM ionomer. It is not promising as a base stable ionomer, given the IEC loss.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The planned next steps are reasonable, particularly the plan to further investigate the incorporation of spirocyclic ionomers into AMFC electrodes. Since the synthesis is limited to a single block copolymer structure, there is not much opportunity to mitigate durability issues by, for instance, adding spirocyclic cations to different backbones. Given the small budget, such synthetic options were probably never realistic.
- The PI plans to leverage the limited promise of the polymer to study it in electrodes, which makes good sense.
- The project should do more work on improving high IEC stability.
- The researchers have identified polymer stability as an issue, as well as the development of more advanced electrode ink formulations. However, there should be some fundamental analysis in the reduction of IEC capacity (and fuel cell performance) with increase in water uptake (as seen on slide 10). There are deep concerns about these spirocyclic materials: they have an inherently rigid backbone structure and form random three-dimensional fragments as they polymerize, which means they have to re-adjust to provide

continuous, directional ionic channels. In less rigid polymers, the polymer backbones are more flexible, and they re-adjust to enable functional groups to aggregate, forming more continuous channels. In addition, in spirocyclic systems, the backbones are so rigid that the channels cannot balloon as they imbibe more water. The rigidity is also an issue with long-term chemical stability. In any case, the reduction in ionic capacity with water uptake should be fundamentally studied. The project team should study why they are losing ionic continuity with greater water uptake.

- This ionomer has poor stability (at reasonable conductivity). It does not make sense to study it further; a new monomer structure with a spirocycle should be proposed.
- The proposed future plans are very vague and do not focus on the project's major issues.

Project strengths:

- This study is very attractive because of its ability to synthesize polymers with spirocyclic cations using a previously used synthetic route, and then subject the polymers to the same battery of evaluations already being used by NREL for other AMFC projects. This is an easy way to evaluate a promising new material set.
- The new chemistry was worth a shot and fit in well with existing work streams at NREL to study AEM polymers. Focusing on MEAs and understanding electrode phenomena is a good route going forward. The work overall helps the AEM space move forward.
- The spirocyclic functional groups look promising, based on their resistance to hydroxide attack; comparison to other ionomers will allow for selection of the best ionomer.
- This is an excellent, highly accomplished, very experienced research team. The work is of very high quality, and the team is well positioned to analyze this class of materials.
- There is great use of limited resources to probe the improved stability of spirocyclic AEMs.
- The project team has probably chosen the direction of the right cation type (spirocycle), but the specific chemistry has problems.

Project weaknesses:

- There is no inherent weakness. However, based on the results provided, there needs to be more fundamental work done to understand ionic conductivity in this class of materials. Results on slide 10 are counter to observations with other ionic polymers.
- The project's only weakness is the lack of synthetic flexibility. The spirocyclic cation was reported to be very stable, and it would be nice to be able to evaluate that stability on different polymer backbones, particularly ones without aryl ethers in them.
- The formation of solid residue during stability testing is an issue that points to instability in the polymer backbone. There needs to be an explanation for the absence of a correlation between IEC and conductivity losses for different ionomers. The interaction between the proposed AEM materials with catalysts remains unknown, though it is very important for making a decision to continue work in this direction. It is unclear how the addition of spirocyclic groups will affect the cost of an AEM or whether the performance improvements justify the cost increase. Strictly speaking, the best results have been obtained for cyclic, not spirocyclic functional groups, so the latter's advantages remain unproven.
- The project team needs to do more complete characterization of copolymer structure, blocks, and improving stability in high IEC.
- The authors did not answer key questions, including why increasing the IEC from 1.3 to 1.7 mmol/g caused significant durability issues or why the conductivity was poorly correlated with the IEC.
- The polymer chemistry is not terribly successful at being base-stable. It has limited promise as a candidate for widely distributed AEM use.

Recommendations for additions/deletions to project scope:

- The project needs to do more fundamental study of water uptake, ionic conductivity, and morphology of the polymer, as well as identification of what mechanisms result in the loss of ionic continuity with water uptake. The team may possibly need to do some work with reinforcements to reduce dimensional changes during water uptake and determine whether ionic continuity can be maintained.

- If it is not already planned, there should be an investigation into why the spirocyclic AEMs with higher IECs are less stable than the ones with lower IECs.
- The study of the interaction between the catalyst and spirocyclic polymer material should be accelerated, and the cost analysis has to be performed.
- The project team should try another backbone or ionomer structure with a spirocyclic cation.
- The team should leverage the unique cation structure to understand electrode phenomena.

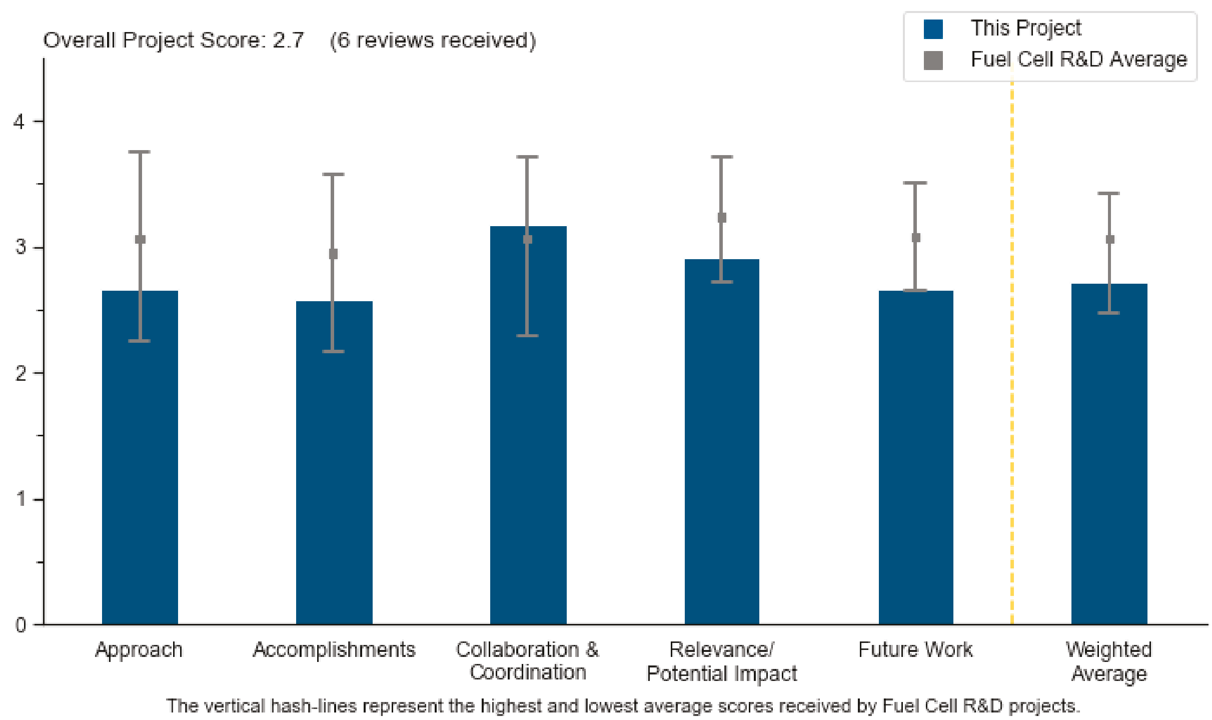
Project #FC-179: Lab Call Fiscal Year 2018 (Membrane): Stable Alkaline Membrane Based on Proazaphosphatranes Organic Super Base

Gao Liu, Lawrence Berkeley National Laboratory

Brief Summary of Project

Lawrence Berkeley National Laboratory (LBNL) is developing new alkaline membranes with improved stability and performance to enable a platinum-group-metal-free (PGM-free) alkaline-membrane-based fuel cell. In addition, proof of concept will be derived for proazaphosphatrane superbases in alkaline membrane applications. The project team has identified a stable and flexible polymer matrix constructed from these superbases; the material demonstrated superior stability in high alkaline conditions. The project has also developed a feasible process to synthesize the superbase-grafted ionomers by connecting the superbases to Kraton Corporation (Kraton) copolymers via methylene chloride modification. The project team plans to address membrane synthesis and membrane electrode assembly (MEA) development and testing in the next phase.

Project Scoring



Question 1: Approach to performing the work

This project was rated **2.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach of adding a superbase group to commercial polymer is a wise choice for this project. It is very good that quantifiable technical targets are stated.
- The project is based on the assumption that the stability and high alkalinity of a proazaphosphatrane organic superbase would result in highly conductive and durable AEMs. These superbase units were grafted to a stable polymer backbone to make them highly conductive and stable against thermal and chemical decomposition. The structure of proazaphosphatranes could be modified to exclude tertiary carbon atoms and thus improve stability.
- The team's approach of using a stable and highly basic organic superbase is excellent. Instead of quaternary ammonium cations, an organic superbase may work for anion exchange membrane (AEM) fuel cells.

However, proazaphosphatranes may not be an ideal superbase, as the molecules are bulky and possibly difficult to make. Tethering the superbase in all hydrocarbon (polystyrene-based) polymers is also a good approach. However, the reaction in the bromoalkyl group will produce the benzyl cation, which would make the polymer unstable.

  - There is not a clear pathway to reach the initial conductivity target (>100 mS/cm, which is better than an ammonium-based system). The pH of the proposed material (1.0 M) is 14, a level similar to ammonium (1.0 M); but the size of the molecule is much larger, which makes it hard to produce a high-ion-exchange-capacity (IEC) membrane.
  - The solvation energy of the cation will likely be low. Therefore, the conductivity of the AEM tethering this superbase will be much lower than that of an ammonium-based system. The principal investigator (PI) should provide a more specific approach to achieving the milestone, rather than just making a general statement based on the funding opportunity announcement.

- The approach is acceptable; however, the project team will not actually make membranes until the project is almost over. The previous work is important, but it is hard to see how the team is going to obtain sufficient results to motivate additional work.
- There are serious concerns about the wisdom of the work in general. Using cations with high molecular weight limits the IEC of a final membrane (such as in the work of Coates) and raises serious concerns about the promise of the membrane to be sufficiently conductive. The literature has suggested that smaller existing N-based cations are sufficiently stable and that attaching them to a polymer backbone in a way that makes them stable should be the focus of AEM work at this point. Also, many groups appear to be close; perhaps focusing on upstream applications of AEMs (such as how they degrade or affect electrode performance) should be more of a focus. However, given the idea, the approach has been generally good, if slow. Testing cation stability as a model system and then leveraging existing styrene copolymers is the right way to evaluate new cations.
- It is unclear why the organic superbase would have improved stability in an aqueous AEM application.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The route to a superbase-grafted polymer has been identified, and surrogate or precursor compounds have been synthesized. The team has studied potassium deuteroxide (KOD) stability with a small surrogate molecule. The project timeline may not allow much time for MEA characterization once the polymer is produced.
- So far, most of the work has been done on synthesis and the stability study of model monomeric compounds. The functional group loading that was achieved is too small. It was shown that the methyl-group-functionalized superbase is stable for four months (after that, some changes in the nuclear magnetic resonance [NMR] spectrum are visible), while the lifetime is less than two months for an isopropyl derivative. The methylene chloride modification to the Kraton polymer was successful, but the reduced polymers were either gels or extremely brittle films.
- The results shown were interesting, but the stability of the materials made to date does not appear all that exceptional. It is not clear that these high-cost materials are worth pursuing. Additionally, the team has not actually made any of the proposed polymers, even though the project is more than half over.
- The progress of this project is rather slow. All that has been accomplished is to check the alkaline stability in a small molecule study. The accomplishment is on the level of a preliminary result before starting the project. It is unclear why the PI spent so much time on the stability of proazaphospatrane derivatives. It turned out that more complex proazaphospatranes have lower stability. The project will not likely meet even the membrane stability target (2,000 hours). The PI will likely not be able to show a fuel cell performance of 620 mA/cm^2 at V = 0.60 V by the end of the project.
- The methyl stability results are confusing. The hydrogen NMR plots show shifts of peaks and new peak growth but are claimed to be stable. There is no clear way to rationalize this. As for the polymer stability, it is not clear that 10 eq $NaOCH_3$ is the best solution for an aging study. It is not clear what the details of that study were or if they were just used as a reference point. The team stated that the copolymer T_g is too low, but no data were presented to quantify the T_g. The details of the membrane casting were not given, so it is

not possible to quantify whether the processing could be causing poor membrane properties. The team tested the Kraton copolymer, but there are no data to suggest that this would be a better material than the initial copolymer tested. It is unclear whether the decomposition rate is good or bad.

- After well over a year of effort, no polymer has been made yet. This work should have been proceeding along with the model compound stability study, but the effort appears to have been sequential. Understanding the promise of the approach requires that evaluation be done in a polymer, especially given the bulky and high-molecular-weight cation; the lack of evaluation severely diminishes the project.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- This is a lab call project, so a minimum level of collaboration is expected. Obtaining materials from Kraton is a good thing for the project. Collaborating with other teams is also a good thing, although the other teams' efforts on this project are minimal so far.
- Despite the modest budget, the team has managed to include three groups at LBNL and a commercial partner (Kraton).
- The project team seems to have relevant partners at LBNL, though perhaps it would be wise to include Ahmet Kusoglu (of LBNL) for some membrane characterization, specifically given the mechanical issues that have been identified. Maybe Kusoglu is assumed to be a part of Adam Weber's team at LBNL.
- The collaboration between team members seems to be working, though a collaboration outside the project is desirable for cost evaluation of the proposed functionalized polymers.
- There is really only one partner (Kraton) that appears to be just a material supplier. However, this is acceptable for a lab call project. Kraton has supplied materials.
- The PI has done well to leverage external polymers as a platform to which to attach his cations, but little tangible progress has been made yet.

Question 4: Relevance/potential impact

This project was rated **2.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- If successful, the project will lead to the development of high-performance alkaline membranes and, based on those, fuel cell systems that would be competitive with current fuel cell systems using Nafion polymer electrolyte membranes. The use of alkaline membranes could lead to replacing Pt-based catalysts with PGM-free ones.
- It seems like there should have been more funding. The project team seems to be addressing current stability problems with available alkaline membranes.
- If the project is successful, then it will have a potential impact on several different areas of the DOE Hydrogen and Fuel Cells Program. The general approach of this project—using organic superbase instead of ammonium—has been tried by groups before, but it has never been successful because of the synthetic complexity and other reasons. It is very challenging to make a reasonable system using superbases. Based on the project's progress so far, the potential impact does not look great.
- The DOE should fund AEM fuel cell work, but it is not clear why this particular AEM approach was funded.
- The project aligns with the DOE's goals of supporting stable AEM research, but it may not be the most successful way to go about it.
- The benefits of using a superbase are unclear.

Question 5: Proposed future work

This project was rated **2.7** for effective and logical planning.

- The future work is focused on synthesizing and evaluating actual polymers, which are sorely needed in this project; this is the correct direction.
- It would be good to see an MEA performance evaluation.
- The team should strive to make membranes as soon as possible to obtain sufficient results to potentially motivate additional work.
- The stated goal is to increase the superbase loading to 30%. It is hard to tell if this is a reasonable goal. Assuming this is possible, the equivalent weight or expected IEC would still need to be determined. This would help quantify whether this 30% goal is adequate, too low, or too high.
- The future work is focused on the development of a superbase polymer based on a polystyrene-hydrogenated-polyisoprene backbone. The work plan is rather generic and based on milestones that have been missed or are yet to be met.
- Most of the proposed future work is unrealistic. The PI has not had any reasonable membranes from this project so far. The PI cannot finish all the tasks and milestones in the years remaining. The project team aims to continue with the stability of the superbase in 2M KOD in a D_2O solution, which has been done extensively during the past year. The PI should stop this task and focus on making AEMs with the superbase and measuring the target properties.

Project strengths:

- The researchers are taking a smart approach to this project in addressing membrane stability, which seems to be one of the primary challenges with alkaline membranes.
- The proposed proazaphosphatrane functional groups that are tethered to a stable hydrocarbon-only backbone could potentially lead to highly stable AEMs and durable fuel cells that use such membranes.
- Leveraging existing polymers to use as a platform for the new cations is a good idea. The evaluation of cation stability has shown some promise in terms of stability.
- The project's strength is in the concept. This is a new idea and a challenging project.
- The team is good, with relevant backgrounds and experience.
- This is a good team with an interesting idea.

Project weaknesses:

- The only weakness is that there has not been any investigation of membrane structure or mechanical properties.
- The proazaphosphatranes are expensive to make and hard to attach to a polymer backbone. Their bulkiness makes creating strong and flexible membranes very hard; this may be a fundamental problem that should be solved by selecting the right backbones. So far, the project has encountered multiple synthetic problems, such as a low level of modification of the styrene units and unsatisfactory mechanical properties of the films. There is no apples-to-apples comparison of stability between the proposed proazaphosphatrane groups and the known functional groups that are much less expensive. Therefore, it is unclear what benefits these groups could bring. The cost analysis of the proposed polymer materials should be done based on synthetic schemes.
- The project's progress is way behind. The PI did not accomplish the milestones for the third or fourth quarters (Q3 or Q4) for fiscal year 2018. There is not much hope for obtaining the rest of the milestones within the project's schedule and budget. The targets for the proof-of-concept project are inappropriate. The PI may not have enough capability to make polymeric materials.
- The work has shown no comparison with baseline benzyltrimethylammonium or other cations to evaluate the base stability of the designed cations. The progress on polymer chemistry has been slow.
- The team is not planning to work on any actual membranes until too late in the project.
- There is not much support (e.g., literature, models) for the advantages of the superbase.

Recommendations for additions/deletions to project scope:

- In the limited time remaining, polymer chemistry is the correct focus. Given the limited funds of the project, no additions/deletions are recommended.
- No additions are recommended. The PI should focus on making stable alkaline superbase AEMs and characterizing the AEM conductivity and stability for the rest of the project's time. The team should not waste more time on investigating the stability of the superbase. The project should not invest time in making MEAs or evaluating cell performance and durability. The team should not investigate more robust connections between the superbase and polymer matrix. If this team shows that the superbase can replace the ammonium-functionalized AEMs with comparable hydroxide conductivity, then this may be a valuable outcome for the project.
- The funding was limited, but the project would have benefitted from some additional modeling to show how a large superbase group would affect phase-separated morphology. Ahmet Kusoglu and the LBNL Advanced Light Source team would be able to look at this and should be considered.
- Cost analysis should be added to help with understanding the cost-competitiveness of the proposed AEMs. The next period of funding should be based on meeting the go/no-go milestone, which does not currently look achievable.
- The project team should accelerate the fabrication of the membranes.

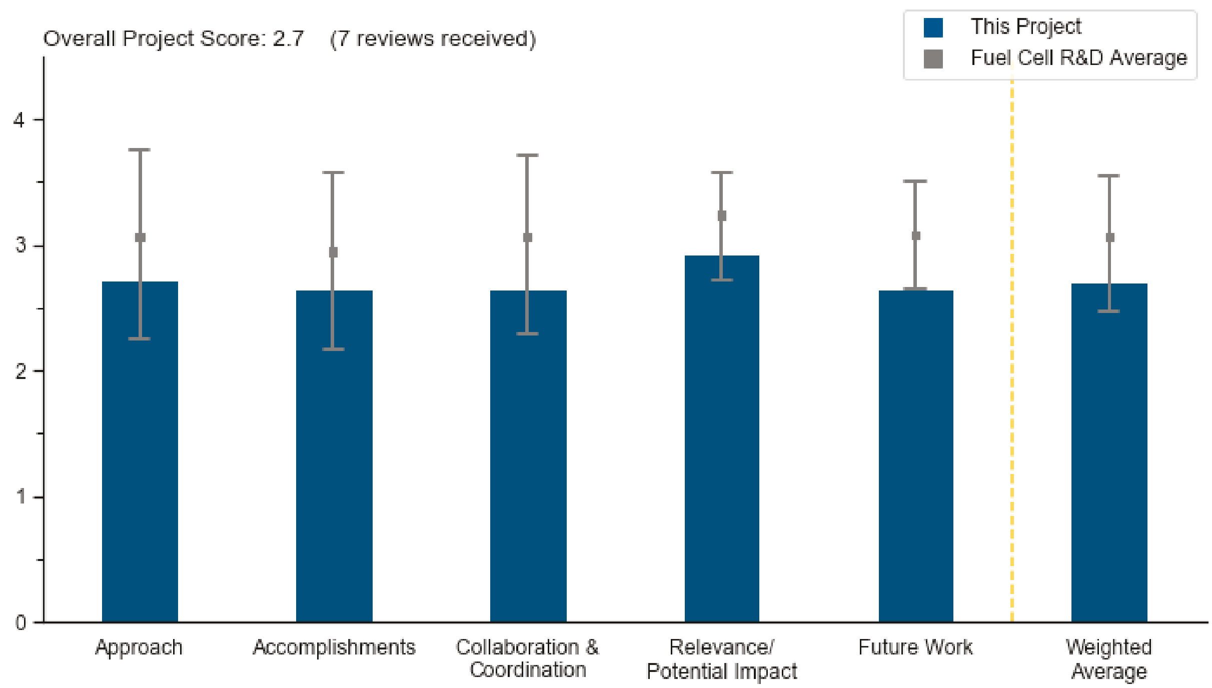
Project #FC-180: Lab Call Fiscal Year 2018 (Membrane): High-Performing and Durable Pyrophosphate-Based Composite Membranes for Intermediate-Temperature Fuel Cells

Cortney Kreller, Los Alamos National Laboratory

Brief Summary of Project

The project objective is to develop a membrane that enables system operation at higher temperatures (200°C) and low relative humidity (RH) with conductivity across the entire range of operating conditions for transportation applications. To do this, the project will tailor the composition of MP_2O_7 (metal pyrophosphates [MPPs])/polymer composite membranes to achieve the U.S. Department of Energy target for membrane area-specific resistance (ASR) of ≤0.02 Ωcm^2. The project addresses the barriers of developing an early-stage membrane concept that can (1) decrease system costs by operating at higher temperature (150°C–400°C), (2) achieve membrane ASR of ≤0.02 Ωcm^2, (3) achieve ASR ≤0.03 Ωcm^2 under low RH conditions, and (4) achieve sufficient conductivity (0.2 → 0.02 Ωcm^2) across the entire range of operating temperatures.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **2.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is addressing mainly system cost reduction, thanks to the development of membranes for fuel cell operation at higher temperatures (about 200°C). It is basic research, based on a material identified a few years ago showing the capability to conduct protons at high temperature and ultralow humidity. The approach is clearly defined; the idea is to make a composite membrane that enables conductivity in the whole range from ambient temperature to 200°C. Nafion™ is a planned part of the composite; current work is focused on the high-temperature side, with the modification of the original material identified at the beginning of the project. SnP_2O_7 has been modified by replacing part of the Sn with various metal cations to improve conductivity. In and Sc have been selected. The integration of the new materials into composite membranes should be done in the coming months. Collaboration for the integration of the membrane into a membrane electrode assembly (MEA) is considered in the approach. A major risk will be getting a thin membrane that does not present the required mechanical or electrical properties on the broad temperature range.

- The project's approach is to produce intermediate-temperature MPP proton conductors, evaluate trends in phosphorous-to-metal (P:M) ratio, produce membranes, and minimize thickness. This is a logical progression with the modest budget.
- The team has followed its research plan and executed it. They have synthesized the MPP materials and made membranes. They have begun to characterize performance.
- The project proposes to develop MPP or polymer-composite membranes with low ASR and the capability to work at 200°C. The main focus was on the effect of substitution on MPP conductivity. However, the data obtained showed that the unsubstituted material has one of the highest conductivity values.
- The objectives are clearly identified, although it is hard to see how this differs significantly from previous work putting other inorganics, such as heteropolyacids, into polymer membranes. If these can conduct protons without water present, that is potentially interesting, but achieving conduction through a matrix of dry Nafion may prove to be very difficult.
- It is not clear when the go/no-go should be completed. Since the project started in January 2018, it seems like the third quarter (Q3) and Q4 milestones should have been completed by the time the slides were due, but it was reported that they were 0% complete. It seems that the team is far behind schedule. It was nice that quantifiable metrics were presented. It seemed like the precipitation method is good because of low temperature.
- The justification for the MPP–Nafion composite membrane does not make sense. It is an interesting idea to have a composite membrane with different conduction pathways as a function of temperature, but the sulfonic acid moieties in Nafion (or another perfluorosulfonic acid [PFSA]) will start to degrade at 200°C, and the PFSA will flow significantly at more intermediate temperatures, such as 120°C and above. It is highly unlikely that such a composite membrane would survive hot and cool cycles without changing morphology, and no proof of concept has been demonstrated in more than a year of project funding.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Good progress has been made toward the project's objectives, with preparation and characterization of various materials going as planned, allowing the project team to select two new ones to be integrated into a membrane.
- If these membranes reach their technical targets, the project will actually contribute to cost reduction as targeted by DOE.
- There is good progress on a variety of metals materials produced. Conductivity has been measured, but there are no results on membrane fabrication.
- A variety of MPP materials have been synthesized and appropriately characterized. The Q3 milestone will be the real indicator of whether this approach is feasible.
- The particle component appears to have been well researched and optimized, but no work on the composite has been undertaken. The entire proof of concept is left unfulfilled at this point.
- It seems there is no trend in conductivity and P:M. Another issue that was identified is that it is not possible to compare dopants unless they are at the same P:M. Bulk pellet conductivity is the primary result related to the go/no-go. There is great concern that since the pellet conductivity is not that much higher than the go/no-go, it will not be possible to achieve the go/no-go when the MPP powder is blended into the polymer.
- As of yet, the main focus has been on the development of conductive MPP materials, with little success on MPP or polymer membrane development. Even the most conductive materials (which are actually not much better than the starting SnP_2O_7) could not achieve the project goals unless they were to be converted into thin composite membranes.

- The data provided was sparse, with only a few slides and limited data points. Based on the data provided, it is hard to determine whether this technology pathway has merit. The impedance and conductivity data appear to be sufficient to down-select a few promising candidates and perform additional testing.

Question 3: Collaboration and coordination

This project was rated **2.6** for its engagement with and coordination of project partners and interaction with other entities.

- There seem to be many team members on a project with a small amount of funding. The team members' roles were not discussed, so it cannot be determined whether all the team members are needed. The low level of funding clearly limits the project team's ability to collaborate with other organizations, so this being a Los Alamos National Laboratory (LANL)-only project seems reasonable.
- One national laboratory is doing the job; however, this is acceptable. UNM is interested in evaluating the membrane as a no-cost partner, and the project team is planning to solicit more partners once the proof of concept is established.
- All the work to date appears to have been done at LANL. The University of New Mexico (UNM) is a partner whose work, evaluating the materials for a specific application, occurs later in the project.
- This project is a laboratory-only call, but the team has a no-cost partner: UNM.
- The project has no partners yet, but this makes sense, given its pre-proof-of-concept status and the fact that it is funded through a lab call.
- Though this lab call project is open to national laboratories only, the project could greatly benefit from collaboration with material scientists and polymer chemists outside the project.
- No collaboration has been undertaken so far. UNM is on the list as a collaborator, but they are described as interested in testing the final product, rather than being meaningfully involved in its generation.

Question 4: Relevance/potential impact

This project was rated **2.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- High-temperature materials for proton-conducting membranes may play a huge role in reducing the balance of plant size and cost, if the ASR and durability targets are met. The proposed polymer electrolyte membrane (PEM) work is at 200°C, which is higher than the optimal temperature for automotive applications, so the system modeling should be done to understand these trade-offs.
- The project team is addressing the barriers that were outlined in the proposal call. The materials seem to have some advantages since they do not require phase change.
- The proposed membranes have the potential to achieve several DOE technical targets and could have an impact on fuel cell design for transportation.
- There is a strong need for intermediate-temperature fuel cells. The proton conducting is novel.
- The core aspect of the project aligns with the goal for system cost reduction. The impact will be positive if the technical targets are reached; the work will have to be continued to enable assessment of the actual potential impact.
- Identifying fuel cell materials that can perform at higher temperatures has inherent value. The question is, of course, whether this group of materials has inherent promise and can provide a pathway to achieving this overall technical goal. The data provided are inconclusive.
- The concept could perhaps be adapted, but as designed, there is no pathway to success that can be seen for a particle–Nafion composite membrane to perform as described.

Question 5: Proposed future work

This project was rated **2.6** for effective and logical planning.

- The researchers have clearly identified what they need to do in terms of making membranes and testing them going forward.

- The plans for next steps are consistent with the original project objectives and the results reached on the new materials during the first period. Materials selected will be implemented in composite membranes for further characterizations. The features identified for validating these membranes are conductivity and thickness; mechanical properties and permeation are missing and should be added to the characterizations to be conducted.
- The future work is satisfactory to attempt to prove the concept.
- The problems with dispersing powder in polymer are concerning, and this needs to be addressed. However, given what seems to be the low conductivity of the MPP powders, it seems that more effort should be focused in this area to achieve higher MPP conductivity, in anticipation that the composite membrane will have lower conductivity than the MPP pellets.
- Milestone 3 will be critical to demonstrating success. Fabricating composite membranes will be tricky, and the presentation does not say much about the anticipated challenges and mitigation strategies.
- It does not seem certain that the year 1 go/no-go criteria will be met.
- The proposed future work targets PEM development, which should be done in year 1, but no MEA work or testing has been done or is planned.

Project strengths:

- The strengths of this project are the good methods that have been applied with systematic analyses and conducted for the selection process, and the actual identification of materials that are potentially able to improve membrane conductivity at high temperature and ultralow humidity.
- The LANL team has tremendous experience in evaluating new materials for PEM fuel cells, and the proposed materials have potentially very advantageous properties.
- The proposed MPP demonstrated high conductivity, and an MPP–polymer composite membrane could potentially work at higher temperatures than conventional PFSA PEMs.
- The use of polyphosphate phases is an important area of research. LANL has the resources and is well placed to do this work.
- The project has a good approach and development of various metal-containing materials.
- The strategy to use materials that do not require a phase change seems like a wise approach.
- There is strong optimization on the inorganic piece of this project.

Project weaknesses:

- For 15 months of full-time activity, the total output seems low. It would have been nice to have more data on actual membranes in situ and in fuel cells to determine the viability of this technology. The project needs a big spur of activity in the next 7 months. It may be that the materials are inherently difficult to work with, and progress will be inherently slow, in which case, this needs to be mentioned. If not, in situ fuel cell data would be great to have as early as possible in the project. There is nothing comparable to in situ, real-life operating data.
- One issue is that after more than 15 months, no composite membranes have been made with new materials. This should be fixed soon. It could be difficult to reach the target of 100 mS/cm with a composite membrane when this is the level that was obtained with just the material alone in pellets. It is also not so obvious that the Nafion will ensure the required conductivity at low temperature with ultralow humidity. A major weakness is the risk of getting composite membranes with poor mechanical properties or permeation, but the project does not seem to consider this aspect.
- It seems that the results are lacking, and the project is behind schedule. It seems like it may be hard for the project to meet the go/no-go point with the MPP materials that have been synthesized so far. It seems there should have been a stronger focus on integrating materials with ionomers since that is part of the go/no-go, though that may only be clear now because of unanticipated challenges with blending.
- It is still unclear how to convert good material conductivity into practical, flexible, and durable composite PEMs with the target thickness and ASR, or how the catalyst activity will be affected by interaction with such membranes. As of yet, the major focus has been on material improvement, although issues with manufacturing the thin composite membranes were not addressed.

- It may be difficult to load Nafion with an inorganic material and get it evenly dispersed without compromising the mechanical properties of the membranes. There are many MPP formulas from which to choose, but discussion on how to prepare composite membranes is limited.
- There does not seem to be a clear strategy for producing the membrane. There may be binders or fillers that need to be added to facilitate sintering. It is not clear what the prospects are for achieving the desired thickness.
- There is a lack of understanding about the behavior of Nafion. There is no collaboration in the design of the experiments.

Recommendations for additions/deletions to project scope:

- The first recommendation is to speed up the process for making membranes with the selected materials. In addition, it is recommended that the team add mechanical properties and permeation as criteria for validating the composite membranes. The project team should also consider integration in MEAs as an important objective. If needed to save resources, the project team could decide to work with only one selected material to enable more membrane and MEA optimization and characterizations.
- The project could consider another (uncharged) binder that serves simply as a matrix for the particle material. This would limit conduction to higher temperatures but could be more successful than trying to find a membrane to conduct across a wide variety of temperatures. For example, hydrocarbon ionomers that could be more resilient to flow at high temperatures would require higher water content to be conductive at low temperatures.
- The scope is appropriate, but most of the effort should be focused on increasing the conductivity of pellets and on the challenges of blending MPP powder into polymer.
- If it is not already planned, the team should include a study of how water-tolerant the composite membranes are. It needs to be determined whether the MPP will leach out if the membranes are used in a fuel cell that operates briefly at high RH.
- The project team needs to identify a route to creation of the membrane, including strategies for barriers and mitigation.
- The project seems to be lagging behind the original schedule, and the go/no-go milestones were not met.
- The project team needs to make membranes and test them as soon as possible.

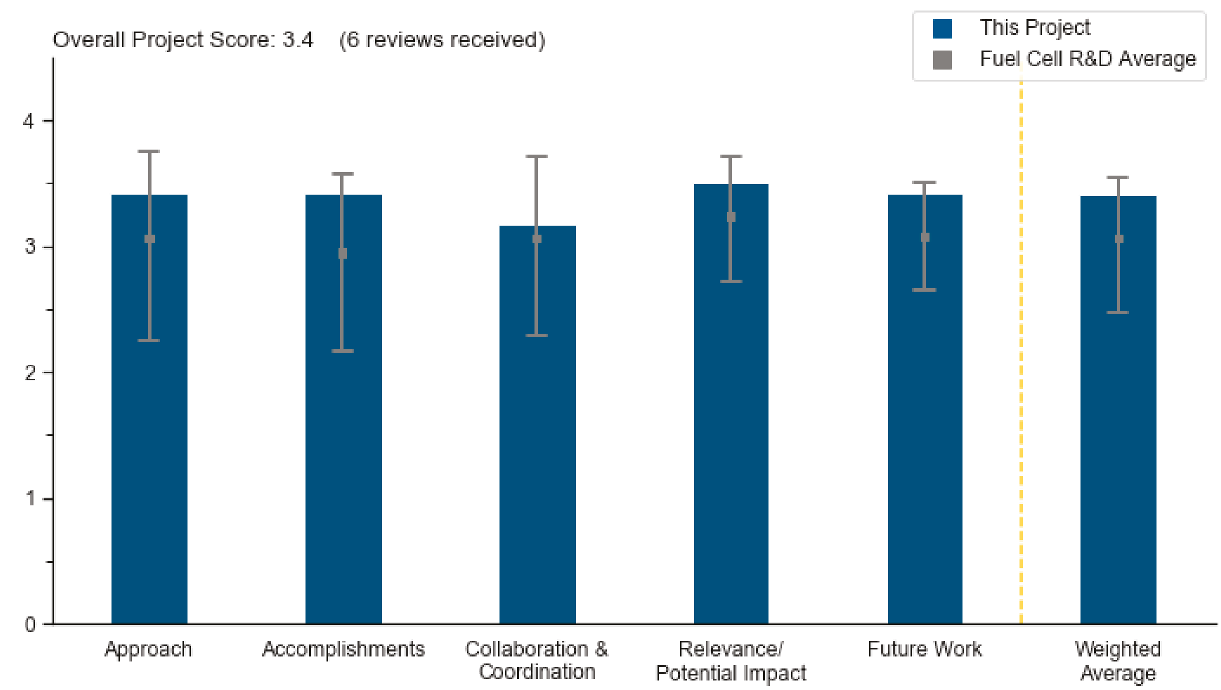
Project #FC-181: Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Microstructured Electrodes and Diffusion Layers for Enhanced Transport in Reversible Fuel Cells

Jacob Spendelow, Los Alamos National Laboratory

Brief Summary of Project

The objectives of this project are to enhance the H_2O and O_2 transport for unitized reversible fuel cells (URFCs), as well as fabricate, test, and validate these devices for high performance and durability. The UFRCs use amphiphilic electrode structures, diffusion media, patterned gas diffusion layer (GDL) substrates, and microporous layers (MPLs) to address transport challenges. Patterned hydrophilic/hydrophobic GDL substrates, MPLs, and catalyst layers (CLs) are used to construct an amphiphilic membrane electrode assembly (MEA) to achieve improved fuel cell and electrolyzer performance and rapid switching between fuel cell and electrolyzer modes.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The team proposes a novel approach for designing electrodes to enhance the transport property of URFCs. The optimized electrode structure is made of hydrophobic and hydrophilic channels to address the challenges of water management, satisfying both electrolyzer and fuel cell modes. Electrode structures composed of micropatterned amphiphilic GDLs and MPLs are expected to bring enhanced transport of H_2O (through hydrophilic channels) and O_2 (through hydrophobic channels), which ultimately results in improved performance in URFCs that require rapid switching modes between electrolyzer and fuel cell.
- The approach proposed is sound and fundamentally relevant to DOE targets. The idea of patterned electrodes is brilliant and should be explored further. The main aim of the work is to improve performance of reversible cells. Cost and durability are not yet addressed in this year's work. It is vital to understand

which would be the most important degradation phenomena related to the mutual interactions of the hydrophobic and hydrophilic MPLs.

- The principal investigator's (PI's) approach to achieving high activity in water electrolysis and fuel cells is to locally pattern the GDLs and MPLs and electrodes to make them hydrophobic and hydrophilic in different regions. This approach is sensible and appears to be working well. The outcome of this project along with other approaches can create MPLs for oxygen evolution reaction on titanium-based electrode layers that will help with water management. This is cutting-edge work.
- The use of an amphiphilic electrode structure is a clever idea to balance the needs of reversible fuel cell technology. The use of a patterned electrode structure to achieve balance between hydrophilic and hydrophobic needs is also very promising.
- The project focuses on a fundamental issue of URFCs: absolutely different humidity requirements for fuel cell and water electrolyzer modes. The proposed approach is logical, and the preliminary results confirm the assumptions.
- The fixed-polarity approach has not been sufficiently justified. From a system design standpoint, the fixed-gas approach appears more robust. The approach of trying to develop catalyst supports to enable increased performance with decreased loading is good.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project is on track and making good progress. The atomic layer deposition of Ir and Pt on TiO_2 appears to be resulting in high-quality catalysts, but unfortunately, the hydrogen oxidation reaction durability was poor. It would have been good to have seen data on the effect of catalyst loading on performance and durability since the TiO_2 support may be helping in this area. The down-selected physical mixture of Ir and Pt black seems to be performing well, but this is a conventional catalyst for reversible fuel cells, so the result is expected.
- Hydrophobic/hydrophilic patterning of GDLs via polytetrafluoroethylene (PTFE)/Nafion™ has made significant enhancement in the fuel cell mode of URFC performance under different relative humidity (RH) conditions, and its impact is greater, particularly at highly flooded conditions. In electrolysis mode, the amphiphilic electrode structure also showed improved performance compared to hydrophobic MPLs treated with PTFE alone. DOE has funded a number of URFC projects in the past. Although optional, a comparison with previous funded projects would be helpful for the reviewers and audiences to understand the importance of this project's progress.
- Progress in making structured electrodes with amphiphilic structure is very good. The results are encouraging. The MPL design and fabrication progress is very good. This can help meet DOE goals for reversible fuel cells. The direct blade coating data look good.
- Project accomplishments are very good. Go/no-go criteria are met. Improved fuel cell performance is seen when TiN-treated Ti felt is used and when hydrophobic/hydrophilic treatments are applied to the GDL. Effects are especially significant in fuel cell mode at high RH, when flooding is likely. A greater focus on confirming the major role of water–gas transport in achieving these results, perhaps via computational models that were apparently used at the start of the project, would be helpful.
- The proposed hydrophobic/hydrophilic patterning improves URFC performance in the fuel cell mode, even at high RH, while not decreasing the performance in the electrolyzer mode. The go/no-go criteria have been met, though the round-trip efficiency is very low.
- Accomplishments are relevant to DOE goals, and the project is fairly on time with milestones.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- Collaborations with the Fuel Cell Consortium for Performance and Durability (FC-PAD) and others on electrode microstructure appear to be good.

- The collaboration with Argonne National Laboratory on catalyst development is quite useful.
- It was mentioned that there is collaboration with multiple DOE projects, but it would be useful to hear more elaboration on their roles and outcomes from the collaboration.
- An industrial collaboration would be beneficial to understanding the scalability of the idea.
- Industry partnerships are highly productive when used smartly. There is no industry partner so far.
- Collaboration with other organizations is limited and could be improved.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Sustainable hydrogen production via water electrolysis and its use via fuel cells, the basic concept of URFCs, would be ideal to address this challenge, but device configuration satisfying both modes is not trivial. Because electrolysis and fuel cells require different levels of water management, their electrodes should be constructed differently. This project proposes an optimized electrode design satisfying both modes.
- Reversible fuel cells are very relevant for energy storage to support greater penetration of renewables. This project provides an opportunity to increase round-trip efficiency. It can also lead to new applications for hydrogen and fuel cells.
- The proposed method could be instrumental in making URFCs that work equally well in both operational modes. Such URFCs could find a wide application in long-term energy storage.
- The project appears to be having significant impact on improving URFC technology, particularly for low-temperature operation.
- Work on reversible fuel cells is extremely relevant to DOE multiyear goals.
- The fixed-polarity approach needs to be better justified to demonstrate the relevance of this work. However, the project is demonstrating good reversible fuel cell performance, which is relevant to the DOE Fuel Cell Technologies Office's increasing emphasis on H2@Scale.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work seems well planned. The approach of investigating separated Pt/TiO_2 and Ir/TiO_2 is good. The work on examining operating conditions and components such as diffusion media and flow fields should be helpful to the community.
- The use of neutron radiography for water management is a nice idea. The synthesis and testing plan is good.
- The project is on track, and the team is well aware of the challenges ahead and offered a number of mitigation strategies. Particularly, scalability of the technique is certainly of importance.
- The team is aware of what the current project lacks and has a detailed future work plan to tackle those weaknesses.
- The PI's proposed future work seems sensible and appropriate.
- The future work plan is satisfactory but not very specific, and it lacks technoeconomic analysis.

Project strengths:

- The project brings together significant expertise in creating and adjusting electrode microstructure to achieve desired behavior for the disparate needs of water electrolysis and fuel cell operation. The work with Ti electrodes is very important and likely to provide guidance to others working on related problems.
- Patterned electrodes and microstructural design are highly relevant for reversible cell performance improvement.
- There is good technical progress so far. The team met the go/no-go milestone. The dual-function electrode performance is good. Amphiphilic electrodes provide a wide range of operation.

- The project is focused on the right critical issue of URFCs, and the proposed approach seems to be working.
- LANL uses a novel approach with solid work progress.
- This is a strong team with a good background in both fuel cells and electrolysis.

Project weaknesses:

- The preliminary data look very promising. A comparison with other earlier DOE-funded URFC projects would be helpful.
- The project work presented at this Annual Merit Review lacked a significant modeling component, and because of this, most findings are interpreted somewhat qualitatively. Results demonstrating improved performance are claimed to be due to improved water–gas transport, but they could be explained by other factors. Now that the PI has data using patterned electrodes, he may find it useful to go back to the models and see if they offer predictive capability that would link specific experimental observations with specific physical mechanisms. In turn, this work could suggest pathways for further optimization.
- URFC performance in the two modes is not symmetrical. Using the proposed technology for energy storage will result in overdesign of the system to match the charge and discharge power and times. The effect of channel alignment/misalignment of GDL, MPL, and CL is unknown and should be studied. The UFRC modeling using real grid data should assist in the system design. The development of bifunctional electrocatalysts is not in the project scope, so cooperation in this area is highly desirable.
- The core approach of using fixed polarity has not been adequately justified.
- There is uncertainty in fabrication cost and degradation performance.
- There is a lack of industry partnership durability data, which would be helpful.

Recommendations for additions/deletions to project scope:

- Technoeconomic analysis of the proposed patterned MEA and stacks should be added to the work scope.
- It is recommended that the team investigate quality and durability of the local structure of amphiphilic electrodes after numerous cycles of electrolyzer and fuel cell modes.
- It is recommended that the team consult with an industrial partner.
- Adding durability data in the work plan will be useful.

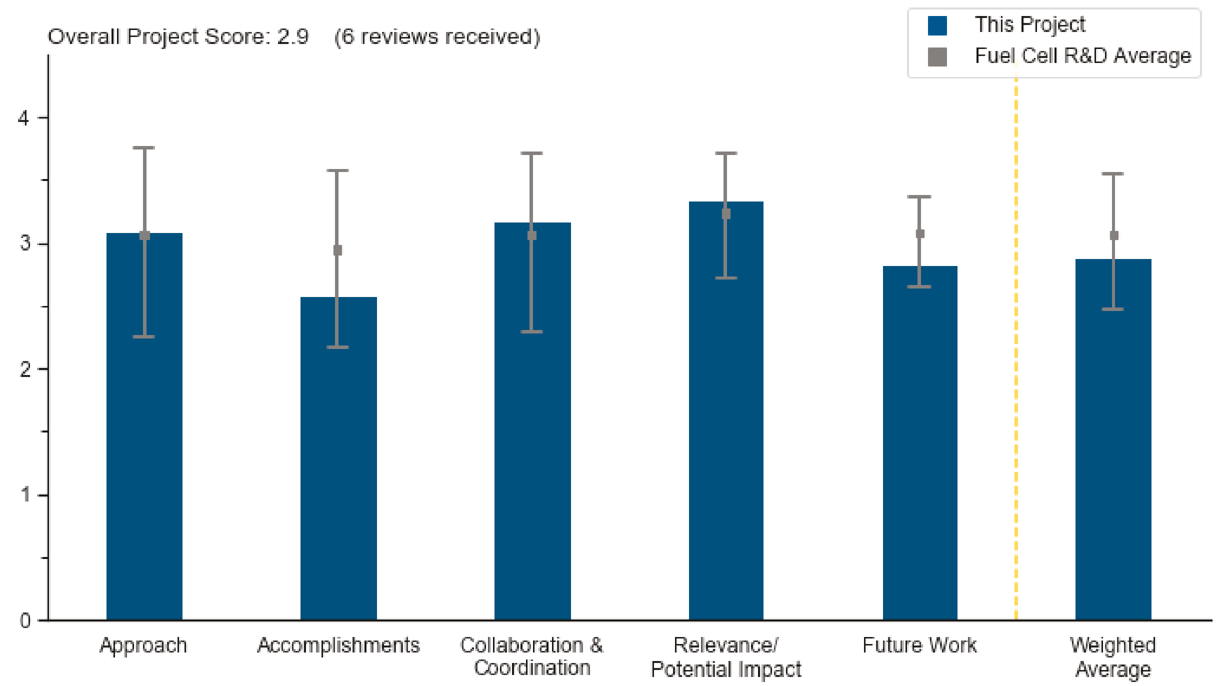
Project #FC-182: Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Bipolar Membrane Development to Enable Regenerative Fuel Cells

Todd Deutsch, National Renewable Energy Laboratory

Brief Summary of Project

This project directly addresses the Fuel Cell Technologies Office's interest in developing reversible fuel cells (RFCs). The project objectives are (1) to fabricate a bipolar membrane (BPM) with a dual-fiber electrospun junction that can be employed in a stable, high-performance RFC membrane electrode assembly (MEA), (2) to fabricate and optimize the BPM junction with available materials (leveraging others' ongoing development), and (3) to obtain BPM device data in both fuel cell and electrolysis mode. The effort will focus on optimizing the BPM junction interface. The project addresses the barriers of cost, durability, and performance.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The use of a three-dimensional (3D) electrode structure is a very innovative idea; electrospinning and interspersing makes it unique. Higher efficiency targets can be reached using the 3D design. Additionally, using graphene oxide (GO) for water disassociation is synergistic.
- This is a unique approach to RFCs using a BPM, one that addresses issues with the BPM junction and interface by co-electrospinning the alkaline and acidic membranes. This approach should improve the interface and decrease the delamination of commercial BPMs that is observed when trying to operate at high current. Other than changing the catalyst content at the interface, it is not clear what parameters of the interface the project team plans to vary (e.g., the thickness of interface layer and gradient versus step change).
- The proposed approach is interesting, as it allows for the intimate mixture of polymer electrolyte membrane (PEM) and anion exchange membrane (AEM) polymer fibers with a water-splitting catalyst to produce

BPMs with different thicknesses (though the target thickness was not defined). However, it is unclear what benefits such a homogeneous mixture can provide compared to a conventional two-layer BPM, or how it will affect crossover through the membrane. This approach still requires platinum-group-metal-based (PGM-based) catalysts at both electrodes.
- The approach is focused on overcoming barriers for electrolyzer and fuel cell performance.
- The approach of the project is to demonstrate regenerative fuel cells using perfluorinated BPMs. The general approach is good; however, the detailed approach for making the proposed system affordable is not clear from the presentation. This is because the target milestone (500 mA/cm^2) is not a measure of the performance without the cell voltage level. If the target is merely 500 mA/cm^2, then commercial BPMs already met the milestone before the project began. In addition, other researchers have suggested the use of 3D structure. There does not seem to be much of an innovative idea except for putting together two available membranes.
- The team was not clear about why the junction should be porous. It was good that they are comparing against a commercial membrane, but they were not clear which one is being used or how it is structurally or functionally different from what they are making.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made good progress but has fallen behind the original schedule. The team has been able to electrospin membranes and demonstrate a lower resistance of the water dissociation reaction by adding GO at the 3D interface. The team has demonstrated performance superior to that of a commercial BPM in an electrolyzer MEA and achieved current densities of 5mA/cm^2 in both fuel cell and electrolyzer MEAs. (This was not achieved with the same membrane, and higher pressure [311 kPa] is needed for a fuel cell.) The project is behind the original schedule, and the team has delayed the milestone of demonstrating an area-specific resistance of <0.2 ohm/cm^2 and achieving 500 mA/cm^2 in both electrolyzer and fuel cell modes. The issues with removing halides from the electrospun AEM could slow progress. It would be beneficial to find a different method or different copolymer to allow for electrospinning the hydroxide form of the alkaline ionomer. The characterization of the membranes, and specifically of the membrane interface, is lacking. It would be nice to see what characterization has been done, even if it would show only the morphology at the interface. If the GO catalyst is dispersed in just one of the ionomers, the team should be able to get some indication of what the interface looks like from the GO distribution.
- One of the intermediate targets—a current density of 500 mA/cm^2 for both fuel cell and electrolyzer modes—has been demonstrated, though for different cells, with high PGM loading for the fuel cell. However, the cell voltage at this current density is unsatisfactory, and it is not clear how durable the BPM produced by electrospinning is (the fuel cell voltage started to decline within 20 minutes). It seems that the major improvement was reached not because of the 3D architecture of the BPM but because of the introduction of GO. No data on membrane thickness have been given, so the comparison with commercial BPMs is not correct. No progress was made in improving the understanding of the electrospun BPM junction interface.
- Progress has been made toward the development of a 3D BPM that demonstrates initial performance characteristics that are close to those of a commercial BPM. The advantages of a 3D design are not very clear, since the voltage–current density curves look very similar. The DOE goals in terms of performance are not clearly defined.
- The go/no-go goal was met, but with two different membranes; this makes RFC application difficult. The complications of 2D-to-3D membranes need to be better understood.
- Demonstrating the electrolyzer and fuel cell performance was a good accomplishment. However, considering the funding level, the National Renewable Energy Laboratory (NREL) team should provide more data. It does not seem like the 3D structure is much better than the 2D structure in cell performance, in spite of the notably lower water-dissociation-reaction resistance. The electrolyzer performance should be compared with the performance of the 2D structure. There is no 3D structure performance for the fuel cell MEA mode; there are no data that show how the 3D structure has been optimized; there are no data on how

to optimize the electrospinning process; and there are no microscopic data on the morphology of the 3D structure. Overall, the progress of the project is disappointing.
- This would have received a "fair" or "poor" rating if not for the no-cost extension and personnel difficulty. The team has not done a sufficient job in characterizing the structure of the created interfaces. The team has not truly developed a baseline or control in this study. In addition to what has been done, the team should also create the electrospun junction without the GO to elucidate whether the improvement is from the project's electrospun polymer or the GO—or if the GO is doing anything at all.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The partnership with 3M and the Colorado School of Mines is positive.
- The collaboration between groups within NREL appears to be going well. Collaboration with the Colorado School of Mines is not evident in the presentation. It is not clear what characterization has been done other than the electrochemical characterizations, which appear to have been done at NREL.
- This is a well-coordinated effort within NREL; however, contribution from the Colorado School of Mines is not noticeable. Collaborating with other institutions outside of NREL may help with membrane characterization and optimization.
- There is clear collaboration with industry and academia and inside NREL, mainly based on the use of materials for BPMs, fuel cells, and electrolyzers. However, there is no apparent coordination between the partners.
- The project needs more involvement from the outside collaborators, if possible. Using 3M's nanostructured thin film catalyst is advantageous for the project. NREL may want to provide data using other available catalysts for comparison, and also change the catalyst loading to see the impact of the catalyst on device performance. No data from the Colorado School of Mines can be seen. Leveraging the research efforts with other DOE projects is excellent.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The relevance and potential impact of this project is high. Bipolar cells could theoretically take advantage of the high PGM-free activity for oxygen reduction reaction in alkaline conditions, and the high activity for hydrogen oxidation reaction in acidic conditions, providing a better PGM-free cell. Issues at the bipolar interface have hampered BPMs; this approach could solve those issues.
- The relevance of the project to the interests of the DOE Fuel Cell Technologies Office is high. As the project's target is to demonstrate RFC technology with high round-trip efficiency, the potential impact of the project on fuel cell and electrolyzer technology may be significant.
- If successful, this technology could move toward the use of RFCs for long-term energy storage.
- The 3D design expands the possibility for operating range and higher efficiency.
- This project is aligned with DOE goals on the development of RFC technology.
- The overall project is directed toward the right goals, but the approach and execution could be improved.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The proposed future work will focus more on instrument-centered research and performance measurement. While the project has shown some promising performance in the fuel cell and electrolyzer modes, more efforts on BPM development are needed. Particularly, the optimization of the 3D structure and the construction of desirable morphology and membrane formation are urgently required to warrant a successful outcome from the project.

- The future work correctly targets demonstrating durability operating in both individual modes (electrolyzer and fuel cell); however, the work focuses mostly on optimization of the current setup (catalyst loading, flow field, etc.) without finding the root causes of instability and low activity.
- The work plan looks good; a staffing issue can slow down progress.
- The proposed future work is more or less straightforward.
- The proposed future work is reasonable. Non-electrochemical characterization of the membranes and interface is lacking here; the team's efforts in characterization should increase. Increased efforts to characterize the interface, ex situ testing (relative humidity cycling) for interface stability, and mechanical testing, etc. should be included.
- The proposed future work is focused on overcoming barriers in terms of performance in fuel cell and electrolysis modes. The performance goals are not clearly defined. For example, 500 mA/cm^2 as a go/no-go decision should be complemented by an operating voltage. "High fuel cell and electrolysis performance" is not a very specific goal.

Project strengths:

- The strength of the project is in NREL's facilities and capability to do the research. Teaming with 3M is another strength. Leveraging project efforts with other existing DOE projects is particularly attractive for increasing the success rate of the project.
- The project team has shown good improvement versus the commercial BPM, especially on the electrolyzer side. Also, the team clearly has the expertise to be successful.
- The project's strengths include its electrochemical characterization and characterization techniques.
- The project's strengths include its novel method for manufacturing BPMs, which may result in the development of RFCs for energy storage.
- The project proposes a novel approach for the 3D design of a BPM.
- The 3D design is a good strength; the partnerships are good.

Project weaknesses:

- The project approach is rather empirical; the material selection for BPMs is limited by the available ionomers and catalysts that are sometimes not designed for selected materials. The leftover salt ions in the BPM electrolyte after water electrolysis seem to be a fundamental problem for the fuel cell operation. The BPM resistance is too high for practical applications. There are no cost estimations or a cost–benefit analysis of electrospun BPMs.
- The research progress is slow. For example, one of the objectives of the project was stated as "The key technical aspects of the project are focused on fabricating and optimizing electrospun 3-D junction… membrane characteristics such as composition, fiber diameter, and the incorporation of catalysts and particulates at the interfacial or junction." However, it does not appear that any of those have been accomplished at a satisfactory level. The project's principal investigator, team members, and the Colorado School of Mines need to spend more time and effort on this project.
- The project's weaknesses include the following: (1) The achievable current density is low. This may be a project-ending issue eventually. These bipolar systems are notoriously lower-performing than AEM- or PEM-only systems. (2) The team does not appear to show a single cell or cell condition in which both the fuel cell and electrolyzer mode were tested and efficiently evaluated. (3) The team did not show a clear protocol for how the unitized RFC would be tested or what the metrics for success are.
- Data for the reversible mode and cycling were not shown; the team needs to make sure that both modes are in good performance and that life data are shown. The efficiency pathway is also not shown.
- The project's weakness is in the lack of membrane characterization and the uncertainty of the project's metrics.
- The project's weaknesses include its membrane and interface characterization.

Recommendations for additions/deletions to project scope:

- Recommendations for the project scope include the following: (1) A more robust physical characterization of the electrospun material and interface is needed. (2) The team should create the electrospun interface without GO and compare the water vapor gas constant value. The team should determine whether it is the catalyst or the structure that is having the effect. (3) In future presentations, the project team should try not to refer to the electrodes as “anode” or “cathode”; they should be “O_2 electrode” and “H_2 electrode.” (4) The fiscal year 2018 go/no-go of 0.5 A/cm^2 should be achieved using a single cell. (5) It should be determined where the Cl goes when the AEM component is exchanged from the Cl- form to the OH- form during electrolysis mode. The team should determine if it evolves as Cl_2 and whether that has any safety ramifications.

- The project team needs to measure the round-trip efficiency and cycle life of the most optimized 3D BPMs. More characterizations of the 3D structure are also required. The progression of the performance improvement, depending on the BPM structures, needs to be presented.
- Modeling would help with the fundamental understanding of BPM performance and its optimization.
- The study of BPM structure and catalyst–ionomer interaction should be added to the project scope.
- Developing cycling data is critical, as is higher efficiency.

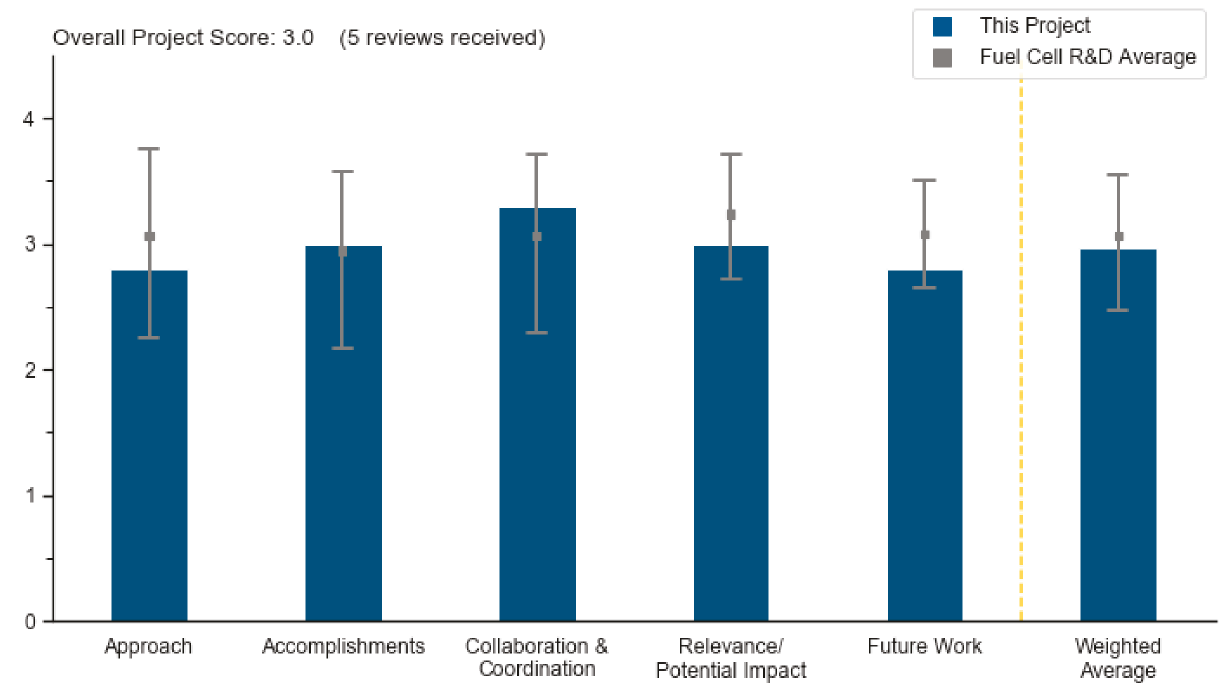
Project #FC-183: Lab Call Fiscal Year 2018 (Reversible Fuel Cells): Technology-Enabling Materials, Cell Design for Reversible Polymer Electrolyte Membrane Fuel Cells

Nem Danilovic, Lawrence Berkeley National Laboratory

Brief Summary of Project

Unitized regenerative fuel cells (URFCs) are energy storage devices that store electricity in the form of hydrogen and oxygen gas (electrolyzer mode) and produce electricity (fuel cell mode). The project will show the feasibility of fixed-polarity URFCs and an engineered bifunctional oxygen evolution reaction (OER, for electrolyzer mode)/ hydrogen oxidation reaction (HOR, for fuel cell mode) catalyst. To do this, Lawrence Berkeley National Laboratory (LBNL) will show the feasibility of the URFC approach in membrane electrode assembly (MEA) testing using state-of-the-art polymer electrolyte membrane fuel cell (PEMFC) and electrolysis materials and developing an application-relevant cycling protocol and accelerated stress test. Argonne National Laboratory (ANL) will demonstrate the feasibility of the engineered supported catalyst approach by (1) developing an atomic layer deposition (ALD) process and (2) characterizing the activity and stability of the supported bifunctional catalyst versus baseline materials for HOR, OER, and cycling.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is original and may be interesting if it fulfills all U.S. Department of Energy targets concurrently, not only at the MEA level but also at the system level. The investigated approach will need purge phases when switching from electrolysis mode to fuel cell mode and the reverse. This will induce some hydrogen and oxygen release and affect the system efficiency and system time operation.

- The project focuses on development of URFCs using an innovative concept of cell fixed polarity and an engineered bifunctional OER/HOR catalyst. This concept may provide a more effective use of bifunctional catalysts but requires more complexity from the UFRC operation.
- The approach leverages the skills of LBNL and ANL with private industry; collaborating with both 3M and Proton OnSite is a very productive combination. The fixed polarity mode concept is an interesting opportunity for regenerative fuel cells. The catalyst design strategy is good for yielding better MEA performance.
- The technical barrier being addressed is the operation of a URFC with "fixed polarity," keeping one side as the anode and the other side as the cathode for the two operating modes. Because of the dual operation, the project is addressing barriers identified for the fuel cell and water electrolysis but with targets being a compromise between the two applications. Thus, clear specific targets have been proposed. The most complicated part of the approach is to use the same electrode as a single anode for operating both a PEMFC and a polymer electrolyte membrane water electrolyzer. The project's core activity is to identify the right catalyst based on materials used for hydrogen oxidation or for oxygen evolution, which are Pt- or Ir-based. The work started with assessment at the rotating disk electrode (RDE) level, then at the MEA level. A major issue is the poor stability of the anode catalyst under voltage cycling (up to 1.6 V to simulate an OER situation, as requested), which is leading to strong losses with the HOR.
- The team does not make a compelling argument for why there would be synergy between the oxygen reduction reaction/hydrogen evolution reaction and/or the HOR/OER. In fact, despite the fact that one electrode is always doing a reduction or oxidation, the potentials are totally different, and the swings in the potential at both electrodes make it seem like it would be higher than that of a catalyst in a typical "fixed gas" URFC. It is unclear why the ALD is necessary, whether it is scalable, or how this process would help with cost.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The experimental data showed better performance of the proposed URFC in the fixed polarity, compared to the conventional fixed gas mode. The high (60%) round-trip efficiency demonstrated at the current density of 1 A/cm^2 is impressive, and the go/no-go milestone has been met. Interestingly, the down-selected bifunctional HOR/OER catalyst is just a physical mixture (9:1) of Ir and Pt black, which outperforms more elaborate structures.
- The cycling data are meaningful and promising. The go/no-go goal has been met. The test stand issue may cause delays. The results need to be illustrated with greater clarity and compared with the project's goals.
- The team has shown proof of concept early on, which is good. They do need to develop protocols more similar to how real URFCs would be deployed in the future.
- The work is ongoing, following most of the future work indicated in the previous year. Some aspects are missing. For example, the project team did not present varying flow fields with discrete MEAs or evaluations of the performance and durability of the traditional versus the proposed URFC concept. In addition, there is no information about the comparison of the different operation modes.
- New results have been provided. However, the stability of the investigated catalysts has not been demonstrated in both modes. No information is given regarding the purge effect or the time spent switching from fuel cell mode to electrolysis mode and the reverse. No information is given on the future stack and system pressure.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- It appears that both members of the team are participating and that ANL materials are being deployed well at LBNL.
- There is a working collaboration between LBNL and ANL, as well as participation from industrial partners.

- ANL's expertise in catalysts is a plus. The project is leveraging LBNL's capabilities.
- The collaboration between LBNL, ANL, and the two industrial partners, 3M and Proton OnSite, appears correct.
- The collaboration between ANL and LBNL is clear and positive for the research side. The contribution of the industry partners is not obvious at this stage of the project and should be increased for the definition of assessment tests.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The proposed fixed-polarity concept could be instrumental in making URFCs work equally well in both operational modes. Such URFCs could find wide application in long-term energy storage.
- The investigation of reverse PEMFCs is of interest but challenging. Even if a relevant MEA is developed, system efficiency and total cost of ownership will be the key drivers when comparing architecture consisting of two systems or two stacks (i.e., fuel cell and electrolysis) to common balance-of-plant components.
- The project is considering several DOE objectives but addressing a very specific device; thus, it is not easy to draw conclusions for the expected impact. If the project's objectives are reached, progress will be made toward cost and performance objectives for PEMFCs and efficiency in hydrogen production.
- The project team needs to show how the materials contribute to higher efficiency on a round-trip basis and other cost benefits. Batteries are a major competitor, and no comparison with these is given.
- The project is focused on meeting DOE targets, but there are some remaining issues to making its possible impact high.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The project's main next steps will be to find out how to improve the anode catalyst by changing the structure. There is a strong risk of failure that should be taken more into account. After that, selecting the best mode for actual validation of durability should be the priority.
- The proposed future work is well aligned with identified challenges and issues but lacks quantifiable metrics. There is no plan to explore decreased platinum-grade-metal loading.
- Everything that is proposed makes sense, but there could be more attention paid to the protocols for testing.
- The chosen operating cycle of four hours is acceptable, but it may be adapted to real duty cycles (i.e., fuel cell and electrolysis duration), depending on its applications. The operating single cell conditions should consider the targeted working pressure of 30 bars.
- The relationship to efficiency and cost goals should be included. Life-cycle improvements were not clarified.

Project strengths:

- Surprisingly, high performance was achieved with first-generation materials. Both team members are working well together.
- The idea of developing a single catalyst layer as a fuel cell and electrolytic anode is innovative and could be a strength, but demonstration is required. The proposal of a specific duty cycle for URFCs should be valuable for further studies on this type of device; it should be validated on the selected operation mode.
- The project has a good combination of component development work (i.e., catalyst and MEA) and technoeconomic analysis.
- The laboratory collaborations are a good strength, with ANL in particular. Industry feedback is important.
- The competence of the project partners is a strength of the project.

Project weaknesses:

- The poor stability of the anode catalyst under voltage cycling (as requested, up to 1.6 V to simulate the OER situation) is leading to strong losses for HOR. This is a major issue, and the approaches planned as mitigation, such as dissociating Pt and Ir, each on its support, are not convincing for solving the problem of Pt dissolution. Information such as the microstructure of the catalysts developed should be added in the characterizations and used in data analyses. At this stage, between fixed polarity, fixed gases, and vapor feed, the best-suited operation mode (i.e., the most stable and most efficient) should already have been selected for further evaluation of durability; this should be fixed soon.
- The switch between fuel cell and electrolyzer modes in the proposed concept is not trivial and may result in a dangerous mixing of hydrogen and oxygen; therefore, a purging procedure should be developed. The URFC's durability under switching operations is extremely important, and the team should pay more attention to this issue. The effect of water management on the URFC performance should be studied, and an optimization should be made.
- It is not currently clear what catalyst will concurrently meet the fuel cell and electrolysis targets and stabilities. The system operating conditions (e.g., output pressure) are not considered.
- The project's weaknesses include the following: (1) The team does not have a reasonable durability test in place. (2) It would seem that ALD will not be a scalable approach, and the team does not justify why it is necessary or what difference it will make at higher metal loadings in future systems. (3) The team does not address electrode development, particularly related to water management.
- Efficiency round-trip and degradation issues are not adequately addressed or correlated with materials used.

Recommendations for additions/deletions to project scope:

- The following are recommendations for the project: (1) In future presentations, the team should better detail the reacting environment (URFC, fuel cell, electrolyzer, RDE, etc.) on the slides. (2) It would seem that deployed URFCs would likely be operated in one mode for longer periods (not voltage-cycled, as was done here). Thus, a better stability test might be to operate these cells at constant current density (e.g., 1 A/cm^2) in fuel cell mode for ~10 minutes to allow for a steady state to be achieved, then switch to electrolyzer mode at 1 A/cm^2 for the same amount of time in order to equally "charge" and "discharge" the URFC. It also seems that controlling the rate would be better than voltage cycling, in which the total charge that is passed could be wildly different for the two cases. (3) Any metrics on performance or durability should be made with a single cell or MEA and materials set.
- Microstructure analyses of the anode catalysts should be added to see if such analyses could help the team understand and improve catalyst behavior. The team should make it a priority to select the best operation mode and complete actual assessment of one URFC on the long term, following the proposed duty cycles. Applying these cycles on "fixed gas" mode could be selected if the proposed approaches do not solve the anode issue for HOR in "fixed polarity" mode. If the issue of the bifunctional anode catalyst is not solved, the difference between the work planned and conducted within FC-313 should be clarified.
- Increasing efficiency is critical for energy storage. Batteries are already >80%, with good cost reductions. Cost and efficiencies should be addressed at a greater level.

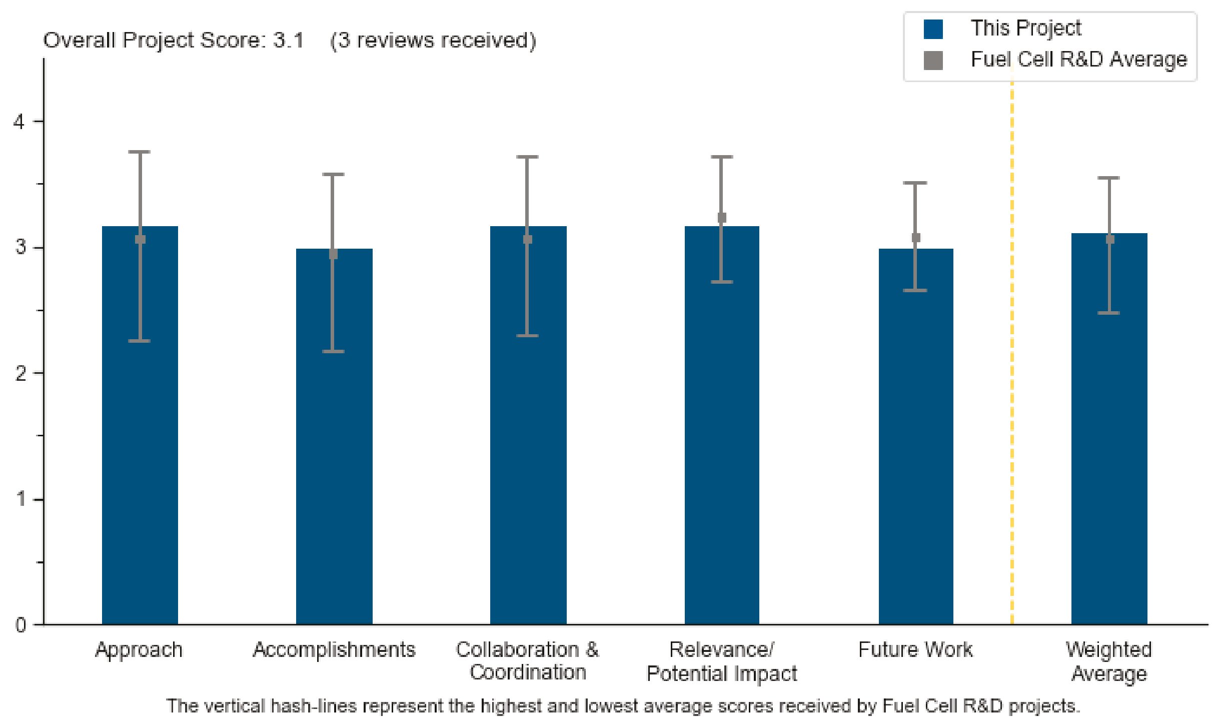
Project #FC-302: Developing Platinum-Group-Metal-Free Catalysts for Oxygen Reduction Reaction in Acid: Beyond the Single Metal Site

Qingying Jia, Northeastern University

Brief Summary of Project

Northeastern University seeks to develop platinum-group-metal-free (PGM-free) oxygen reduction reaction (ORR) catalysts with high activity and durability in polymer electrolyte membrane fuel cells (PEMFCs). These PGM-free ORR catalysts are developed via the following concurrent pathways: (1) M_x-N-C catalyst development featured with multiple metal centers (MMCs) and (2) M_x-N-C catalyst synthesis using surface deposition methods. These catalysts are developed to attain the following performance targets: (1) 0.035 A/cm^2 at 0.9 V in an H_2/O_2 PEMFC (1.0 bar partial pressure, 80°C); (2) loss in activity ≤40% after 30,000 square wave cycles with steps between 0.6 V (3 s) and 0.95 V (3 s), and (3) power density of 0.5 W/cm^2 in an H_2/air PEMFC with a membrane electrode assembly (MEA) size ≥50 cm^2.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach in this project is based on the use of multiple metal (apparently Fe) sites that should be incorporated in carbon materials to improve ORR activity and durability. This approach can be justified as much as all other PGM-free funded projects that are supposed to deliver carbon-based materials with some amount of low-cost transition metals, while maintaining high catalytic activity and durability. Considering that the Fuel Cell Technologies Office (FCTO) has recognized that as its main direction in catalyst development, the approach must be well justified.

- The proposed approach is focused on producing multi-metal active sites that can better facilitate the ORR. The key focus is on the synthesis characterization, but there are also MEA and modeling components to the project.
- In this PGM-free cathode catalyst development project, it is expected that multi-metal-site catalysts will perform better than single-metal-site catalysts. The success of this project hinges entirely on this hypothesis, and therefore a go/no-go decision would make a lot of sense for this project.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This is the first year of the project, and it is challenging to evaluate what has been accomplished toward DOE goals considering that, so far, the principal investigators (PIs) have mainly managed to synthesize and characterize materials. No MEA data were presented that would support the main expectations of this project. For that reason, all claims from the approach fall into the category of predictions and are speculative. The PIs should be acknowledged for the materials that were made and for the fact that structural characterization is consistent with what was proposed. The main issue that remains is how to justify the idea in this approach. It is not clear why these systems should be more active and durable, as well as what the foundation is for such claims.
- It is the beginning of the project and too early to evaluate accomplishments. The initial activity of the MMC catalysts seems low, based on rotating-disk-electrode (RDE) half-wave potential. It will be useful to devise a means of estimating the MMC site density such that the turnover frequency can be evaluated to better quantify whether the MMC site is more active.
- On slide 6, the results should be shown with respect to reference and/or state-of-the-art materials. This project has just started, and the accomplishments are sparse, as would be expected. The initial results demonstrate the project’s capability for the work to be conducted.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration between the participants is well coordinated.
- There is collaboration from one academic institution, one national laboratory, and the Energy Materials Network. The technical back-up slides show how the consortium members (perhaps ElectroCat) are being utilized. More details on the roles would be helpful to understand the levels of interaction better. For example, it is unclear who is doing the MEA integration work, how the feedback loop from the testing is given, or how the preliminary evaluation is aligned with subsequent diagnostics.
- There is collaboration outside of Northeastern University with Lawrence Berkeley National Laboratory. The value of the mass transport modeling will be apparent only if the catalyst activity becomes sufficient; otherwise, there is too much uncertainty in future catalyst morphologies that will meet activity targets.

Question 4: Relevance/potential impact

This project was rated **3.2** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project’s topics are right on target with the interests of the FCTO in PGM-free catalysts for fuel cell systems. Although not mentioned in the presentation, these catalyst types could reduce cost significantly if they could achieve higher performance and lifetimes.
- The potential impact would be significant if it could be demonstrated that a multi-metal active site was more active and could be reliably synthesized at high density.

- The project's main issues were, are, and will be the insufficient activity and poor durability of PGM-free systems. A modest knowledge of material science and electrochemistry does not imply that carbon-based materials doped with Fe would ever evolve to the level that would enable application in PEMFC cathodes, considering that even Pt-based catalysts suffer from degradation. Nevertheless, keeping in mind that the goal of this project is to improve activity and durability, the relevance is satisfactory.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed work seems reasonable. Densifying the MMC sites is a key part of the future work.
- Overall, this is a sound approach for the work on the catalyst side. It is unclear why ion-beam-assisted deposition and electro-spinning are highlighted for MEA fabrication. Electrode integration and optimization should be an important aspect. Furthermore, some evaluation of catalyst degradation at the end of the project should be added to the scope.
- The future work should provide feedback that would clearly address the approach of this project.

Project strengths:

- The project's strengths include clear communication about what is targeted and what was accomplished. The project also has had successful synthesis and structural characterization, as well as well-executed collaboration.
- The project has an interesting approach that could have the potential to improve PGM-free catalyst performance significantly.
- The project's strength is its focus on an active site that is more novel than the common MN_4 site.

Project weaknesses:

- The project's weaknesses include the lack of evidence that the proposed approach can effectively address the activity and durability of PGM-free catalysts, as well as the lack of RDE durability measurements or MEA data.
- The project's early weakness is likely the density and verification of the MMCs.
- Everything is based on one hypothesis.

Recommendations for additions/deletions to project scope:

- It is recommended that the project have a go/no-go decision point that shows some indication that the hypothesis is true.
- MEA testing is required.

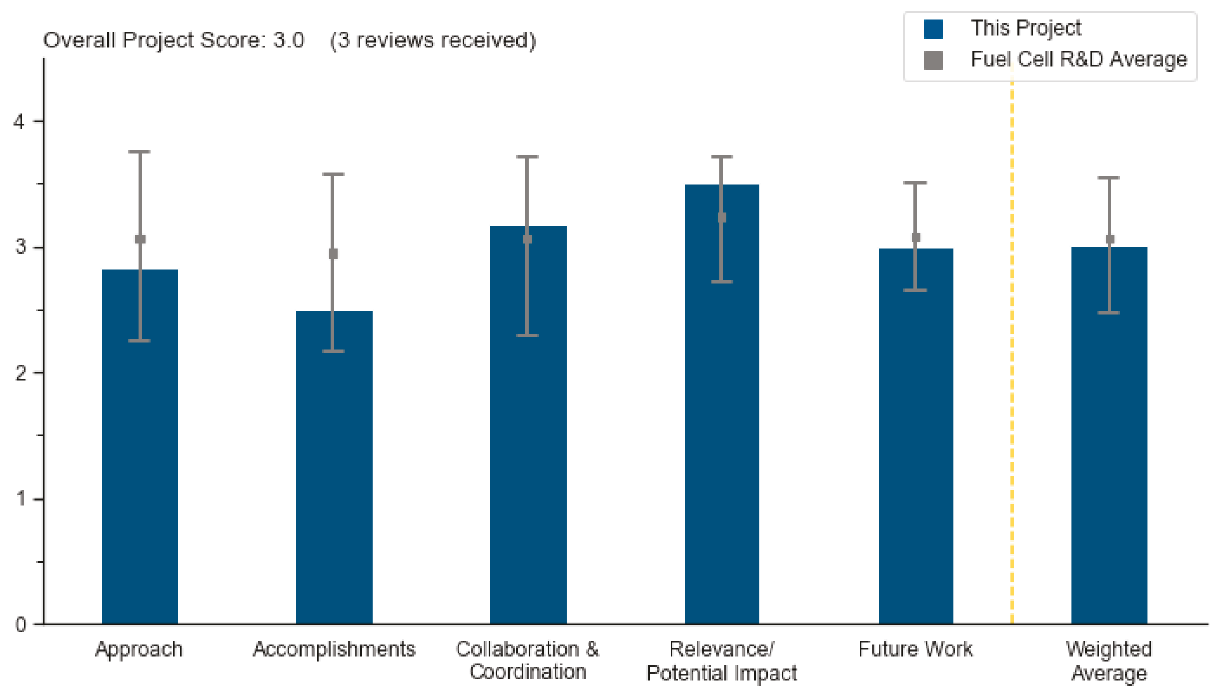
Project #FC-303: Mesoporous Carbon-Based Platinum-Group-Metal-Free Catalyst Cathodes

Jian Xie, Indiana University–Purdue University Indianapolis

Brief Summary of Project

Indiana University–Purdue University Indianapolis (IUPUI) will use controllable synthesis to design and develop advanced hierarchically porous carbon sphere (HPCS) M-N-C catalysts for precious-group-metal-free (PGM-free) cathodes in polymer electrolyte membrane fuel cells. The project team also aims to develop membrane electrode assemblies (MEAs) using the novel ionomer–catalyst interface by controlling the surface charges on catalyst particles to obtain improved catalyst activity, utilization, and high-current-density performance. The project goals are addressed on both intra-particle and inter-particle levels respectively via the following approaches: (1) develop high-performance PGM-free catalysts with mesopore structure and (2) construct an ideal Nafion™ ionomer–catalyst interface within a catalyst layer of MEAs.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has four different tasks. Task 1 is the development of HPCS-based M-N-C catalysts with high mass activity. This approach is very solid and led by the University of Buffalo. Task 1.3 addresses the stability of M-N-C catalyst on mesoporous carbon support (MCS@M-N-C). Some milestones need to be added to monitor the durability of these catalysts. Task 2 is the development of cathode layers using the HPCS-based catalysts. The approach to this task has some serious issues. The HPCSs are approximately 500 nm in diameter, and it is expected that most of the active sites would be buried in the smaller (micro- and meso-) pores within this large particle. The approach involves functionalizing only the surface of this large particle and not the mesopores. Controlling only the ionomer coverage on the outside of these particles might not be enough. It needs to be made clear whether this project relies on just surface proton transport or liquid water to provide access to the active sites within the mesopores and micropores of the carbon particle. This needs to be addressed early in the project and will be key to achieving good MEA performance. Tasks 3 and 4 are MEA preparation, testing, and cost analysis; that approach is sound.

- This is a polymer electrolyte membrane low-temperature electrolysis technology project, as well as a catalyst synthesis and integration project, pursuing the development of HPCSs. From the images on slide 5, it is not apparent how this approach differs from traditional electrode structures. Slide 9 indicates that the hope is that improvement will be made with the particle itself and in its coating with ionomer. The images of slide 5 show a Pt catalyst system, while the project is aiming at PGM-free catalyst development. Images on slide 8 and the following slides are much more aligned with the description of the project, though from the images on slide 11, it is not clear how the ionomer thickness and distribution are being controlled.
- While the project is good in terms of scope, the approach is not well defined in terms of achievability. It seems a bit overly optimistic and ambitious. It is not clear that adding mesoporosity will increase the non-PGM mass activity, as it is unknown whether it is mass-transport-limited; what is really needed is an increase in the number of active sites. Similarly, the idea of an ideal ionomer–carbon interface is very good, but again, the approach is unknown in terms of its feasibility, as it relies on several understandings and assumptions that are not well known as of yet. For example, it is unknown what morphology or properties are wanted with the ionomer backbone interactions versus the side chains. Ink formulation by itself is perhaps a very large effort, and here it seems to be trivialized. The exact surface groups being examined are not well discussed.

Question 2: Accomplishments and progress

This project was rated **2.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Considering that this project is just starting, there has been great progress, especially in regard to Task 1. The University of Buffalo has already demonstrated $E_{1/2}$ of 0.82 V versus a reversible hydrogen electrode, which was a milestone. The team should look into and report on the durability of this catalyst in parallel with the electrode design tasks.
- No accomplishments and/or signs of progress were presented. This is understandable, as the project has not spent any money yet and obviously has not started yet.
- The project has not started.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The project has a good team, with the University of Buffalo providing catalysts, IUPUI making electrodes and MEAs, and the United Technologies Research Center providing testing and cost analysis.
- The project has a good team that is wide-ranging in terms of tasks, but there should be more effort devoted to characterization. The understanding gained from discussions with a national laboratory would be helpful.
- The project has an academic lead, with collaborators from one university and one industry research center. Beyond listing the partners, it was not clearly laid out how the partners would communicate and/or interact with each other. It would be helpful if there were more information about the actual collaboration and some understanding of how the partners work together and/or exchange information.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project topics are right on target with the advancement of the technology and the goals of the DOE Hydrogen and Fuel Cells Program. Reducing the costs of available cost-effective catalyst materials is important. It is unclear how well this seemingly complicated catalyst fabrication process could be scaled up, or what impact scaling up might have on the cost of the material. This will, however, be addressed in year 2, quarters 1–3, of the project.
- This project supports ElectroCat, and the milestones are well aligned with the consortium's goals. The team should work closely with the ElectroCat laboratories to determine the stability of these catalysts. The laboratories can provide key capabilities that would complement the team's ability to understand these materials and electrode structures.
- Nominally, the project is tackling very important and critical fuel cell issues. However, it is not clear whether the approach is the correct one to solve those problems.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- Overall, this is a very sound, comprehensive project plan. The role of the ionomer will be critical for the success of this project. There seems to be too little attention being paid to understanding the effect of ionomer loading on transport phenomena and, ultimately, performance. PGM-free catalysts face significant durability challenges. Some durability evaluation needs to be conducted at some point to put this system in context with other PGM-free systems.
- The proposed work is perhaps too wide-ranging and ambitious, as it relies on understandings that are still not well developed. There is concern about Task 2 in terms of how many functionalities can be examined and the need to develop full catalyst layers. Simpler studies and setups are recommended. For Task 1, it is unclear whether the system is mass-transfer-limited or whether the catalyst site density will be increased and activity per site maintained.
- The project's future work is almost identical to its approach since this project is just starting.

Project strengths:

- This project is tackling a very relevant problem from two related angles and has some interesting aspects. The functionalization of carbon is a good idea, although the team needs to ensure it is maintained and is positive in terms of increasing performance.
- The project has good teaming with clearly defined roles. The project team has novel ideas about M-N-C catalysts and HPCS development that show promise for making better PGM-free catalysts.
- Multiple approaches have been suggested for achieving the project's goal. Overall, there is very sound project planning.

Project weaknesses:

- The surface functionalization and ionomer incorporation are unproven and need to be demonstrated early in the project. There is not much science or understanding on how functionalization will affect ionomer distribution. To provide DOE with lasting value from this project, some fundamental studies of how functionalization affects ionomer coverage and thickness need to be added. With advanced characterization techniques from ElectroCat, these studies might be accomplished with a systematic study.
- It is unclear how the partners interact and help each other to achieve the project goals. It is also unclear how the ionomer thickness is controlled or to what extent ionomer will fill the pores and hinder gas transport. Understanding the effect of ionomer distribution and being able to control it will be key for the success of this project.

- The project relies on a good deal of understanding or empirical luck to occur quickly. It is not certain that the objectives can be met within the proposed time, scope, and budget.

Recommendations for additions/deletions to project scope:

- It is recommended that the team add more model-type studies and more characterization so that understanding can be gained before just trial and error. The scope should perhaps be readjusted to be more focused.
- The team should add a durability milestone, at least at the end of the project. This is a known issue with all PGM-free catalysts, and it needs to be explicitly addressed, at least toward the project's end.
- Results and/or signs of progress need to be demonstrated. The project has apparently not started yet. It is also recommended that the team do some long-term testing to probe the durability of this catalyst structure.

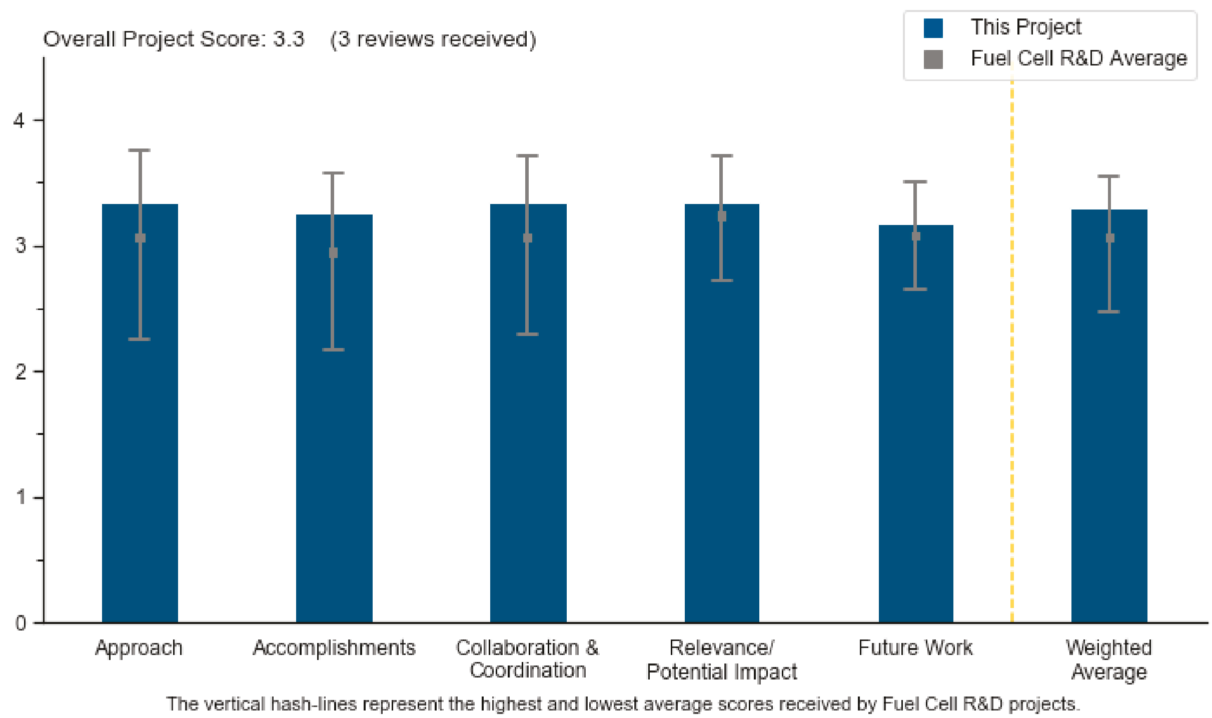
Project #FC-304: Fuel Cell Membrane Electrode Assemblies with Platinum-Group-Metal-Free Nanofiber Cathodes

Peter Pintauro, Vanderbilt University

Brief Summary of Project

This project will fabricate, characterize, and evaluate electrospun nanofiber mat electrode membrane electrode assemblies (MEAs) with platinum-group-metal-free (PGM-free) oxygen reduction reaction (ORR) cathode catalysts for H_2–air fuel cells. The novel electrospun electrode structure has potential to overcome shortcomings of conventional fuel cell electrodes (e.g., prepared by slot die coating) to improve MEA performance and durability. This is especially true for PGM-free ORR catalysts that have issues with catalyst durability (associated with metal leaching) and high cathode catalyst loading (i.e., thick cathodes, with the potential problem of significant O_2 and H+ mass transfer resistance). The project seeks to better understand and further improve the power output and durability of nanofiber mat fuel cell cathodes and MEAs with state-of-the-art (SOA) PGM-free catalyst powders (from project partner Pajarito Power). The project will also optimize electrospun nanofiber mat cathode composition and morphology for MEAs to meet U.S. Department of Energy performance and durability targets.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has a well-organized approach with a good understanding of the properties and requirements of electrodes. The principal investigator recognizes potential difficulties and has anticipated a research approach to resolve or test these difficulties.
- The project's approach is effective and contributes to overcoming most barriers. The objectives and critical barriers are effectively identified and are being addressed.

- The project's approach is to utilize nanofiber technology to enhance the performance of thick non-PGM catalyst electrodes.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This is a new project. Past work demonstrated the ability to form and attach catalysts to nanofibers. This is key to developing a high-performance, PGM-free electrode. The work has demonstrated a break-in period for the nanofiber PGM-free electrodes, with increased performance after 50 hours.
- The project had just started upon slide submission, so few specific project results were available. The pre-project results shown indicate good initial feasibility.
- The project has just started; all of the results shown were prior results.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The technical, synthesis, and fabrication areas are covered by team members. The project may need additional help in cost analysis. There is extensive collaboration with national laboratories for testing nanofibers and catalyst performance. Collaborators have demonstrated technical capabilities in measuring electrode properties and performance. Industry partners were identified that could move the successful project toward the manufacturing of nanofiber PGM-free fuel cell systems.
- The project plan indicates good coordination between the formal project organizations and the Electrocatalysis Consortium (ElectroCat).
- There is good collaboration between the three partners and good interaction with ElectroCat.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- PGM-free catalysts have low power density, and the use of nanofiber mat electrodes offers an approach to increasing the nominal power density. However, there will be a question of catalyst utilization for the mat electrodes, and it is not clear that a ten-fold increase in power density will be feasible. If successful, the potential impact will be important.
- For PGM-free catalysts to be incorporated in commercial devices, questions of power output and durability— which this project seeks to address—must be investigated.
- The project has good prospects for advancing the performance of PGM-free catalysts. However, PGM-free durability is a severe fundamental challenge, and the project is not addressing this issue.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed future work is logical, based on the project objectives.
- The future work is reasonable, but it would be good to see a risk and mitigation table.
- The future work emphasizes catalyst agglomerate size. However, for the PGM-free electrodes to be successful, a three-dimensional electrode needs to be developed. The future work does not include studying the effects of mat thickness. The future work does not appear to evaluate catalyst utilization.

Project strengths:

- The project brings together an alternative PGM-free cathode catalyst with nanofiber fabrication to improve the power density of a PGM-free cathode and yield short-term stable performance (300 hours) at 0.5 V, after initial wetting of the mat nanofiber electrode.
- The project will utilize SOA PGM-free catalysts and nanofiber electrode technology, which has been shown to be very effective with PGM catalysts.
- This is a good team with experience in the areas being investigated.

Project weaknesses:

- The project addresses improved catalysts but does not address the varied thickness of nanofiber mat cathodes. A three-dimensional dispersion of PGM-free catalysts is necessary to get nominal power density at levels similar to electrodes that contain PGM catalysts.
- This is a large monetary award for a university-led project. The scope of the work seems small when considering this budget and the relatively low overhead at universities and companies.

Recommendations for additions/deletions to project scope:

- A recommended addition to the project scope includes the development of nanofiber, PGM-free mat electrodes of different thicknesses, with measurement of the catalyst utilization as a function of mat thickness. It could be anticipated that thicker mat electrodes could have lower catalyst utilization, similar to what has been observed with PGM electrodes. This would suggest that with thicker nanofiber PGM-free electrodes would have reduced effectiveness and present limits on increasing the power density of the fuel cell system and, therefore, an inability to achieve performance at a level competitive with PGM fuel cell systems.

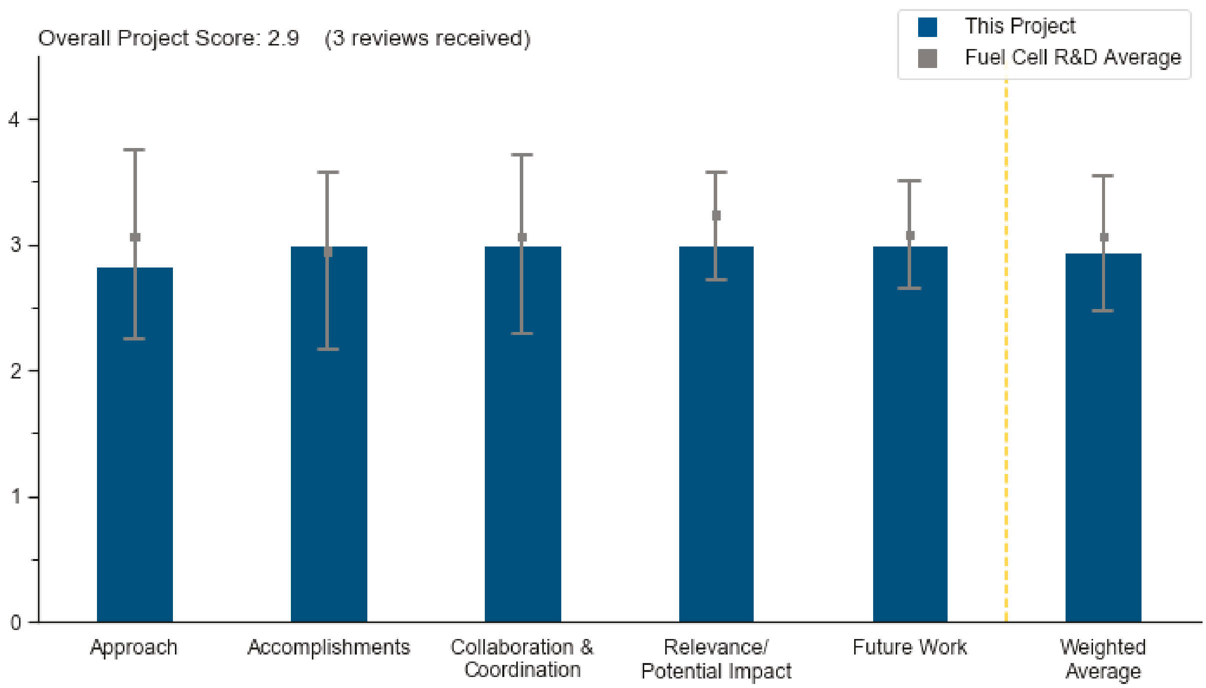
Project #FC-305: Active and Durable Platinum-Group-Metal-Free Cathodic Electrocatalysts for Fuel Cell Application

Alexey Serov, Pajarito Powder

Brief Summary of Project

The project objectives are to (1) develop platinum-group-metal-free (PGM-free) electrocatalysts for oxygen reduction reaction (ORR), (2) scale up production of the catalysts to 50 g batches, (3) integrate PGM-free catalysts into the industrial state-of-the-art membrane electrode assemblies (MEAs), and (4) comprehensively evaluate the catalysts using electrochemical methods. The project addresses existing barriers by (1) increasing the activity of PGM-free ORR catalysts, (2) decreasing the cost of PGM-free catalyst manufacturing, and (3) increasing PGM-free catalyst durability. Improved understanding of the electrochemical processes relevant to PGM-free materials in mass-produced MEAs will allow commercial manufacturers to develop inexpensive, highly active, and stable PGM-free ORR catalysts that demonstrate performance levels required by the U.S. Department of Energy.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Utilizing sacrificial silica substrates has been a successful approach at small scale, but scaling up to 50–200 gr batches will be beneficial. The proposed use of probe molecules should provide good quantification of active sites. Use of more than one probe molecule should provide more information. The approach of optimizing MEAs with PGM-free catalysts using high-throughput screening is beneficial. Capability for spatially graded catalysts and ionomers, especially in the thickness direction for thicker PGM-free catalyst layers, may prove beneficial.

- The project approach is satisfactory and clearly specific to using morphology techniques to optimize catalyst performance.
- The approach is focused on large-batch manufacturing of a PGM-free catalyst, producing MEAs, and characterizing fuel cells. The approach does not include a significant effort to develop a new catalyst. The preliminary data are from a 2013 Annual Merit Review report.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- It is the beginning of the project, so it is too early to comment on accomplishments. The principal investigator (PI) and Pajarito Powder have made significant advances in large-batch synthesis of a PGM-free catalyst. The progress toward PGM-free targets depends on the ability to significantly increase activity while maintaining the present durability.
- The project began only in January, so not much progress is expected, and there is not much to show to date. Pajarito Powder has been able to show increased graphitization over the baseline. Performance of the graphitized samples has not been demonstrated yet. Initial stability (over a limited 12-hour hold) looks good, and the team has achieved the first milestone of 25 mA/cm^2 at 0.83 V iR-free.
- Although the project is in the beginning stages, the team has already achieved a performance milestone.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- The project has just started, but collaborations between partners appear to be working well. Plans for collaboration with ElectroCat are not apparent. It is unclear whether the team will take advantage of ElectroCat's capabilities of—and if so, which ones—or if the interaction will just be supplying catalyst to ElectroCat.
- The team is well aligned, and the roles are assigned clearly; there is no duplication of effort. Verification testing at Hawaii Natural Energy Institute in the different cell architecture is essential.
- The partners are appropriate for MEA development and testing.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project is relevant to DOE's fuel cell efforts and fits in with the recent emphasis on PGM-free catalysts and low-technology-readiness-level material development. The project seeks to address barriers of performance, cost, and durability for PGM-free catalysts and PGM-free-catalyst-based MEAs.
- The team set well-aligned performance targets with the DOE objectives; however, the durability targets of the project are less clear.
- The learning in mass producing PGM-free catalysts is valuable as more active catalysts emerge.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The PI's plans for scale-up and testing are good. Effort to develop activation protocols is important, but it is not clear whether an activation protocol will be universal for all PGM-free catalysts, or even all $Fe\text{-}N_4$-type PGM-free catalysts, because of the different precursors and preparation routes used. It is not clear what changes are targeted for Generation 2 (Gen 2) or what properties will be changed to improve performance.

- Proposed work is relevant to the milestones and Hydrogen and Fuel Cells Program work scope.
- There should be a key focus on increased activity with the Gen 2/Gen 3 catalysts.

Project strengths:

- The strength of the project is the team, including catalyst and MEA developers, as well as performance verification by the third party.
- The strength is the experience in mass producing a consistent PGM-free catalyst with good durability.
- The project team is strong.

Project weaknesses:

- No weakness has been identified at this point.
- Gen 1 catalyst lifetime is questionable; therefore, the mitigation approach needs to be defined.
- The weakness is the current catalyst activity and performance in MEAs.

Recommendations for additions/deletions to project scope:

- The team should include specific stability and durability targets in addition to the performance milestones.
- More planned interactions with ElectroCat could be beneficial.
- No changes are recommended.

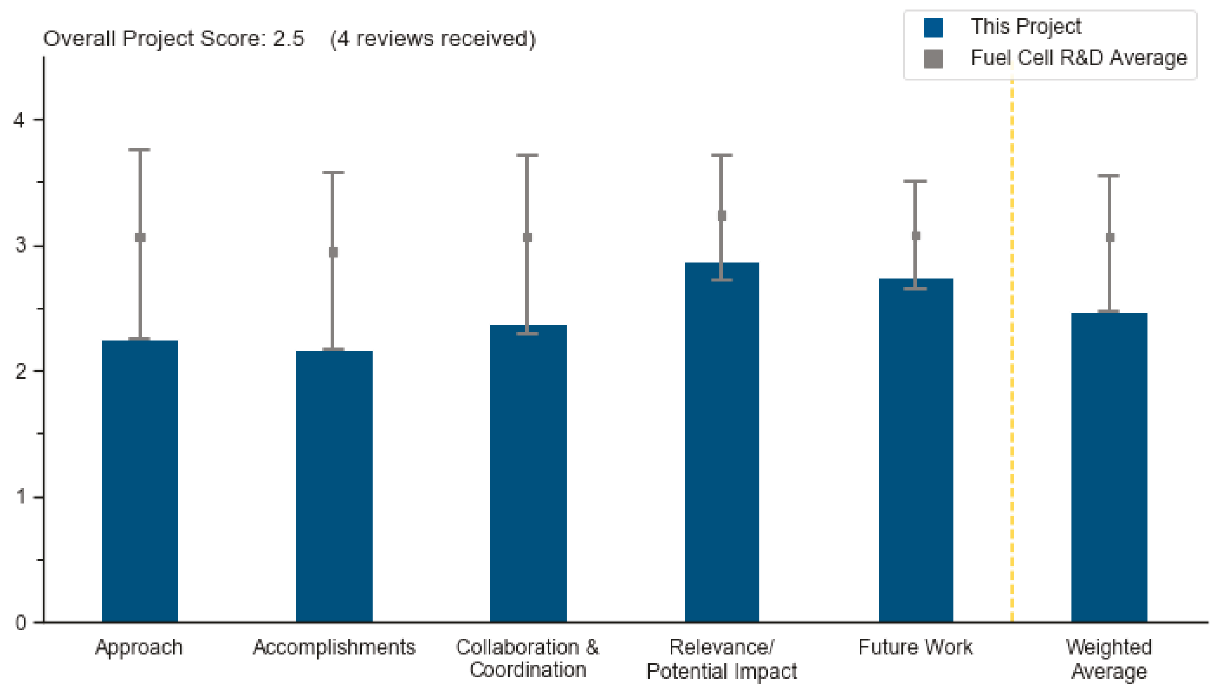
Project #FC-306: High-Performance Non-Platinum-Group-Metal Transition Metal Oxide Oxygen Reduction Reaction Catalysts of Polymer Electrolyte Membrane Fuel Cells

Timothy Davenport, United Technologies Research Center

Brief Summary of Project

The project's objective is to develop acid-stable non-platinum-group-metal (non-PGM) metal oxides and optimize oxide catalytic activity for oxygen reduction reaction (ORR) reactivity. The project will (1) utilize high-throughput computational methods to develop acid-stable complex doped transition metal oxides, (2) leverage high-throughput experimental electrochemical testing to optimize identified acid-stable oxides for ORR electrocatalytic activity, and (3) utilize a rapid development process to optimize ink formulation and optimize membrane electrode assembly (MEA) fabrication for metal oxide electrocatalysts. The project addresses barriers required to achieve U.S. Department of Energy 2020 targets for non-PGM MEAs: (1) reduce catalyst mass loss by 40%, (2) decrease performance loss, and (3) increase PGM-free catalyst activity.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **2.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project applies metal oxides as ORR catalysts for polymer electrolyte membrane fuel cells (PEMFCs). It is different from most existing projects and represents a new approach, if perhaps not a new concept.
- The project is at technology readiness level (TRL) 1, the concept phase. It is quite ambitious to get to and be successful at TRL 4, which is component testing in the relevant environment with a small MEA, in only two years. It was assumed that this funding opportunity announcement was for getting a TRL 2–3 technology to TRL 4. For this to happen, the project must have a specific plan and approach and be

aggressive with the timing. These are lacking in this project. The Massachusetts Institute of Technology (MIT) will work on theory and propose target chemical composition for the catalyst. The United Technologies Research Center (UTRC) will evaluate the catalyst. However, it is not clear how or who will do the most important part: developing the catalyst. UTRC will likely produce the catalyst, but considering the capabilities and resources required, this appears to be troublesome.
- This project just started, and its objectives and critical barriers have been clearly identified. This is the only effort that aims to develop cathode catalysts based on complex metal oxides. The approach is based on published work in alkaline electrolytes, which had rather poor activity. It is hard to envision that these systems would be efficient cathode catalysts in PEMFCs.
- The theoretical approach is rather insufficient and lacks any specific data.

Question 2: Accomplishments and progress

This project was rated **2.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- If the principal investigator could provide some preliminary data, it would be really helpful for evaluating the approach.
- The project is in the beginning stage, and progress is limited.
- The project has just started, but the plan is not very specific.

Question 3: Collaboration and coordination

This project was rated **2.4** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration between industry and the university is a good start.
- The proposed collaboration is well justified.
- The project has just started, but it is not clear who will do the most important part or how it will be done: developing the catalyst.
- MIT's work is on a parallel path with UTRC's. It is unclear why the duplication of effort has been chosen.

Question 4: Relevance/potential impact

This project was rated **2.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Transitioning away from platinum-grade-metal catalysts can reduce cost if the new catalyst is as active and durable. The project offers an alternative to the highly unstable metal nitrogen-doped carbon catalyst.
- If successful, this project might have significant impact on DOE technical targets.
- The project's chosen outline and approach are more appropriate for fundamental science, rather than applied science, and the impact of yielding new catalytic formulations by the end of the project seems quite remote.
- It is difficult to evaluate the impact without any preliminary data.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- Considering the project is starting from TRL 1, it will benefit from having frequent down-selections and implementing fast evaluation methods, commonly done during the TRL 2–3 stages.
- The go/no-go should include simultaneously demonstrating voltage performance and acid stability with the same formulation.
- The principal investigator has a good justification for the future work, but the preliminary support for the justification should come sooner.

- The proposed work relies on published work in alkaline electrolytes. There is no evidence that these systems would perform in acidic environments at a level that would be of practical relevance.

Project strengths:

- The project elaborates on the acid stability of transitional oxides and could find some stable formulations.
- The project has good teaming and a new approach that is outside of the current DOE portfolio.
- The project's strengths include its area of research, which is less clouded and less explored.
- The project's strengths include its team members.

Project weaknesses:

- The project's weaknesses include its catalyst synthesis capability and the demanding progress, milestones, and timing of a project funded by the DOE Office of Energy Efficiency and Renewable Energy. The project might be better suited to an Advanced Research Projects Agency–Energy or National Science Foundation setting.
- There is a lack of evidence that complex metal oxides can be active, stable, and conductive under the relevant conditions for PEMFCs.
- The idea is not entirely new and has been in the literature as one of the "not so promising" methods. Therefore, some of the previously known limitations need to be addressed as soon as possible.
- There is a lack of data for the chosen approach.

Recommendations for additions/deletions to project scope:

- An immediate electrochemical characterization would be more beneficial than lengthy combinatorial modeling.
- The project should clearly identify acid stability and include acid stability in the go/no-go decision point.
- The project should generate preliminary data as soon as possible.

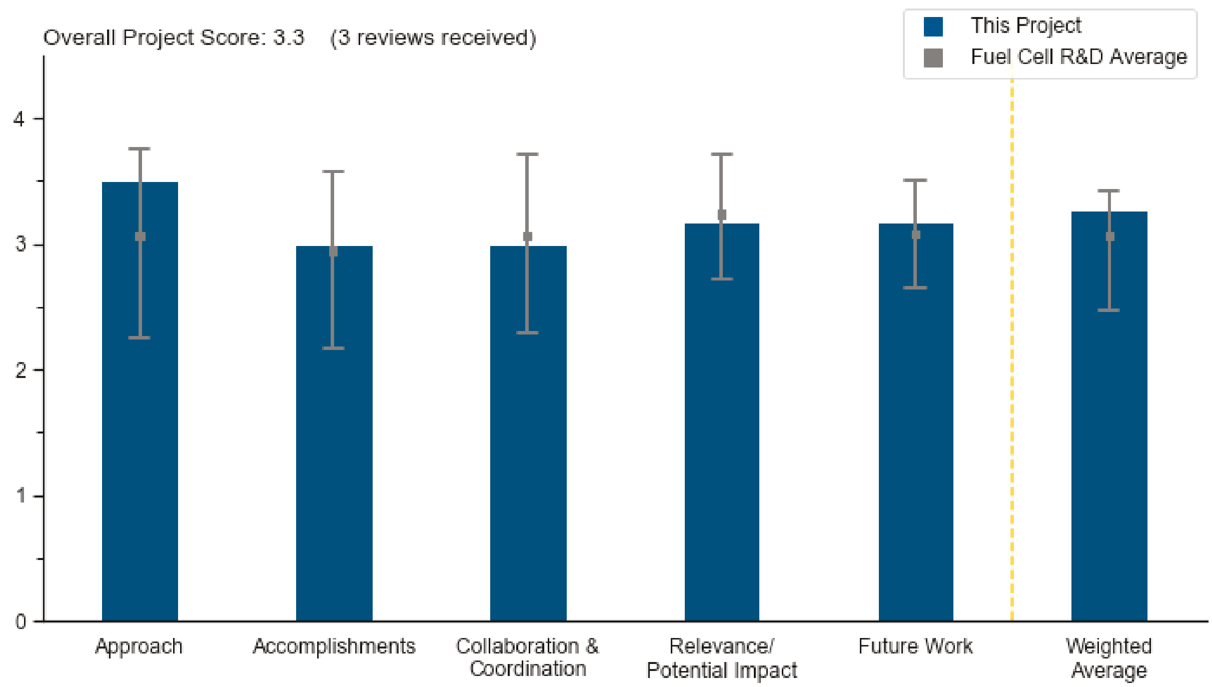
Project #FC-307: Cyclic Olefin Copolymer-Based Alkaline Exchange Polymers and Reinforced Membranes

Chulsung Bae, Rensselaer Polytechnic Institute

Brief Summary of Project

In this project, Rensselaer Polytechnic Institute (RPI) will develop a series of innovative ethylene–norbornene copolymer (ENC)-based alkaline exchange membranes (AEMs) that would overcome the challenges of the state-of-the-art AEM. Specifically, the project team plans to (1) develop ENCs with tunable backbone rigidity, (2) incorporate alkyl chain-tethered quaternary ammoniums (QAs) of different structures to the polymer by simple post-functionalization method, (3) impregnate the anionic polymers into a mechanically stable matrix (reinforced AEM), and (4) demonstrate the membranes' performance and durability in fuel cells using Pt-based and platinum-group-metal-free (PGM-free) catalysts. The reinforcement of AEM will allow RPI to produce thinner (e.g., 10–15 µm) membranes, affording lower area-specific resistance and better water management in MEAs, particularly with a PGM-free catalyst.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The technical approach is novel and reasonable, namely using no heteroatom (O or N) in the backbone for alkaline stability, using high molecular weight for good mechanical properties and dimensional stability, getting tunable rigidity by varying the ratio of ethylene and norbornene and cyclic olefins in the backbone, and using a pore-filling reinforcement framework for enhancing the durability and extending the lifetime of MEAs. Whether this is inexpensive remains to be seen. The more complex the synthesis in the commercial stage, the more impractical and expensive it will be to manufacture.

- The project addresses a number of issues with these polymers, including avoiding phenyl groups that poison the catalyst, as well as some chemical weaknesses in a system that should be fairly low-cost to produce.
- The project's approach is laid out in straightforward terms. The project team's partners are there to help with key parts.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has just started, so only the polymer has been synthesized. However, that is often done before the proposal, so the project might have gotten a little bit further done in the first tasks, especially some work toward the functionalization.
- This is a new project, but prior work indicates the team can do what they say.
- The project is around two weeks old; it is too early.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- There is a good combination of collaboration from academics (led by RPI), industry (Xergy), and national laboratories (LANL), with well-defined tasks and complementary skills.
- Kim at Los Alamos National Laboratory (LANL) is one of the premier scientists in this area, though it is not completely clear what his role will be; if it is only for testing, then that is a waste. Also, expanded polyethylene is likely a poor choice for a support material, and the team advertises that the base material should be strong, so it is not clear that this is needed.
- It is too early to answer in much detail.

Question 4: Relevance/potential impact

This project was rated **3.2** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project addresses a number of concerns for AEMs.
- The project offers some uniqueness of approach that opens up new possibilities.
- This relevance falls under a speculation on a speculation, which is not a good place to be. The authors have responded to the funding opportunity announcement, but the wisdom of this line of work (AEMs) is questionable. It is not certain that there is proof that AEMs will lead to making good and practical fuel cells and fuel cell power sources. These workers received a "good" rating for these reasons. Making these membranes is a bit speculative, and if there is success, then a good alkaline membrane is achieved—but it is not clear what good having a good AEM does for making a fuel cell and fuel cell power source. The former is the job of the research team; the latter is the responsibility of DOE management and remains to be seen.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- Durability is the last thing that the team studies, and it should be addressed much earlier; there is no point in pursuing these materials if they will not be stable. The other characterizations and testing are appropriate—it is just the order that is in question.
- The design of the experiment is reasonable for this new project.

Project strengths:

- The project's relevance is a strength, and the team is aware of the issues. As a collaborator, Kim should help and is a good choice for making MEAs. The approach is good, but it is doubtful that the project will get to MEA testing within 16 months from now; this schedule is a bit ambitious for a new polymer that has not even been functionalized.
- The project has good teaming. The academic team is good in small-scale synthesis, Xergy has proven support technology, and LANL is proven in assessing AEM technology.
- There are multiple opportunities for success in this project. The project seems focused in scope so as to better enable success.

Project weaknesses:

- The resistance targets seem quite ambitious. There is the additional difficulty of adding in reinforcement, which perhaps may dilute some from the core synthesis effort. Scaling up to larger batch sizes is listed as a challenge, but no clear path or process was given. There may be many challenges, including ionomer cleaning, separation, fabrication, testing, etc. It would be nice to see a few more details about this effort.
- Chemical durability should be moved ahead, and the project team should have some strategies for what to do next if the product is not stable; that is not addressed.
- There are no clear weaknesses at this stage of this new project.

Recommendations for additions/deletions to project scope:

- The real benefit of this work is to see whether this new synthetic approach leads to chemically and physically stable ionic membranes under fuel cell conditions. Once that is clear and a membrane gives satisfactory properties, then the next step is to see whether that membrane (or multiple membranes) is amenable to mass manufacturing (i.e., low cost).
- The project's tasks are all relevant, but moving chemical durability up earlier is suggested.
- The project team could perhaps provide a better breakdown of synthesis risks and mitigations.

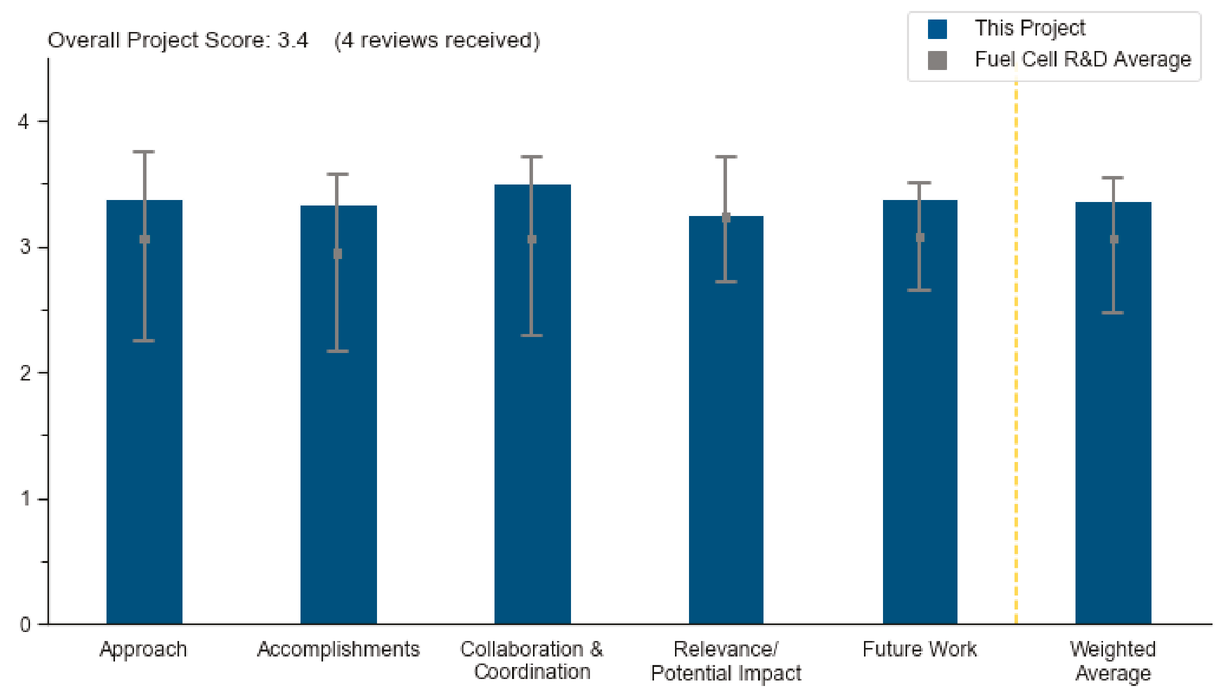
Project #FC-308: Advanced Anion Exchange Membranes with Tunable Water Transport for Platinum-Group-Metal-Free Anion Exchange Membrane Fuel Cells

Michael Hickner, Pennsylvania State University

Brief Summary of Project

This project will enable high-performance, long-lifetime, low-platinum-group-metal (low-PGM) (PGM loading ≤0.125 mg/cm^2) anion exchange membrane fuel cells (AEMFCs) through (1) synthesis and fabrication of novel thin, mechanically supported anion exchange membranes (AEMs) and electrode ionomers with validated outstanding water transport properties and stability; (2) integration of these new polymers with high-performing low-PGM and PGM-free catalysts and electrodes; and (3) precise control over the distribution of water in operating cells. What makes this project unique are the team's capabilities in new material synthesis to tune water transport and the world-leading knowledge in membrane integration with electrodes to achieve the current world-record performance in AEMFCs.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The two membrane metrics are reasonable and in the team's control: (1) develop novel poly(olefin) AEM chemistries with tunable water transport and (2) incorporate these novel ionomers into mechanical supports and integrate the resulting membranes into AEMFCs. The third performance metric seems beyond the scope of this project. For the third metric, the project title says "platinum-group-metal-free" (PGM-free), but the project talks about low-to-moderate Pt loadings. There is no path to PGM-free given, except on slide 12 of the presentation, which says that "risk will be mitigated by taking advantage of state-of-the-art catalyst for alkaline membranes that are reported." The project's approach is to develop novel poly(olefin)

AEM chemistries with tunable water transport. To facilitate high AEMFC performance, the fuel cells will have the following properties:

- OH- conductivities greater than 60 mS/cm at 60°C, 100% relative humidity (RH)
- Less than 10% degradation in conductivity after 5000 hours in 1 M NaOH at 60°C and 2000 hours in 1 M NaOH at 80°C
- A water diffusion coefficient >$5*10^{-6}$ cm^2/s (a 50% improvement over existing AEMs.

Additionally, the project team will incorporate these novel ionomers into mechanical supports and integrate the resulting membranes into AEMFCs. During operation inside the AEMFC, the membranes will have:

- Area-specific resistance values less than 100 mOhm×cm^2 over 2000 hours of operation
- Water flux greater than $2*10^{-5}$ mol $H_2O/cm^2 \times s$ to be able to back-diffuse 80% of produced + electro-osmotic water from anode to cathode at 600 mA/cm^2.

Finally, the project will demonstrate of all of the following DOE metrics in a single MEA with hydrogen and oxygen fuel:

- Greater than 2000 hours of AEMFC operation at 600 mA/cm^2
- An operating voltage greater than 0.6 V with less than 10% decay over 2000 hours
- Operating T ≥60°C and P ≤1.5 atm with PGM loading less than 0.125 mgPGM/cm^2

- There is very good focus on barriers relevant to AEM implementation. The poly (norbornene/olefin/long-chain quaternary ammonium) system appears to be well chosen, based on the principal investigator's prior experience and the rationale stated in the poster materials. The project has a target to more than double the water-diffusion coefficient from values in existing AEMs. The proposal does not provide the rationale for how the project team thinks they can accomplish that. One question is whether these polymers are more gel-like than existing AEMs. If so, it may be that the membrane mechanical properties are compromised by the liquid-water-like character. The information given in the poster is not enough to tell.
- The Pennsylvania State University (Penn State) is developing novel AEM chemistries with improved water transport. This will in turn result in improved AEMFC performance. The polyolefin-based chemistries hold promise for AEM membrane development. While the relationship between water transport and performance is clear, the link to durability is unclear and needs a better scientific basis. The team should add experiments to understand the link between enhanced water transport and improved durability.
- The approach of the project is to prepare polyolefin membranes for AEMFCs. Synthesizing polyolefinic membranes may improve alkaline stability, although this approach has been tried by one of the project team members and other researchers. The approach to preparing membranes with a high water-diffusion coefficient is not well justified, although there are not any major issues with it. First, the slide does not show a clear relationship between the water-diffusion coefficient and AEMFC performance. Second, the diffusion coefficient target ($2*10^{-6}$ cm^2/s) is rather arbitrary. Third, the presentation does not explain how the proposed polymer can have a high diffusion coefficient. The final issue is that, while the project title indicates these membranes are for PGM-free AEMFCs, the benefits of these membranes for PGM-free AEMFCs are not apparent. It is not clear how high water transport helps use PGM-free AEMFCs.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Slides 6 and 7 show syntheses done up to the 4 g level. This is very impressive for a new project that began a half year ago (in late 2018). If the team keeps up this pace of work, then the "nobornyl concept" for making stable and conductive water-transport AEMs should be checked during this work.
- This project is about 16% spent in 5 months. Given the early stages of this project, there is significant progress, especially from Penn State and the University of South Carolina (USC), with over 80 polymerization batches conducted, membranes developed, and initial fuel cell performance reported, albeit at very high loadings.
- Good progress has been made on synthesis, but in other areas, progress is hard to determine at this early stage. Lifetime testing will be especially hard to gauge until membrane fabrication is well along.
- It seems the project has started with some tryouts for polymer synthesis. However, it is too early to review the progress of the project at this moment.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The project's teaming is excellent, comprehensive, and complementary for four team members' making membranes. The work for low-PGM is reasonable; for no-PGM, the work is questionable. The four teams are (1) Penn State, which makes new polymer; (2) USC, which is responsible for electrode formulation, cell testing, and water transport studies, including neutron radiography; (3) National Renewable Energy Laboratory (NREL), which is responsible for lifetime testing and water balance studies; and (4) 3M Company (3M), which is responsible for membrane coating and supported membranes.
- The team is well organized. Penn State has been working in this area for a long time. USC is known to be an expert on MEA fabrication and fuel cell testing. NREL can accomplish the job as stated. 3M has extensive experience in synthesizing chain-growth polymers.
- This is an excellent team. Penn State is making the polymers and membranes, USC is developing electrodes, NREL is responsible for lifetime testing and water balance, and 3M is developing the supported membranes. This is a very experienced team.
- The first round of newly synthesized polymers have been sent to partners at NREL and USC, and the early-stage results for hydrogen and oxygen cells are in hand. This is good progress for only a few months in. There are no results from the collaboration with 3M yet; presumably that comes later.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project has a goal to meet all DOE targets simultaneously (>2000 hours at 600 mA/cm^2 with V >0.6 V and <10% decay with T >60ºC, P <1.5 atm, and PGM loading <0125 mg/cm^2). If the project meets these goals, it will have significant impact on the DOE Hydrogen and Fuel Cells Program.
- The project's relevance and potential impact are excellent.
- This work is commendable, but it remains a speculation (of whether the membranes can be made with suitable properties) on a speculation (that John R. Varcoe of the University of Surrey is correct that AEMs are good). Yet another speculation is that PGM-free catalysts will work. The only durable alkaline fuel cell is the one that is used in space, which uses pure oxygen and hydrogen, as well as noble metal catalysts. Once again, the DOE has "bid on questionable work" from outside the country. The team has responded with great relevance to the funding opportunity announcement. The potential impact for making a practical fuel cell and fuel cell power source system is questionable for the reasons stated above. The question of making a practical fuel cell and fuel cell system is the responsibility not of this project's research team but of DOE management.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The two membrane goals are good. The catalyst goals are highly speculative and questionable. The first membrane goal in fiscal year (FY) 2019 is to synthesize larger-scale batches of polymer with vinyl-norbornene motif and to fabricate supported membranes. The team will also continue to optimize electrode structures and cell conditions to meet milestones and the year 1 go/no-go for performance and durability at required loadings. The team will also measure water transport in membranes using pulsed field gradient and nuclear magnetic resonance (PFG-NMR) and connect cell water transport observations using water balance measurements. Next year, the second membrane goal in FY 2020 is the fabrication of high-performance supported membranes and the optimization of electrode structures and cell conditions that will allow for progress on year 2 milestones. The project team will also develop strategies for increasing durability by modifying cell water transport. The team will also develop a holistic picture of water transport in AEMFCs using neutron radiography. The catalyst goal is that risk will be mitigated by taking advantage of state-of-the-art catalysts (PGM-free seems improbable) for alkaline membranes that are reported. The major risks will be in approaching required (possibly PGM) catalyst loadings while still reaching durability targets. Particularly worrisome is the durability of PGM-free catalysts. If these existed, they would presumably be being used in the space program.

- All the 3M work and NREL work is proposed in FY 2020. Currently, all major milestones are related to AEMFC performance, which is very good for judging progress. However, it would be good to have some milestones associated with the water transport work and durability work and how those are linked.
- The project's proposed future work is good. More membrane characterizations beside the water transport measurement should be listed (e.g., ex situ membrane stability, conductivity, etc.) before putting the membranes in the MEAs. No pathway for incorporating PGM-free catalysts can be seen.
- The project's proposed future work seems reasonable.

Project strengths:

- The overall strength of the project is teaming for the project. The team is capable of preparing a series of membranes for optimum performance. Penn State has a good track record for delivering the products, so much progress is expected next year. The other strength of this project is that the performance milestone is challenging, which is very much appreciated. Just one suggestion would be that the go/no-go decision (in month 12) should include the catalyst loading target (0.3 mg/cm^2). If the team does not meet the interim loading target, then it is likely that the team will not meet the quarter 6 (Q6) target with loading <=0.125 mg/cm^2.
- The project's strengths include its good teaming. The team has a complementary and comprehensive set of skills, including Penn State's skills in new synthesis, USC's skills in characterization, NREL's skills in durability, and 3M's membrane supports. However, new catalysts are an "Achilles' heel"; it is doubtful a PGM-free catalyst will be seen in our lifetime.
- The project's strengths include its use of a robust polymer synthesis system and its choice of partners, which will enable the team to make and evaluate large amounts of AEM using methods suitable for scale-up and manufacturing.
- This is an excellent team with complementary strengths.

Project weaknesses:

- The overall weakness is that the project is based on the idea that water transport is the single most important factor for AEMFC performance and durability. It may be true, but in case this is not the decisive factor, then the whole project may go in the wrong direction. The membrane milestone is not challenging (40 mS/cm at 60°C). Those targets with quaternized polyolefinic polymers have been achieved by a couple of projects. USC has demonstrated over 2 W/cm^2 peak power density with its polyolefinic membrane and ionomers. It is unknown how much better performance can be achieved with highly water-permeable, "more advanced" polyolefinic membranes. It is understood that this is not an AEMFC project but an AEM project. However, if the project does not achieve better performance, better durability (>2,000 hours in fuel cell operating conditions), or low PGM loading (<0.125 mgPGM/cm^2), the advantage of using the proposed AEMs for AEMFCs may be too small. A clear pathway for achieving those challenging targets is not apparent.
- The project team needs to quantify "larger-scale" batches. The current loading (as seen on slide 8) is way too high and needs to be lowered soon. It seems like the cell has some transport issues, even in oxygen. A systematic study of those limitations and how they can be overcome with advanced membranes should be added.
- The linkage between polymer structure and the desired AEM property improvements has not emerged from results to date. This may reflect the fact that the project is still in a synthesis-heavy phase, with the first round of feedback from measurements not yet completed.
- PGM-free catalysts are highly speculative, and an especially speculative idea is that there are ones that are durable.

Recommendations for additions/deletions to project scope:

- A recommended addition would be to the go/no-go decision point: an interim total PGM-loading target is needed. Regarding deletions, the target for the later stage of the project is overly challenging. Either the 500-hour H_2/air (CO_2-free) or 2000-hour H_2/O_2 target can be deleted and modified to some progress measure, e.g., 100-hour H_2/air (CO_2-free) for Q7 and 500-hour H_2/air (CO_2-free) for Q8.
- The project team should forget about catalysts and do what they do best and check whether they can make durable membranes that operate under fuel cell operating conditions with low-PGM catalysts.
- The project is off to a good start. Seeing the progress in the coming years is gladly anticipated.

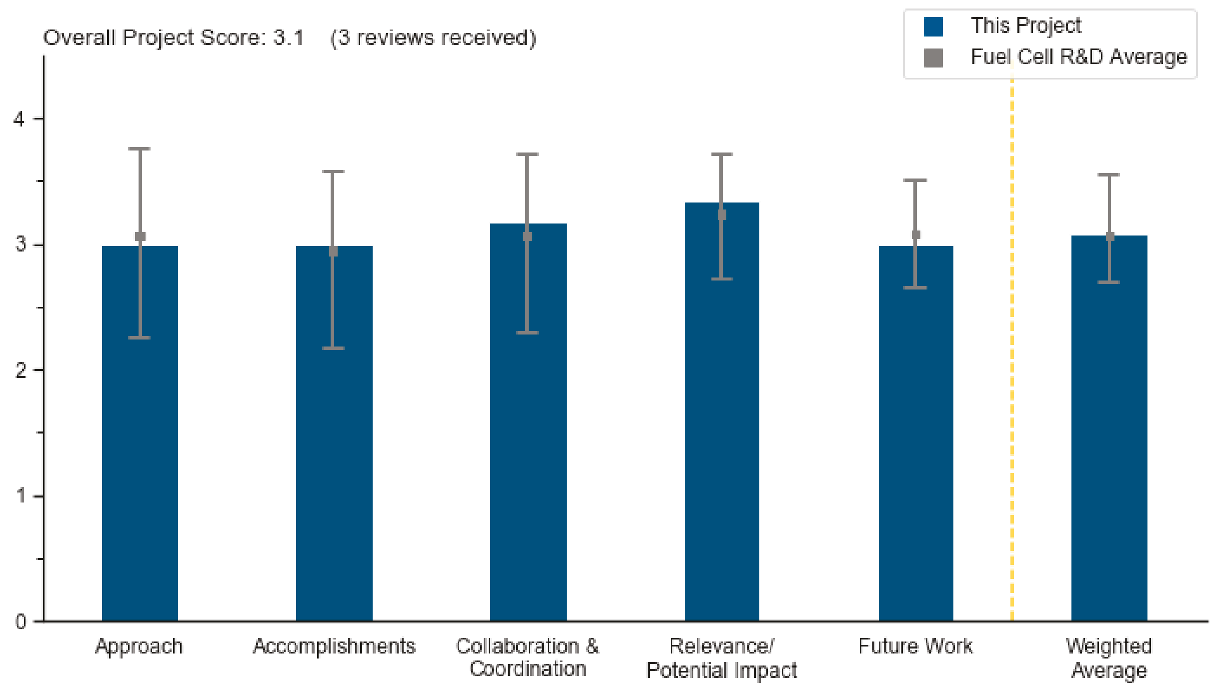
Project #FC-309: Polymerized Ionic Liquid Block Copolymers and Ionic Liquids (PILBCP-IL) Composite Ionomers for High Current Density Performance

Joshua Snyder, Drexel University

Brief Summary of Project

The project's goal is to develop a polymerized ionic liquid block copolymer/ionic liquid (PILBCP/IL) composite ionomer to replace traditional perfluorosulfonic acid (PFSA)-based ionomers and address their associated limitations. The expected outcomes include (1) development of a cathode that meets U.S. Department of Energy targets for low and high current density (HCD) and (2) improved understanding of how interface engineering affects HCD performance. The project will develop the PILBCP/IL ionomer and then develop and study membrane electrode assembly (MEA) performance and durability. The project addresses the primary technical barriers associated with (1) oxygen transport through ionomer thin films, (2) ionomer-specific adsorption onto catalyst, (3) inaccessible catalyst in porous carbon supports, (4) distribution and retention of IL in catalyst layers, and (5) humidity tolerance at HCD (Pt utilization).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- PILBCP/IL is a good concept for enhancing catalyst mass activity and thereby achieving increased cell performance under low humidity conditions. Covalently bonding the IL is a great approach to immobilize the IL into the catalyst ionomer interface and provide consistent higher catalyst mass activity and proton transport. The team should address the issue of IL leaching during fuel cell operational conditions.
- Using protic IL additives to improve access to catalysts is sensible and has been shown to work in prior efforts. The present approach builds on this prior work using copolymers with immobilized ionic groups to

prevent the loss of IL. This approach may work, though it appears that gradual IL loss could occur if the ionic groups from the two parts of the polymer combine with each other to release their counterions. This situation could result in dissolution of bis(trifluoromethanesulfonyl)imide (HTFSI) into the fuel cell exhaust. If this happened, it could result in significant and irreversible long-term performance loss. The team should be on the watch for this. Also, the polymers the researchers are proposing may be subject to degradation during long-term fuel cell operation.
- Some groups have tried to use ILs in catalyst layers without much significant success, but this group's approach with PILBCP/IL may work. This project is also targeting key technical barriers.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This is a new project that started in October 2018. The team has demonstrated increased cell performance and higher catalyst mass activity using IL [MTBD] [beti]. The team has also demonstrated higher electrochemical surface area and lower Pt dissolution using IL. The team has also shown intermediary IL thin-film formation with the Nafion™ ionomer.
- This project has started recently, and the team can leverage a lot on a previous General Motors Company (GM) project, which studied similar technical barriers. The team tried some IL deposition techniques and preliminary ex situ tests, which is also encouraging. Establishing a baseline or benchmarking against conventional Nafion should be the first step in MEA. This is planned, as outlined in future work.
- The project is at an early stage (7% complete, having started in October 2018), so few new results are expected. The poster mostly presented results from the prior funding period using [MTBD] [beti], which is intriguing. The new findings on the capacitive deposition of IL are intriguing but are at an early stage.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The team is composed of excellent research institutions conducting effective research in fuel cells. The team is a good combination for pursuing the proposed work and includes the principal investigator, Drexel University, and sub-contractors GM, Texas A&M University, and the National Renewable Energy Laboratory (NREL).
- Collaboration among team members is key, and this team has all the relevant and capable members (from industry and academia) to make it successful.
- The team appears to be well chosen, but the poster did not clearly show how the work was distributed among team members.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Improving HCD performance could result in cost reduction, so this project is well aligned with the DOE Hydrogen and Fuel Cells Program's (the Program's) research and development objectives. Improving HCD performance with a low Pt-loading catalyst has been a great challenge in recent years, so positive outcomes in this project would be very helpful.
- The project is relevant to developing a fuel cell cathode that meets the DOE targets for low and high current density and performs under low humidity conditions. The use of IL to boost specific and mass activities of the catalyst is directly linked to DOE's goal of catalyst performance enhancement.
- The project is targeting improvements in metrics relevant to the Program's goals.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The team has listed and described the future work very well. All the relevant tasks needed for the success of this project have been captured.
- The future work looks like it would take lot of knowledge gained from past GM projects, which is a plus. Additionally, the team should try MEA testing first to make sure it works before spending too much effort on understanding the underlying fundamentals using ex situ tests.
- The future work seems appropriate. The project is still at an early stage; the team needs to make progress on the synthesis work on new polymers so that other project areas can move forward.

Project strengths:

- The team is very strong and capable of meeting the challenges of this project. The tasks are appropriately shared between the prime and sub-partners, as per their technical expertise. This approach is very effective in enhancing the catalyst activity under stressed operational conditions, such as low relative humidity. The inclusion of an industry partner (GM) and a national laboratory (NREL) allows the team access to a significant fuel cell network for accomplishing the project.
- The very capable team is the project's strength. Each team member has the respective expertise to make this project successful. GM's significant previous work can be leveraged by the team to move the project along quickly.
- The project provides a rational approach to improving electrolyte access to all catalyst particles in high-area supports, which should improve performance under high-rate conditions.

Project weaknesses:

- The project's weaknesses include cost; the DOE mandates low-cost fuel cell systems to meet commercialization targets, and IL is expensive. The incorporation of IL in block copolymer is also a very cost-intensive proposition. It is very unlikely that the proposed effort is going to be a cost-effective approach to the development of high-performance fuel cell MEAs. The project also faces weaknesses in terms of durability. To meet the desired cost objectives, DOE targets high-durability MEAs. Being hydrophilic, the IL additive is expected to leach out through the product water in the cell. This leaching will lead to the loss of catalytic activity and catalyst–ionomer interfacial proton conductivity and, therefore, an increase in cell impedance, resulting in poor cell performance and the loss of stack performance over time. Plug Power Inc. and the Rensselaer Polytechnic Institute team experienced the same phenomenon with their DOE-funded project for phosphoric-acid-doped polybenzimidazole membrane development. The copolymerized IL from the block copolymer may be stable and not leachable; however, the free IL has a very high chance of getting leached and affecting the stack performance durability. Also, the leached IL may contaminate the balance of plant, leading to unintended consequences. The project also has a weakness in terms of ink fabrication. The capacitive deposition of IL onto the catalyst surface adds increasing steps, which may increase the cost of ink fabrication. This increased ink cost will ultimately increase the total MEA cost, which is not aligned with DOE's mandate.
- The use of IL additives may suffer from a weakness of poor long-term durability due to eventual loss of IL in the exhaust, especially if the IL has high water solubility. The team should watch for this. Additionally, the polymer's chemical structure may suffer its own degradation, e.g., from hydroxyl radicals or other oxidative species known to be present in H_2/O_2 fuel cells.
- Based on some preliminary results, it is assumed that PILBCP/IL will work in MEAs, which can be very tricky. There are many unknowns with this material; Nafion in the catalyst layer systems has been studied extensively by various groups, so it is pretty well understood. Pt and Pt-alloy interaction with this new polymer IL is unknown, and its effect on durability is also unknown.

Recommendations for additions/deletions to project scope:

- The team should consider developing a means of monitoring IL loss into the output stream, perhaps using methods similar to those used to monitor the fluoride loss associated with polymer electrolyte membrane degradation.
- No additions or deletions to this project are needed. The project is fine as proposed.

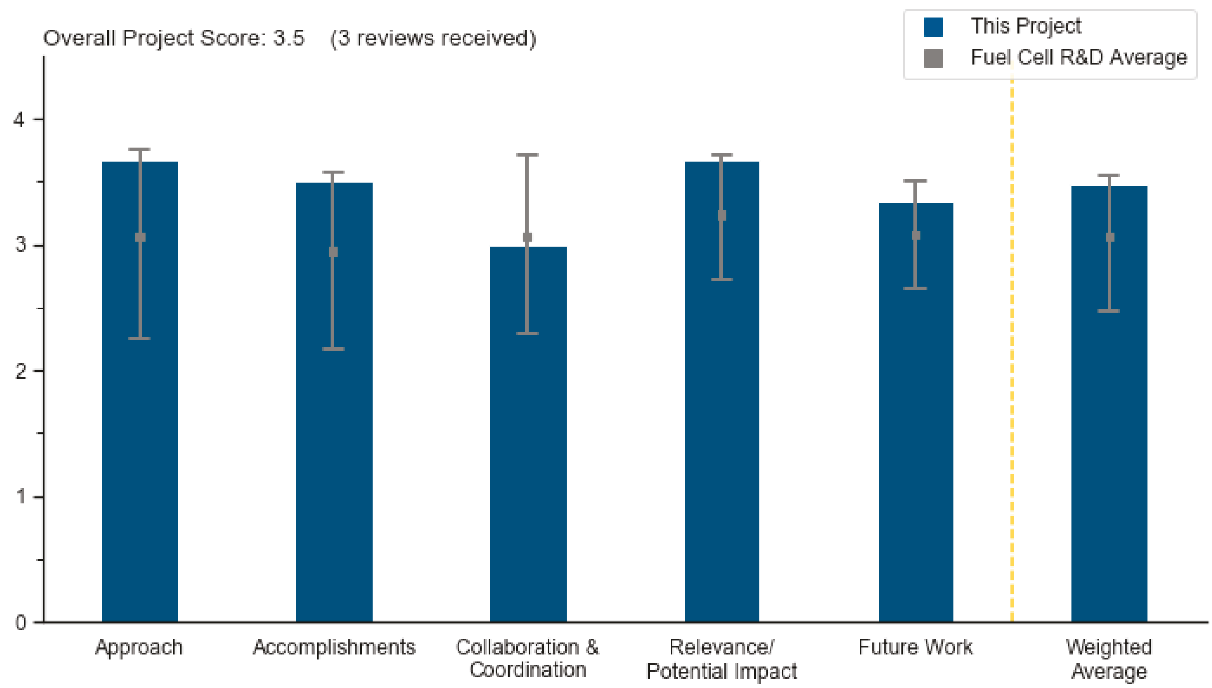
Project #FC-310: Composite Polymer Electrolyte Membranes from Electrospun Crosslinkable Poly(Phenylene Sulfonic Acid)s

Ryszard Wycisk, Vanderbilt University

Brief Summary of Project

The project objective is to fabricate a novel electrospun, non-perfluorosulfonic acid (non-PFSA) fuel cell membrane that meets all 2020 technical targets in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan. The project approach is to develop/fabricate a robust, low-cost composite all-hydrocarbon membrane via dual fiber co-electrospinning of a crosslinkable poly(phenylene sulfonic acid) (cPPSA) and poly(phenyl sulfone) (PPSU) mixture mat, followed by mat densification via solvent-vapor-induced softening of PPSU fibers and thermal crosslinking. The project addresses the barriers of (1) the high cost of PFSA membranes, (2) low proton conductivity at reduced humidity (water partial pressure), and (3) performance drop above 80°C.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project takes over from prior work performed at Case Western on similar composite membrane systems. The team has just started working on this project, and it is too early to assess performance. Generally speaking, the idea of combining fibers with ionomers remains very promising. In this project, the fibers and ionomer share similar chemical structures, which ensures excellent interfacial properties. The researcher has a strategy for eliminating voids in the structure, and it will be interesting to see cross-sectional views of the overall structure once membranes are produced. One concern with this technology is the viability of the chemistry, from a chemical resistance and durability standpoint, inside fuel cells and electrolyzers. Durability should be investigated. In addition, the principal investigator (PI) mentioned that

there is some issue with brittleness in prior structures produced at Case Western. Therefore, mechanical properties will need to be investigated. Nevertheless, this project is off to a good start.
- The approach and combination of electrospun and previous high-performing polymer is interesting and provides good synergy, assuming that it is processable.
- This is a polymer electrolyte membrane fuel cell technology project. The approach is membrane synthesis using a combination of electrospinning and subsequent densification (solvent vapor + thermal crosslinking). The project tries to combine individual successes of two previous projects into one material.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has started to get materials and equipment together. The first materials were successfully synthesized.
- It is too early to comment. Overall, this project is off to a good start. The PI has properly identified issues to study.
- The project just started, with minimal work accomplished before the slides were due.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- This is an academia-lead project with one university. It was unclear how the partners would communicate and/or interact with each other. The roles of individuals was laid out, but no interaction between the institutions was presented that showed any material, sample, or information exchange. Slide 6 states that Los Alamos National Laboratory (LANL) is performing fuel cell testing in year 2, but it is unclear how LANL is tied into this project.
- The overall collaboration is sufficient, although further testing and characterization is recommended, perhaps at a national laboratory.
- It is too early to judge collaboration and coordination. Collaborations were not discussed specifically.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Ionomers are inherently weak. Any approach to making new and different composites should be investigated in addition to fundamental work on ionomer synthesis. Both processes must be done. This is a novel approach, and it will be interesting to see progress reports in future Annual Review Meetings.
- The project topics are right on target with the technology’s advancement and DOE’s goals. Reduction of cost toward available cost-effective membrane materials is important. If at the same time the resistance can be improved, specifically at temperatures greater than 80°C, performance improvement could be achieved.
- The project aligns well with the membrane targets, assuming cost projections and durability are met. It has yet to be determined whether compatible electrode ionomers will be found, which could be an issue that minimizes impact.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- Overall, this is a very sound, comprehensive project plan.
- The project just started. The statement of work seems appropriate.

- There needs to be further property testing and full characterization of the membrane, including mechanical properties, uptake, conductivity, water diffusivity, etc. The focus on synthesis makes sense, although it is unclear how it is a true composite membrane.

Project strengths:

- This is a different approach to composite membrane production. It should be explored, and it should be determined whether the approach has merit. It is more about the approach than the specific chemistry of the project. The industry needs to develop “technology platforms” that can be useful with different chemistries for different applications. Some similar work has been reported at other institutions, and this area should be reviewed as part of an overall approach. The industry needs to fundamentally understand whether this approach has merit.
- The project has a strong background and previous success in similar projects, which makes this project very promising. Successfully developed materials would not be limited to one application but could be applied to multiple technologies.
- There is good synergy of a processing technique and a novel polymer that have both demonstrated good results independently.

Project weaknesses:

- It is unclear how the partners interact and help each other to achieve their project goals.
- It is unclear whether this chemistry is fundamentally stable in actual applications and whether the final mechanical properties meet application requirements. Both research questions need to be tested as part of this project.
- The project seems too empirical and relies on the need to address several key issues, such as carrier polymers, solutions, heat treatment, etc., by formulation processes.

Recommendations for additions/deletions to project scope:

- It would be good to see more knowledge gained in terms of key processability and transport parameters that can be used for other polymer systems. More experimental characterization of polymers would be helpful.
- In situ (or application-oriented) testing must be done. Perhaps the PI needs industrial partners that can assist with this effort. That should be added as part of the scope of work.
- So far there are not significant results or progress, which is expected since the project has just started.

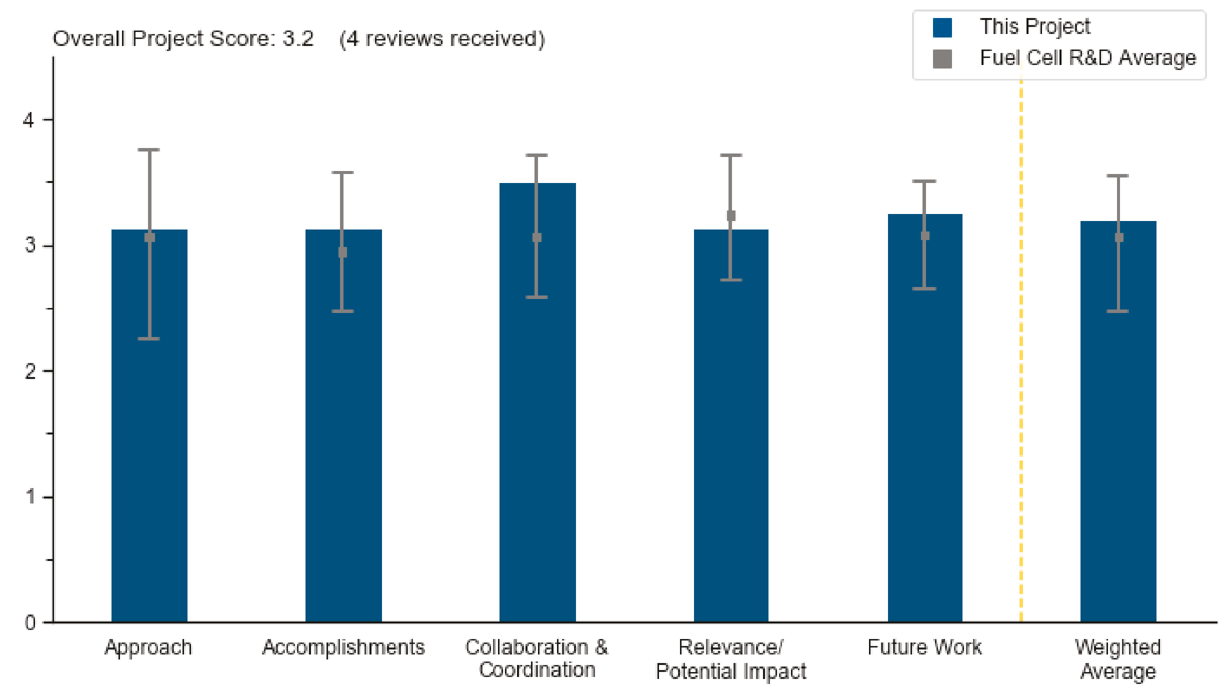
Project #FC-311: Novel Non-Perfluorosulfonic Acid Proton Exchange Membrane for Fuel Cell Application

Taoli Gu, Xergy, Inc.

Brief Summary of Project

This project seeks to develop a novel composite polymer electrolyte membrane (PEM) using uniquely designed hydrocarbon-based aromatic sulfonated polymers and reinforcement technology to meet the U.S. Department of Energy's durability, cost, and performance targets for PEM fuel cell electric vehicles (FCEVs) and provide enhanced characteristics over state-of-the-art PEMs. The project will synthesize a novel BP-Ar_3 ionomer, incorporate the ionomer into porous support materials, characterize a membrane electrode assembly (MEA) based on the technology, and conduct a cost analysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Xergy, Inc. (Xergy) has an interesting and novel approach for hydrocarbon membranes. One of the long-standing challenges of aromatic sulfonic acids is the low conductivity at low relative humidity (RH). The side chain structure might change the morphology enough to improve this property. Comparisons of conductivity as a function of RH with traditional perfluorosulfonic acids (PFSAs) would be valuable and a true measure of advancement over the existing hydrocarbon options.
- The synthesis of a partially fluorinated, aromatic sulfonated hydrocarbon membrane (called BP-Ar_3 PEM) and the optimization of the sulfonation of ionomer precursor to synthesize the BP-Ar_3 PEM ionomer are reasonable new membrane technology. The questions to be answered are about physical stability (i.e.,

shrink and swell) and conductivity as a function of humidity. These can be solved but certainly need to be optimized.
- The approach of using multiple proton-exchange sites in a single side chain is not new. In the past, 3M has demonstrated this strategy with PFSA-based ionomers to achieve higher proton conductivity. This approach is expected to provide higher proton conductivity per unit area, with the possibility of increasing the performance density of the fuel cell stack.
- The approach is interesting in that it will result in highly aggregated functional groups, which has been shown to be very beneficial for low-RH conductivity. The concept completely ignores years of history and learning in sulfonated aromatics, and there is no reason to believe that these polymers will have better durability than those membranes. There are numerous vulnerable spots for OH to attack, on both the main and the side chains, and especially the functional group itself. Also, a post-sulfonation of the aromatic groups will leave a sulfonate group that can easily be removed, as McGrath showed conclusively. A review of the history of sulfonated polystyrene/divinylbenzene, as well as the Ballard membrane and many other membranes that have been tried over the years, would make one hesitate before going down this path. Finally, using porous polyethylene will be very difficult, particularly if the team wants to hot press electrodes at some point, as that will erase the polyethylene porosity.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project started in March 2019, and the team has developed, optimized, and scaled up the synthetic pathway of the BP-Ar_3 PEM ionomer precursor. The proton nuclear magnetic resonance (NMR) shows that the team is able to make pure BP-Ar_3 PEM ionomer precursor.
- Slide 6 shows that polymer has been made on a small scale at Rensselaer Polytechnic Institute (RPI). Slide 9 shows that support of the membrane is available from Xergy. Characterization in fuel cells can be done at the University of Delaware (UD), according to slide 10.
- The project has just started, so it is hard to know; the team has made the polymer, so that is a good start.
- This project is in its first quarter. The plan looks good, but expectations for progress are minimal at this time.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The project has good teaming and division of labor. RPI is doing polymer synthesis, Xergy supported the membrane-making, and UD is doing MEA and fuel cell testing.
- The collaboration between the principal investigator (Xergy) and subcontractors (UD and RPI) makes sense. With their unique expertise, all three entities are complementary to each other in running this project.
- Xergy, RPI, and UD are all well-respected organizations. The project looks to have a good balance of skills.
- The partners are well qualified but not yet engaged, so the collaboration cannot be judged at this time.

Question 4: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The development of a novel PEM that uses hydrocarbon ionomer and low-cost reinforcement is needed to meet DOE’s performance, durability, and cost targets for the commercialization of FCEVs. The proposed project addresses the key issue of increasing fuel cell power density via an increase in membrane conductivity, which will help FCEV manufacturers make miniaturized, high-power-density fuel cell stacks.

High-density fuel cell stacks would also make a big impact on miniaturizing the balance of plant of fuel cells in the vehicle.
- This project could lead to low-cost fuel cell (BP-Ar_3 composite) membranes, but the durability of the novel BP-Ar_3 composite membrane is unknown and remains the greatest challenge.
- This project might develop some knowledge regarding structure and property relationships, as these polymers should have very high local charge densities. There is no reason to believe these polymers will have appreciable lifetimes in a fuel cell operating at relevant temperatures.
- While a low-cost, high-performing membrane is always desirable, it is unclear that this approach can truly compete with well-established PFSA technology. A lower cost alone will not be enough unless the performance and durability match, or exceed, that of PFSAs.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The team has clearly described the project's future work for fiscal year (FY) 2019 and FY 2020. The future work has been adequately divided between the team members on the basis of individual team expertise.
- This project has the potential to advance the state of the art in hydrocarbon membranes. The project's future plans look reasonable for evaluating this approach.
- As the greatest question with these polymers is of durability, this should be addressed early. The investigators recognize that this is the largest challenge for these films, but they address only mechanical durability, not chemical.
- The researchers have restated their goals, but there are no design-of-experiment details for how they will meet these goals. The team is to scale up in 2019 and develop a membrane in 2020. The team sounds confident, but this seems improbable. It is unclear how the team can scale up and make membranes when the team members do not even know the stability of the optimized polymer membrane yet.

Project strengths:

- The project team is very strong and knowledgeable in the field of the proposed work. The tasks were appropriately divided between the team members on the basis of their technical expertise.
- The main strength of this project lies in the unique aromatic sulfonic acid side chain. If this structure can improve on the conductivity at low RH compared to traditional, backbone, aromatic sulfonic acids, then the project will be a success.
- The project has a good division of labor, with RPI on synthesis, Xergy on support, and UD doing testing.
- The polymer structure addresses the need for high localized charge density.

Project weaknesses:

- A major weakness for all hydrocarbon membranes is oxidative stability. The team has a good plan for mechanical stability through reinforcement, but chemical stability may still be insufficient for many applications. If the conductivity as a function of RH is the same as with other hydrocarbon ionomers, then this approach has not much advanced the state of this class of membranes. However, the project is well suited to answer this question.
- The approach of using multiple proton-exchange sites that are anchored to the single side chain has been attempted in the past by 3M in a DOE-funded project. That project suffered significant issues with swelling and high water retention (MEA flooding), despite the expanded polytetrafluoroethylene (ePTFE) reinforcement. The current team's similar approach may encounter similar hurdles.
- The project completely ignores scores of years of experience that says that these chemistries are not stable in a PEM environment.
- Very little detail was given on how the project's goals will be achieved.

Recommendations for additions/deletions to project scope:

- No addition or deletion is needed in this project. The project is fine as proposed.
- As the team states on slide 9, the "durability of the novel BP-Ar_3 composite membrane is unknown and the greatest challenge. Team will systematically identify failure modes." This is the top priority, as this is really the main thing this project offers.
- The project needs to add a chemical durability component, as well as ways to mitigate this issue. This may perhaps be partial fluorination. Ce has been shown to be ineffective in these systems.
- Comparison to well-established PFSAs and traditional hydrocarbon ionomers (if available) would highlight the potential (or lack thereof) for this approach.

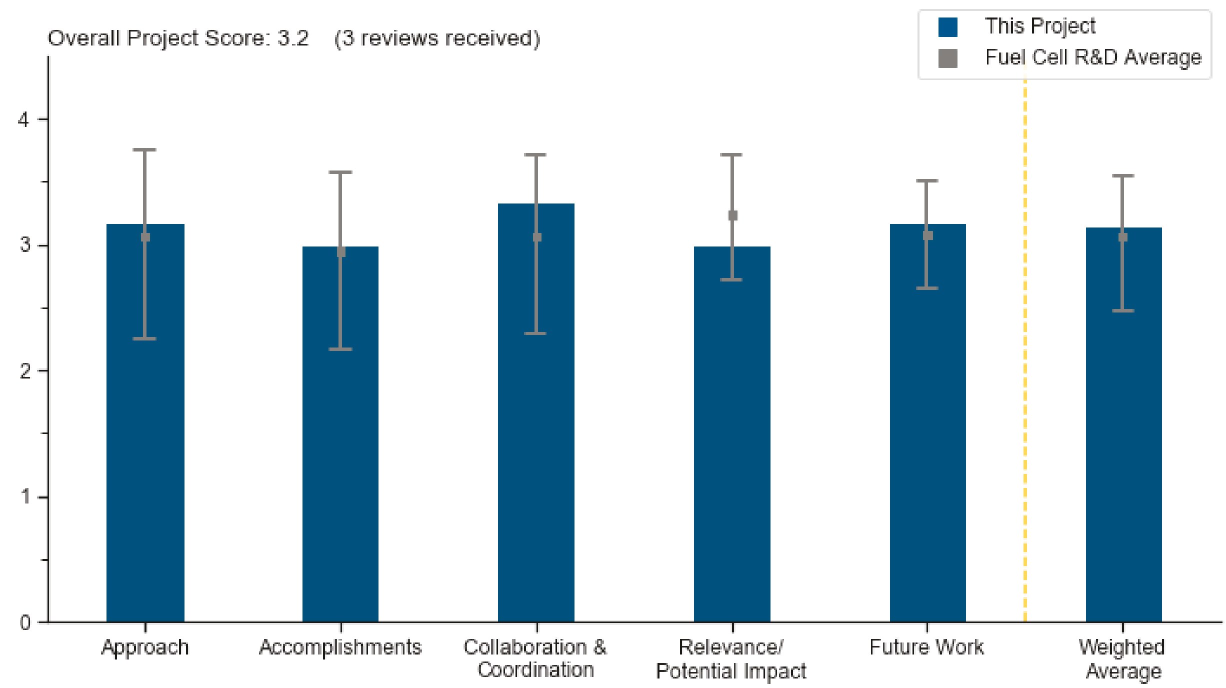
Project #FC-312: Molten Hydroxide Dual-Phase Membranes for Intermediate-Temperature Anion Exchange Membrane Fuel Cells

Patrick Campbell, Lawrence Livermore National Laboratory

Brief Summary of Project

This project will demonstrate the performance of molten hydroxide dual-phase membranes as anion exchange membranes (AEMs) in intermediate-temperature, air-oxidant compatible hydrogen fuel cells. The dual-phase molten hydroxide/ceramic support membrane being developed utilizes steam-based carbonate management and works at intermediate temperature to enable superior fuel cell performance and simplified operation. The project aims to (1) achieve ionic conductivity of greater than 600 mS/cm, (2) produce a complete fuel cell assembly with a membrane area greater than 50 cm^2, (3) validate that a steam-based carbonate management approach is effective during long-term operation, and (4) demonstrate high performance across an intermediate temperature range of 150°C–400°C.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach of molten hydroxide/ceramic support membranes utilizing steam-based carbonate management has been demonstrated to work at intermediate temperatures. This is expected to enable superior fuel cell performance and simplified operation due to efficient carbonate management.
- This is an interesting approach to alkaline fuel cells, utilizing a porous ceramic support for molten hydroxide ionomer. The method for carbonate management is novel and has the potential to reduce the impact of CO_2. The project has achieved high ionic conductivity so far, but the membranes are thick, and the area-specific resistance (ASR) is high at 0.5 ohm cm^2, more than an order of magnitude higher than

polymer electrolyte membranes (PEMs). The thickness of the membranes and supports needs to be <100 microns to get close to the ASR for polymer AEMs or PEMs. This will require a membrane 5x–10x thinner than what the team is making. The durability of porous ceramic membranes that are less than 100 microns thick could be an issue. Mechanical durability does not seem to be addressed in the approach.
- The project's approach involves dual-phase molten hydroxide/ceramic support membranes with steam-based carbonate management. The dual-phase membrane approach seems reasonably straightforward and sound. However, there is very little detail on the steam-based carbonate management. It is not clear what the mechanism is or whether peroxide is formed from the water to convert the carbonate to CO_2. This needs to be better demonstrated in this project; a detailed mechanism should be proposed and validated. The approach should also target thinner membranes to get to lower ASR.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has achieved good pore size distribution with a majority of pores <100 nm. The approach of dip coating for edge sealing has promise, but the team needs to demonstrate that it is gas-tight. The test station is assembled, which allows for testing. The project has just begun and is only about six months along.
- Good progress has been made, given that this project started in October 2018 and is only 20% spent. The team has already made porous supports and incorporated 1:1 NaOH–KOH into those. However, the ASR of 0.5 ohm cm^2 is still too high. The 50–80-micron-dense yttria-stabilized zirconia (YSZ) coatings over the sealing area seem to work. It will be good to see fuel cell results from these soon.
- The team has successfully demonstrated the fabrication of <500-µm-thick porous membrane support with no defects. However, in typical AEM fuel cells, the electrolyte thickness is <50 µm to achieve low cell resistivity and high power density. Porous membrane supports that are <500 µm thick may be adequate for the solid oxide fuel cell (SOFC) architecture, as it operates at much higher temperatures (>800°C), but it is not clear how such a thick electrolyte will perform at intermediate temperatures. Preliminary electrolyte conductivity measurements with 1:1 NaOH–KOH at 200°C showed a conductivity of 196 mS/cm, which is lower than the project goal of >600 mS/cm. The electrolyte thickness needs to be decreased to achieve such high electrolyte conductivity. The team may also need to determine the conductivity improvement that the present electrolyte could achieve by increasing the temperature to 300°C or 400°C.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The team has a very good commercial partner, OxEon Energy LLC (OxEon), who will be providing fuel cell and electrolyzer expertise that is needed for this project. The team also has the right collaborating partner for design consulting and testing capabilities. FCA US LLC is well known for providing support to these aspects.
- Lawrence Livermore National Laboratory (LLNL) has a technology and has partnered with OxEon for this project. LLNL also has three patents and/or applications on this technology. The team should clarify whether OxEon plans to license these patents if this project is successful.
- The initial efforts suggest that the collaboration between partners is working okay.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The success of this project will help to achieve orders of magnitude of improvement in ionic conductivity compared to existing intermediate-temperature AEMs. Present AEM technologies are unable to achieve such high electrolyte conductivity. Validation of the proposed steam-based carbonate management

approach will be very effective during long-term operation. The carbonate mitigation strategy is already built in the electrolyte technology, and it will help the electrolyte to sustain long-term fuel cell operation. The formation and demonstration of such dual-phase membrane electrolytes in a >50 cm^2 cell will validate the viability of this technology in cells with larger footprints in the future.
- The project has high relevance and the potential for a new type of intermediate-temperature fuel cell that could potentially be low-cost. This could potentially provide a platinum-group-metal-free intermediate-temperature fuel cell.
- This project needs quantitative milestones to be more relevant to DOE. For example, the first go/no-go is "satisfactory membrane and cell component performance." These need to be quantified. The project should aim to achieve DOE's membrane ASR targets and to get close to DOE's target of 600 mA/cm^2 at >0.6 V at some temperature. The only quantitative target listed on slide 5 is >600 mS/cm. This needs to be significantly improved with more quantitative milestones and ASR and fuel cell performance targets.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The team has adequately described the future work for fiscal years 2019 and 2020. The team has identified and defined different phases and milestones of the project very well. The team has also correctly identified the go/no-go steps to judge the actual progress of the project. The team has maintained a true balance between the scientific challenges and the feasibility of technical success in the project.
- The proposed future work addresses the challenges of sealing and shows efforts to prove the carbonate mitigation strategy. The proposed work does not seem to be directed at making thinner membranes, which is important to achieving good fuel cell performance. The supports need to be one-fifth to one-tenth as thick as current supports. That will take significant effort.
- The plan seems sound and will result in 50 cm^2 fuel cells and an eventual commercialization plan. The project needs more quantitative targets; also, the mechanism for the carbonate mitigation using steam needs to be determined.

Project strengths:

- The principal investigator, team, and collaborators of this project are strong. The team has a good industrial partner in OxEon, who has great insight into this problem. The team has a good fuel-cell-hardware collaborator in FCA US LLC, who can guide the team with appropriate fuel cell hardware and setup conditions to mitigate testing and hardware-related issues that may become an obstacle for the project.
- This is a good team and a nice concept. A laboratory technology is being transferred to industry.
- The project has a novel idea and concept.

Project weaknesses:

- No weaknesses are identified at this point.
- Sealing is a big challenge in high and intermediate SOFCs that possess ceramic materials. The team did not explain much of the project's sealing strategy with the proposed porous-ceramic-support-based electrolyte. The team has proposed using "glue" as sealing material; however, there are many other issues with traditional glue, including leaching and creep issues. The team did not specify the humidification and carbonate mitigation strategy, so it is not known how the team will manage these two complex issues.
- There is a lack of quantitative milestones.

Recommendations for additions/deletions to project scope:

- The whole project, as presented, is fine and does not need any additions or deletions.
- The team should determine the mechanism of carbonate mitigation via steam operation.
- There are no recommendations at this time.

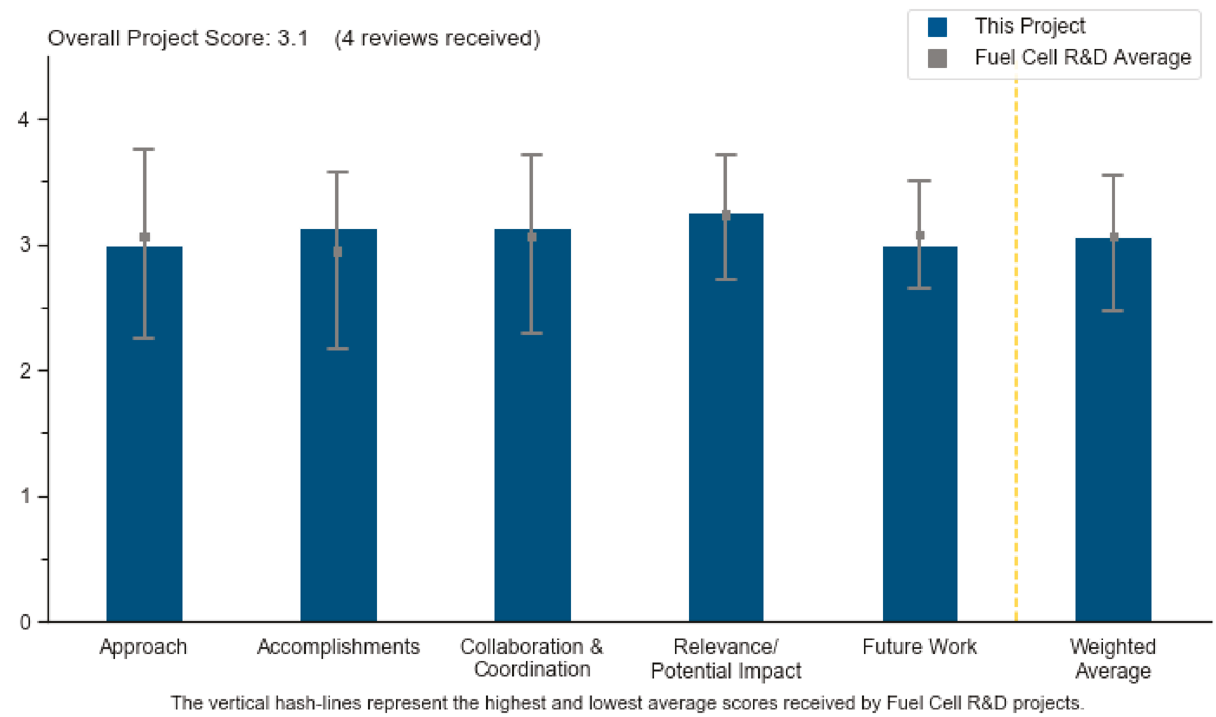
Project #FC-313: Novel Bifunctional Electrocatalysts, Supports, and Membranes for High-Performing and Durable Unitized Regenerative Fuel Cells

Nem Danilovic, Lawrence Berkeley National Laboratory

Brief Summary of Project

The main focus of this project is to demonstrate a highly efficient and stable unitized regenerative fuel cell (URFC) achieved through a novel membrane and supported electrocatalysts. The goal is to achieve 50% round-trip efficiency utilizing advanced membranes and bifunctional oxygen evolution reaction/oxygen reduction reaction catalysts on engineered supports. Project tasks include (1) developing membrane/ionomer and catalyst supports, (2) integrating the membrane into a membrane electrode assembly (MEA) and integrating the bifunctional catalyst onto supports, (3) demonstrating MEA performance and durability in electrolysis testing, and (4) demonstrating MEA performance and durability in fuel cell testing.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The proposed approach addresses the performance and durability of reversible fuel cells (RFCs). The team has identified major project risks and has appropriate mitigation strategies for them.
- The objectives are clearly articulated and clearly address the barriers that are identified. A strong multi-sectorial team has been assembled to tackle the various problems. The major technical barrier being addressed is to manage a huge breakthrough in the URFCs. Because the approach is logically based on developments for both fuel cells and water electrolysis, the project is addressing barriers identified for the two of them but considering specific targets. The targets are outstanding compared to baseline URFCs but are less challenging than individual targets for each technology. Only durability is expected to be

demonstrated at much lower levels compared to fuel cells or electrolyzers. The targets are particularly challenging for the water electrolysis mode: it is difficult to get how the approach on materials will allow for long-term operation with thin membranes at such loadings. Specific targets are identified, and the project plan is to reach them thanks to the work done on core materials, the membrane, and oxygen-side catalysts for improving both fuel cell and electrolyzer efficiency. The lack of information about the development routes prevents proper assessment of the approach. However, the overall approach is simple and consistent, starting with materials development, followed by their implementation in MEAs and testing in dedicated cell devices for fuel cell, electrolyzer, or URFC modes. Only one partner seems to actually be involved in the URFC.

- There are issues in this project that need to be addressed. (1) This project is confusing. It is regenerative, but in barriers it states “no regenerative-fuel-cell-specific barriers.” (2) The proposal is quite broad, with membranes and supported catalysts all in one project. (3) It would be nice to see a flowchart of how the contributors are interfacing. (4) It was stated that key personnel may have changed, which has impacts on the approach. (5) The challenges list the gas diffusion layer (GDL) and porous transport layer (TPL), which seem to be out of scope. (6) There is no mention of what will be unique about the membranes; they seem to be just commercially bought.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Lawrence Berkeley National Laboratory (LBNL) has made reasonable progress in the short time the team has been active. Baseline MEA fabrication has been completed, and initial baseline testing has been done at LBNL. Subcontracting to partners is still not completed.
- The work started recently; it is too early for proper ranking. However, baseline materials were defined, and the first results are available as planned.
- Despite subcontract negotiation issues, which are common to these collaborative efforts, good progress has already been made.
- It is early, but it seems that a lot must be done in two years.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- Coordination and plans for coordination are good. Bringing in Pajarito Powder, LLC (Pajarito) as a subcontractor should improve the project. Coordinating with Max Wei (LBNL) for URFC targets should be beneficial.
- This is a highly collaborative project with participants from industry (U.S. and foreign), national laboratory, and university sectors.
- Pajarito was added at the beginning; this seems relevant and required. Therefore, it is not clear why this role was not planned at an earlier stage. There are overlaps between partners for manufacturing and testing. Only one partner is actually involved in the URFC, even though this is the core objective of the project. The link with Solvay is indicated as a collaboration, but Solvay seems to be a supplier. If a common development with Solvay is planned, this should be mentioned clearly, including how they are collaborating and on what aspect of the membrane.
- Based on discussions at the presentation, there seems to be some flux with the contributors. There perhaps needs to be more clarity on what exact formulations will be made and why (e.g., how much Ir with Pt).

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- RFCs are highly relevant to DOE's H2@Scale efforts. The potential impact of this work is high, and participation by Ballard Power Systems, Inc. (Ballard), Proton OnSite, and Pajarito should increase the probability that the project will have an impact.
- The milestones and targets are aggressive and could significantly advance RFC technology.
- The project is considering several DOE objectives but addressing a very specific device; thus, it is not easy to conclude on the expected impacts. If the objectives are reached, progress will be made toward cost and performance objectives for polymer electrolyte membrane fuel cells and toward efficiency on the hydrogen production side.
- Using existing commercial membranes does not create much new impact. Pt–Ir systems have been around for a long time. The main impact, it seems, is the Washington University in St. Louis's supports for stability.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed work should advance RFC performance. The proposed supports should provide improved durability, while the bifunctional catalysts should improve performance.
- Good risk mitigation plans are presented.
- In year 1, the next developments are planned for the catalyst's support and integration, but nothing is mentioned for the membranes; this should be justified, considering the title of the project, including the membrane aspect. MEA optimization should focus on the reversible operation; performance for discrete operation could be second in the order. This is the same for the accelerated stress test (AST); it would be better justified to focus on defining the right duty cycles for URFCs or a specific AST for URFCs, if needed. In year 2, scale-up and discrete testing are planned; it should be that scale-up and reversible testing are planned for validation.
- The GDL and PTL seem to be out of scope. It seems there is flux in the project.

Project strengths:

- The collaboration between industry and laboratories is a positive aspect, allowing for combined interest in innovative developments and applicability. The targeted technical improvements, if they are reachable, are project strengths. The idea of selectively combining fuel cell and electrolyzer catalyst materials for the manufacturing of the reversible electrodes is the most interesting aspect of the ongoing work.
- The project has assembled a team with large industrial participation.
- The project's strengths include the new supports and the breadth of the team.
- A strong team has been assembled to address several barriers.

Project weaknesses:

- The complementarity between partners is not always clear, particularly for MEA manufacturing and testing; the choice to double some actions should be justified. More efforts seem to be put on the separate assessment in fuel cell or electrolyzer modes instead of pushing URFC tests, which is the core scope. There is a lack of technical information about developments concerning the membrane in particular. Concerning catalysts, results could have been shown (electrochemical analyses or microstructure observations could have been mentioned, if available). The differences in the level of information expected from 25 cm^2 and 50 cm^2 is not obvious; the choice of considering these two areas for evaluating up-scaling should be clarified. For the validation task, the reason that Proton OnSite and Ballard are performing fuel cell or electrolyzer testing only is not justified. Validation should be done at larger scale for actual URFC cases.

Duty cycles are defined as a challenge; this should be considered more of a required objective for final validation.

- The project has a broad, unfocused scope. Out-of-scope challenges are listed. The project has confusing targets and seemingly arbitrary baselines. Using a 175 µm membrane as a baseline needs explanation as to why it is so thick. Also, the team is in flux.
- Contracting issues have delayed the work.

Recommendations for additions/deletions to project scope:

- It is recommended that the project clarify whether the membrane development aspects are still needed for the project outcomes and, in this case, what the routes explored and next steps are and what the possible role of Solvay might be. Focusing on the assessment and validation of materials and devices in URFC conditions with the definition of proper duty cycles would add value to the project (instead of focusing on discrete validation), since other projects are already considering the specific developments for fuel cell or electrolyzer materials and improvements. For the next review, more details should be given and more results shown.
- The project should eliminate or clarify the membrane part and flesh out the catalyst development paths and reasoning. Out-of-project components should be eliminated.
- There are no recommendations at this time.

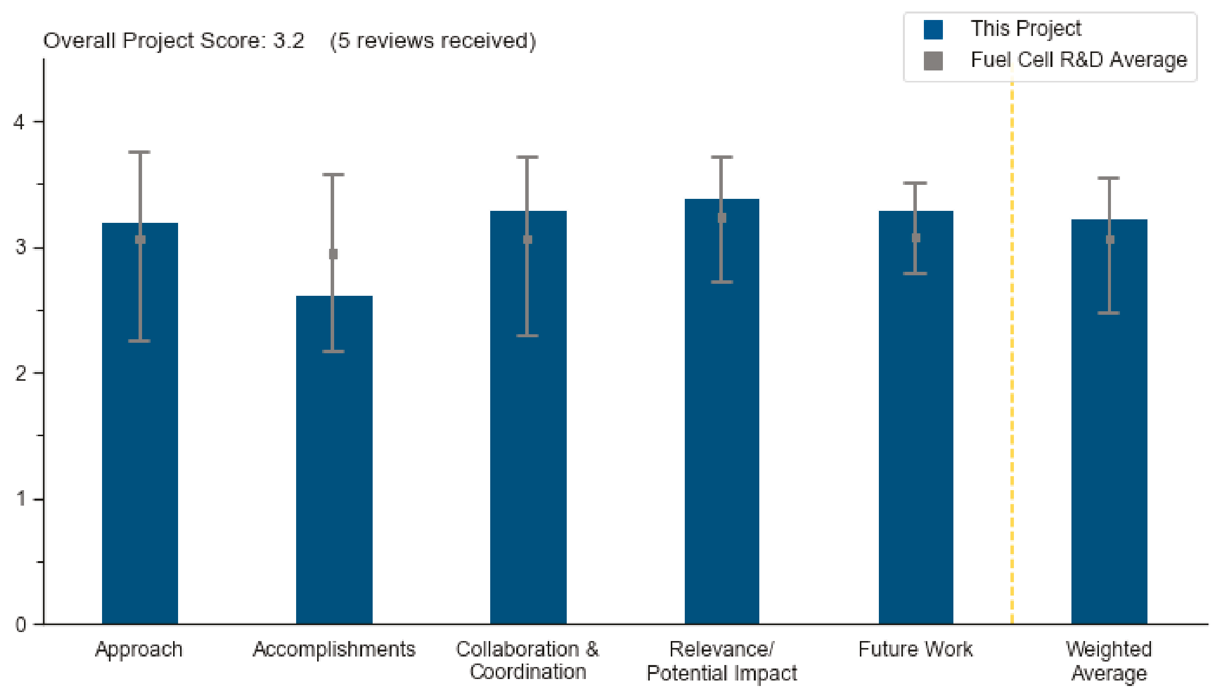
Project #FC-314: Efficient Reversible Operation and Stability of Novel Solid Oxide Cells

Scott Barnett, Northwestern University

Brief Summary of Project

This project will develop and test reversible solid oxide cells (ReSOCs) for electrical energy storage applications, including system concepts for high efficiency. The ReSOCs will be designed to operate efficiently and durably in both fuel cell and electrolyzer modes. The project approach employs novel high-temperature cells with the potential for high power density, long-term stability, and high round-trip efficiency. The ReSOCs will be designed to achieve the low area-specific resistance (ASR <0.15 Ωcm^2) required for high round-trip efficiency at high current density (>1 A/cm^2). One focus is on durability improvement via a combination of materials development, mechanistic degradation model development, and accelerated stress testing to determine the factors that affect long-term stability, including reversible operation cycles. Multiple cell designs will be investigated. The team will also fabricate and test large-area cells and determine the effects of pressurized testing. System modeling (system concept development and technoeconomic analysis [TEA]) will inform designs that can achieve cost and efficiency targets for renewable electricity storage.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is a novel concept: high-temperature solid oxide fuel cells (SOFCs) capable of achieving high power density, long-term stability, and high round-trip efficiency in ReSOCs. The project will fabricate and test large-area cells based on current button cells. The team will focus on the relationship between long-term stability and operating conditions.

- The technology barriers for durability, cost, and performance are clearly identified. Project objectives are to develop, fabricate, and test large ReSOCs; determine the effect of operating conditions on cell performance and durability (including operation at high pressure); assess systems efficiency; and validate technology viability using TEA.
    - There is a significant emphasis on the degradation studies. The team needs to be careful not to test cells under unrealistic conditions (e.g., overly high cathode/anode overpotential, temperature, local oxygen partial pressure) to force earlier and more pronounced degradations.
    - When reporting ASR or degradation rates, including those in the go/no-go milestone (slide 6), the specific test conditions (temperature, pressure, cell voltage, etc.) should be provided. It would be beneficial to compare to the state-of-the-art performance and list the target values.
    - The round-trip efficiency is typically discussed for a device or system because it ties into storage rather than for a single button cell, as in this work. From thermodynamics, cell efficiency is always high for a high-temperature cell, but there are penalties for storage and compression. The efficiency itself may not be as important as the cost per stored amount of energy. Efficiency can also be measured in many ways; how it was calculated should be explained.
- In general, the approach is good. It appears that the work is very focused on small-scale tests and materials characterization. This is cost-effective, but the project could benefit from access to samples taken from larger systems. This may simply not be possible, as there are not a large number of solid oxide electrolyzer cells (SOECs) and systems in operation, even at a laboratory scale.
- The approach and down-selection to look at three different cell designs is appropriate. The use of a 3D-printed cell design has some potential for improvements. The thermal energy storage concept could provide advantages and ease thermal stresses during transitions between SOEC and SOFC modes. The round-trip efficiency target of >70% is aggressive.
- The approach to addressing performance and durability is very good, but it is limited to small cells. It appears that work on scale-up will not occur until quite late in the project. Since making cells of a practical size is a major challenge for SOFCs and will undoubtedly be required to meet the cost targets for the intended application, this major challenge should also be a focus of the project. A similar comment can be made with respect to fabricating a robust cell stack, which is another major SOFC challenge.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project is just starting. Models for high-temperature reversible fuel cell (RFC) systems have been established. Desired operating conditions have been determined.
- A number of results were presented, and it appears the project is generating some reasonable outcomes.
- The project contract was just recently finalized, so no work has been done yet.
- This project was only recently funded. It contains no new results, and it is not possible to evaluate progress.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The team members will utilize their best strengths and support each other. Northwestern University will develop and fabricate cells, test and characterize them, and provide experimental data to Colorado School of Mines (CSM) to perform stack and system modeling. CSM will provides input to Northwestern University regarding desired cell characteristics and operating parameters, ensuring that test results are relevant.
- Collaboration between Northwestern University and CSM should be good. The combination of modeling and experiment should be beneficial.
- It appears that the team has clear roles and a good plan on how they will collaborate throughout the project.
- The team is collaborating with CSM. CSM will perform stack and system modeling and TEA.

- There are only university partners in the project. It can be challenging to do fundamental research on materials degradation with industrial partners, but the team should establish some link with an organization that manufactures and is currently developing or producing SOFCs or SOECs. This would not need to be a paying partner, just an adviser who could suggest whether the approach taken and materials selected are relevant to what will likely be a commercial product in the future.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- It is still an open question whether energy storage using RFCs is going to be viable since the round-trip efficiency is typically much lower than other options (e.g., batteries). However, the cost of the storage media is low relative to the cost of battery-active materials, so RFCs may be viable for long-duration storage. SOFCs can potentially enable higher round-trip efficiency than lower-temperature fuel cells, so this does appear to be a promising technology for the intended application. Of course, in addition to performance, substantial durability and scale-up challenges must be overcome.
- SOEC is an important technology, and little work is done on degradation, so the project will likely have significant impact.
- The project has high relevance and is applicable to the Fuel Cell Technologies Office H2@Scale efforts. If the target round-trip efficiency of 70% is reached, it will have a large impact.
- Development of RFCs is very important for advancing energy storage and power generation technology.
- This project is related to an existing project on hydrogen production. The overall objective is to develop a system with high round-trip efficiency and low storage cost.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed future work is relevant and addresses issues of degradation and thermal effects from cycling between modes.
- The project seems to be well planned and organized.
- The proposed future work is reasonable, though no details on specifics of cell fabrication, testing, characterization, or scale-up approaches are given.
- Identifying realistic performance targets is helpful.
- The future work will be directed at achieving low ASR ($<0.15\ \Omega cm^2$) for high round-trip efficiency at high current density ($>1\ A/cm^2$). The project will carry out tests to determine factors that affect long-term stability. Future presentations may better illustrate the methodology and approach to achieve stated objectives.
- More focus on scale-up earlier in the project would be a good addition.

Project strengths:

- The principal investigator has useful experience in identifying cell degradation at high current density and the possible benefit of cyclic potentials. Use of multiscale modeling tools for system design, analysis, and optimization may help in further understanding the degradation mechanisms.
- The project will develop and test novel, efficient, and stable ReSOCs. Teaming is excellent, and the work is well coordinated.
- The combination of system modeling and cell development is a strength.
- This is a good fundamental study of materials degradation.
- The project focuses on performance and durability.

Project weaknesses:

- A weakness is not evident at this time.

- There is no significant weakness.
- It is really tough to work on the degradation of a technology still in development. It is a simple fact of life that no one knows what materials will be in an SOEC in the future, so there is a chance that this work may not be relevant to future systems. That should not be taken as a reason not to do the work, but it is a potential weakness.
- What makes the team's SOFC technology different—i.e., why this should be better than other SOFC systems—is not really clear. Also, there is not enough focus on scale-up of cell size and stack technology.
- It is not clear what is "novel" in novel ReSOCs. The materials set listed is well known and has been previously tested and characterized.

Recommendations for additions/deletions to project scope:

- There are no recommendations on the project approach; the approach is very reasonable.
- An industrial partner might be beneficial for stack-level testing.
- The project should have some form of industrial engagement, even in a fairly informal way.
- At the next Annual Merit Review (AMR), the team should communicate the following:
    - What differentiates the team's SOFC technology
    - What the issues are with making larger cells, and how these risks will be reduced in this project
    - What the issues are with making cell stacks, and how these risks will be reduced in this project

  If the answers to the above questions are known but were just not clearly communicated during the AMR, then the team should also modify the plan.
- It is too early to change directions or add tasks.

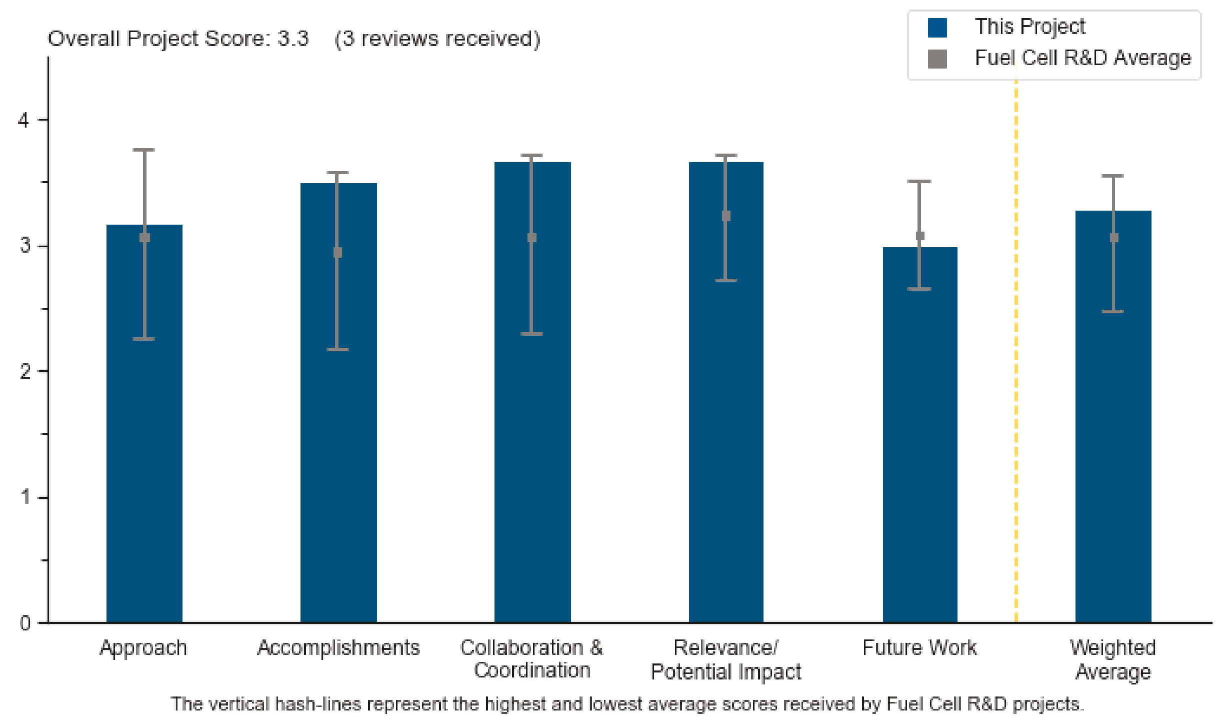
Project #FC-315: High-Efficiency Reversible Alkaline Membrane Fuel Cells

Hui Xu, Giner, Inc.

Brief Summary of Project

Reversible fuel cells can store renewable energy as batteries do, with one advantage: the ability to accommodate much higher energy density. An alkaline membrane system may reduce the associated capital costs, thanks to adopted inexpensive materials (e.g., catalysts and bipolar plates). The project team is investigating the following technical approaches to enable reversible alkaline membrane fuel cells (AMFCs) for stationary energy storage: (1) bifunctional catalysts for hydrogen oxidation reaction (HOR)/hydrogen evolution reaction (HER), (2) bifunctional catalysts for oxygen reduction reaction (ORR)/oxygen evolution reaction (OER), and (3) high-performance alkaline membranes (with high OH- conductivity, oxidative resistance, and mechanical stability). This project will demonstrate, for the first time, a reversible AMFC with greater than 50% roundtrip efficiency at 1 A/cm^2 without introducing any salt or base in the aqueous feed.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project is extremely ambitious. The work scope includes advances in membranes and bifunctional catalysts at each electrode, with project funding of only $1.25 million over only two years. This seems like a good deal to tackle. However, the project team is excellent and comprises leaders in each relative area. The principal investigator and the project team have among the best records of broad collaboration in the electrochemical space, and a unitized reversible test cell is a big step forward for this type of work.
- The project team members are very experienced in the development and testing of electrolyzers. They understand that there are many benefits to using OH- membranes but equally understand that these

membranes have many stability issues. The combination of materials experts from university and industrial partners with device expertise is clearly beneficial.

- The general technical approaches to using hydroxide exchange membrane (HEM), HER/HOR and OER/ORR catalysts are suitable. However, it seems all components used for the reversible fuel cells have already been developed for fuel cell or electrolyzer applications. There is no clear explanation of how these materials produce the best reversible fuel cell performance. High-temperature AEMs >100°C is something new, but that is a risky approach. No AEMs have demonstrated excellent stability at >100°C with water vapor, even in ex situ conditions. This approach likely will fail.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This project has only just started; the project team is making reasonable progress, but it is still early in the project.
- It is too early to see progress in this project, as work has been ongoing for only three months.
- The project is at an early stage. Therefore, not much progress is reported.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- Leaders in ORR/OER and HOR/HER bifunctional catalysts have been selected, along with a very successful AEM chemist. The project is well designed for collaboration; now the project team needs to deliver.
- The project is at a very early stage, but it appears that both partners have been assigned clear, complementary tasks to complete.
- The project's collaboration exists. Giner, Inc., is managing project coordination.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Reversible fuel cells are probably best suited with an AEM, given the wider array of catalysts possible in a basic environment. This moonshot approach is well suited for the current DOE emphasis on early-stage research and development (R&D) work. Success in this project would be very impactful in the electrochemical device field.
- The project target aligned well with the DOE Hydrogen and Fuel Cells Program. Developing platinum-group-metal-free catalysts for reversible fuel cells is relevant to the DOE approach to reducing device cost. Applications for regenerative fuel cells exist. If the project is successful, the product of this project will find markets and have impacts on them.
- The development of a stable OH- system could potentially reduce electrolyzer and fuel cell costs, but it also has the potential to allow for more novel electrochemical devices to be manufactured.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The correct work has been proposed. The project hits all areas of reversible fuel cell R&D necessary to be successful.
- The project plan seemed reasonable.

- Similar or the same poly(aryl piperidinium)-based AEMs can be seen in multiple AEM-related projects. The base membranes have been reported in the literature. All milestones related to the AEMs seem similar to what the University of Delaware already has. The project target is >100°C under vapor conditions; the fuel work should align with the device condition, not 80°C conditions. Likewise, the catalyst development milestone should not target xx grams of catalysts; it should target xx activity. Having inactive catalysts with quantity will not help the project. The participants seem aware of this issue, so they need to need to rewrite the milestone. The go/no-go milestone needs some more description. For example, it needs to be known if the reversible fuel cell will use caustic solvent and, if not, what voltage limit it will have, what the target temperature is, and how many cycles will be analyzed. Milestone 4.2 should also carefully define the degradation rate of <1%; the voltage, temperature, and other conditions should be defined specifically. Also, the diagnostic works of the MEA should be included.

Project strengths:

- One project strength is that Giner, Inc., has experience in reversible fuel cell technology. The other strength is that all critical reversible fuel cell components will be developed in one project, in an organized manner. By the end of the project, the project team may bring results that identify the bottleneck of alkaline HEM reversible fuel cells.
- The unitized cell is a big advance in studying these MEAs. The team is excellent and broadly capable of delivering on the ambitious targets.
- Overall, this is a sensible, solid project for developing a new set of materials that could benefit many different electrochemical devices. However, reversible fuel cells offer very limited benefits over a separate fuel cell and electrolyzer combination. Clearly, DOE and many in the field disagree, but it would still be better to test the materials developed in this project in separate devices (fuel cell and electrolyzer) rather than in a combined device that offers little benefit in terms of cost or performance.

Project weaknesses:

- This is a challenging project. It will be very difficult to have to have an efficiency of about 70% of the performance of acid reversible fuel cells, even if all those proposed materials work extremely well. This project does not provide good metrics to evaluate component performance. This type of project should be supported in the innovative concept category with a lower funding level.
- There is little value in combining a fuel cell and an electrolyzer. That device is called a metal hydride battery, and significant compromises must be made in the way the oxygen and hydrogen are stored because of the different balance of plant for each of these two devices. There is some value in doing this with high-temperature devices because the round-trip efficiency is higher, but there is no value in doing this if the device operates below the boiling point of water.
- The project is hugely ambitious and may not have enough funding to be successful. The reduction–oxidation (redox) reaction cycle and oxidation concerns in AEMs is a new idea, and the materials did not explain well why it is important.

Recommendations for additions/deletions to project scope:

- A recommended addition would be SMART (Specific, Measurable, Achievable, Relevant, and Timely) milestones for each component. The AEM performance needs to be measured at the relevant device conditions, including stability at >100°C at a reduced relative humidity. The HER/HOR and OER/ORR catalysts need to be evaluated in rotating disk electrode testing with control sample performance.
- This is very valuable work for the fuel cell and electrolyzer fields, but it would be better to focus on the development of a high-performance fuel cell or electrolyzer. There is very little value in combining the two. In reality, this would make little difference to the project, as the team would still make the same cell and test it first as a fuel cell and then as an electrolyzer. However, it is important to recognize that either a good fuel cell or a good electrolyzer would be valuable individually, whereas a combined device is likely always to be a compromise that might simply not be worth the effort.
- It would be desirable to see some more focus on explaining the concerns about AEM oxidation within the reversible fuel cell concept.

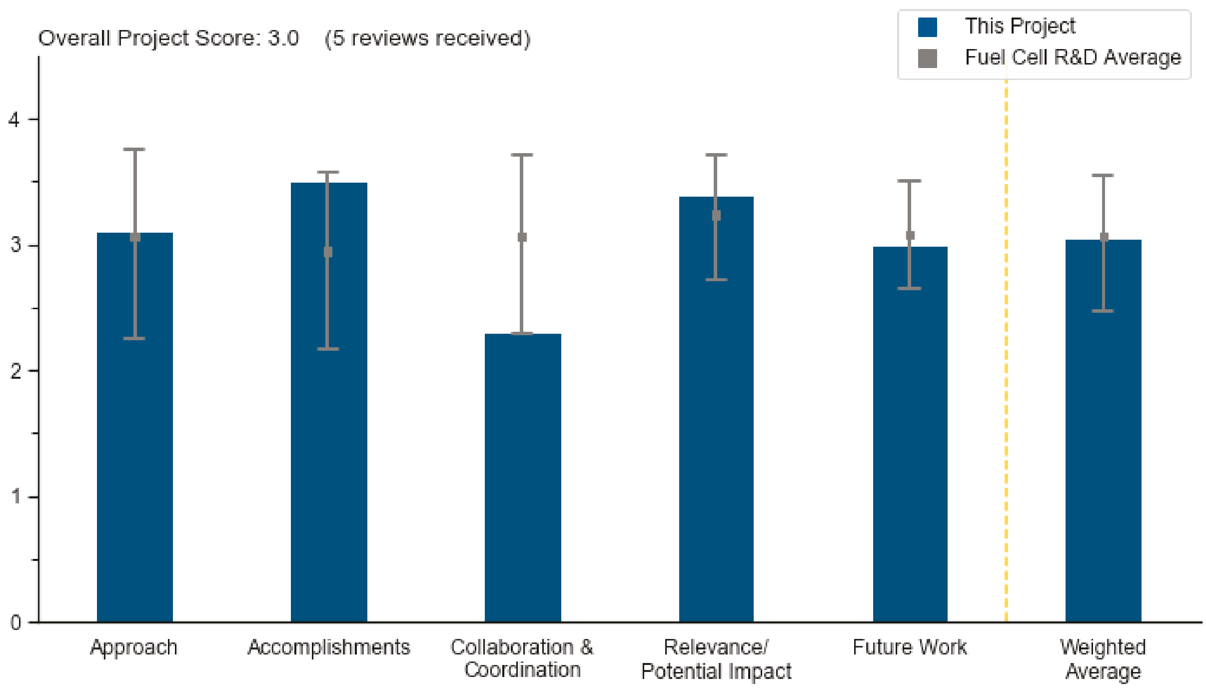
Project #FC-316: Durable, High-Performance Unitized Reversible Fuel Cells Based on Proton Conductors

Meilin Liu, Georgia Institute of Technology

Brief Summary of Project

This project is developing a robust, highly efficient, and economically viable high-temperature unitized reversible fuel cell (URFC) based on proton conductors for large-scale co-located energy storage and power generation. Project activities focus on two main areas: (1) gaining better understanding of the degradation mechanism of cell and stack materials and interfaces, using various in situ, ex situ, and operando measurements guided by theoretical analysis; and (2) integrating nanostructured components into the cell design and interfaces between electrodes and electrolyte, which will be modified with active bi-functional catalysts and protection coatings to achieve >70% roundtrip efficiency at 1 A/cm2 in both operating modes.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an excellent approach; the principal investigator (PI) is experienced and focused on U.S. Department of Energy goals for high-temperature URFC technology.
- The approach to develop high-temperature, high-performance reversible fuel cells (RFCs) based on proton conductors has some advantages, as it may produce pure or dry hydrogen without downstream separation or purification. According to the PI, the system can tolerate sulfur impurities at a parts-per-million level.
- Understating the degradation mechanisms in RFCs is essential for designing a robust, reliable system. Thus, the fundamental focus of this project is very important and in line with Georgia Institute of Technology's (Georgia Tech's) strengths. There are a few comments to consider.

  - There is some disconnect between the technology barriers—listed as (1) capital cost, (2) system efficiency and electricity cost, and (3) operations and maintenance—and the project's immediate objectives and approaches. It seems that the barriers are more related to a large-scale system, while the objectives and approaches (i.e., to gain a profound understanding of the degradation mechanism of electrolyte, electrode, and catalyst materials) are related to the cell development. Thanks to the high operating temperatures, cell efficiency will be high, but the system efficiency is unknown. Another barrier that was listed, capital cost, is not discussed in the poster.
  - There is significant emphasis on the degradation studies of all three cell components—electrode, electrolyte, and catalyst—without stating the issues with each of these components. It would be helpful to introduce the limitations of the state-of-the-art materials first. The approach suggests that there are issues with charge transfer and mass transfer in the electrode materials associated with the reversible operation of a fuel cell. It is not clear if this is the issue with all (or any) of the materials, or only with those (state-of-the-art-materials) that were down-selected for this study, or with those developed at Georgia Tech.
  - This project aims to test the proton-conducting reversible cells at very high temperatures, 700°C–850°C. Typically, such cells offer an advantage over oxygen ion conductors when operated at lower temperatures, such as 500°C–650°C. At >650°C, the oxygen ion conduction in BZY-based materials becomes significant, as most of the "proton conductors" are in fact mixed conductors. Degradation is also expected to be lower if operated at lower temperatures, especially since the use of nanoparticles was proposed here to avoid their coarsening.
  - It is not explained why the new coating materials for the electrolyte are needed or how they would affect the cell resistance, performance, and cost. It would also be very helpful to list the targets for durability to understand what "required durability" means.
  - The roundtrip efficiency is typically discussed for the device or system, rather than for the single button cell, as in this work. Giving the Faradaic efficiency instead is probably more reasonable.
- The approach to addressing performance and durability is very good, but it is limited to small cells. It appears that work on scale-up will not occur until quite late in the project. Since making cells of a practical size is a major challenge for solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs) and will undoubtedly be required to meet the cost targets for the intended application, this major challenge should also be a focus of the project. Although the team does have a target of 10 mm cells, these are still a very long way from the size that will be required in a future product. A similar comment can be made with respect to fabricating a robust cell stack, which is another major SOFC/SOEC challenge.
- The communication skills of the scientist who was presenting the poster were very poor. It can be tough when English is a second language, but in discussion, it was hard to understand what experimental work had been conducted. A simple diagram of the proposed system is strongly recommended. Good spoken English should not be a requirement for any scientist, but an image that can be pointed at to explain the principles of the system would be a valuable communication aid. This can be useful, especially when presenting to a group that does not speak English as a first language.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made good progress, particularly in cell fabrication and microscopy characterization. This work appears to be a continuation of something the PI has been doing for a long time. The present results are reasonable for a project that has been in place only since October. One project goal is to unravel the mechanisms of charge and mass transport; this appears not to be happening quite yet, as the results are not yet discussed in terms of mechanism or of why certain materials and processes show improved behavior. Presumably, that comes at a later stage.
- This is a new project. To date, it has developed a new electrolyte coating material that has high conductivity and high stability against water and CO_2. The project has evaluated the electrochemical performance of single cells and has already demonstrated a roundtrip efficiency of ~72% at 1 Acm^{-2} at 700°C.
- This project was only recently funded. Thus, most of the data presented are likely from previously performed fuel cell activities. Some good progress has been made since the beginning of the project in

January: the team has synthesized electrode materials and fabricated and tested small cells with <1 cm diameter.
- Many results are presented here, considering that the project has just started.
- The project has early initial results.

Question 3: Collaboration and coordination

This project was rated **2.3** for its engagement with and coordination of project partners and interaction with other entities.

- The PI does not appear to have any partners involved in the work; the project resides solely at Georgia Tech. The PI says he is looking for an industrial partner.
- This project does not yet have a formal partner. Georgia Tech would need to identify an industrial partner for scaling up the cell and developing a roll-to-roll manufacturing concept.
- This project would be greatly enhanced if it included an industrial partner, since it is not clear that the team has much experience on what is required to potentially enable a viable product.
- As far as can be seen, there is little or no collaboration in this project.
- So far, there are no outside collaborators or contributors.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The development of RFCs is very important for advancing energy storage and power generation technology.
- There is significant potential to develop a URFC system with >72% roundtrip efficiency.
- The project's prospects for advancement are excellent.
- It is still an open question whether energy storage using RFCs is going to be viable, since the roundtrip efficiency is typically much lower than it is with other options (e.g., batteries). However, the cost of the storage media is low relative to the cost of battery active materials, so RFCs may be viable for long-duration storage. Proton-conducting SOFCs can potentially enable higher roundtrip efficiency than lower-temperature fuel cells, so this does appear to be a promising technology for the intended application. Of course, in addition to performance, there are substantial durability and scale-up challenges that must be overcome. A key advantage of proton-conducting SOFCs is supposed to be lower operating temperatures, which can enable improved durability and lower-cost sealing materials; however, the team does not appear to be focused on operating temperatures significantly lower than those used with conventional SOFCs.
- High-temperature systems offer much higher roundtrip efficiencies, which has the potential to allow for better economics. It would be simpler to operate the SOEC as an electrolyzer and then use the hydrogen in a PEM, as the same high efficiency could be achieved with a simpler and potentially much cheaper system.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed future work is clearly outlined: (1) synthesize electrodes and electrolyte powders with desired properties and (2) complete the fabrication and/or microstructure modification of electrode support with targeted 30%–40% porosity before reduction.
- The researchers have a plan, and they are following it. Once there are more results, there will be an opportunity to refine the plan.
- The proposed future work is reasonable.
- The team should focus more on the key challenges of scaling up the technology and develop methods to reduce these risks as much as possible during the project.
- The proposed future work is very extensive and covers all of the aspects of cell fabrication, testing, in situ characterization, scale-up, and the development of manufacturing concepts for mass production. This is

perhaps too broad and not realistic for the budget. The goal of testing cell performance under “various operating conditions” seems ambiguous. Instead, identifying realistic performance targets would be more valuable.

Project strengths:

- This is a good start to the project, as electrode and electrolyte materials with desired particle size and morphology have been synthesized. The team has made good initial progress in fabricating symmetrical cells and single cells.
- Georgia Tech has an excellent reputation in developing new fuel cell materials and in situ characterization of fuel cells. The same approach will be used to assist in developing high-performing materials for reversible cells.
- This is quite a simple project, with the objective of making a relatively simple cell. This is appreciated, as there is a culture of trying to oversell projects. This project will achieve its objective and add value to the field.
- The high-temperature approach is attractive, and the PI has much experience in this area.
- There is a major focus on performance and durability with small cells.

Project weaknesses:

- The project’s focus so far seems to have been mostly on presenting findings but not proposing the rationale for why improvements are seen over existing materials and devices. Going forward, it would be good to focus on understanding the mechanisms and relationships that the materials and structures have with device performance.
- The project needs to put more emphasis on scale-up issues. The results that were shown are not consistent. For example, the claimed fuel cell performance is based on results obtained at 700°C, and the durability results shown are at 650°C (as seen on slide 12). Similarly, the claimed cycling performance is based on results obtained at 700°C, and the durability results shown are at 650°C (as seen on slide 13). The project needs to clarify what temperature is the focus.
- There is no collaboration or any real path for the work to deliver impact. This is acknowledged, but with no partner pushing to get results, this project will continue trying to achieve harder and harder performance goals, without ever getting to the point where a system is built.
- There is an inadequate understanding of degradation mechanisms. Precise control of the morphology, composition, and thickness of the catalyst coatings remains a challenge. Scaling up from button cell to large-area cell may be a challenge.
- The scope is too broad; the team is attempting to solve any potential problems without clearly starting the problem.

Recommendations for additions/deletions to project scope:

- At the next Annual Merit Review, it is recommended that the team communicate the following: (1) what the issues are with making larger cells, and how these risks will be reduced in this project; and (2) what the issues are with making cell stacks, and how these risks will be reduced in this project. If these answers are not obvious (i.e., known by the team but not clearly communicated in the presentation), then the team should also modify the plan.
- The team should focus on the solid oxide electrolyzer aspect. If it works as a fuel cell as well, then that is great, but the team should optimize for the solid oxide electrolyzer. Hydrogen fuel cells of good quality are already available, so the focus should be on producing low-cost hydrogen. The team should find someone who will want the technology beyond a cell.
- The team should split the scope into smaller, well-described tasks and clearly explain why each task is needed and what will be achieved.

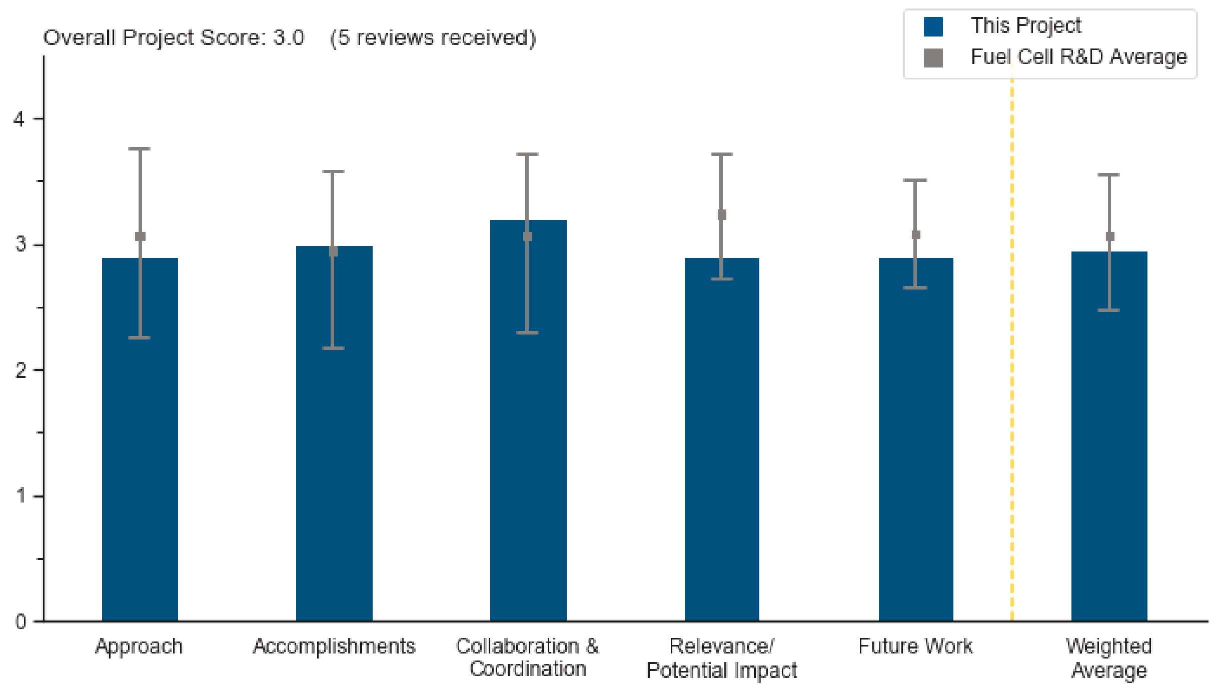
Project #FC-317: Stationary Direct Methanol Fuel Cells Using Pure Methanol

Xianglin Li, University of Kansas Center for Research, Inc.

Brief Summary of Project

The project goal is to develop stationary direct methanol fuel cells (DMFCs) using pure methanol as the fuel. The project will address three critical challenges from material to system levels: (1) reduce noble catalyst loading and cost, (2) enhance cathode tolerance of methanol poisoning, and (3) decrease methanol crossover. The end-of-project goal is to deliver a 50 cm^2 membrane electrode assembly (MEA) and prototype that produces peak power density of ≥300 mW/cm^2 with total loading of ≤3 $mgPGM/cm^2$. The project addresses the barriers of high-platinum-group-metal (high-PGM) catalyst loading, catalyst poisoning by methanol, and high fuel crossover.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **2.9** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project combines an aligned carbon nanotube as anode and a PGM-free catalyst as cathode. Both approaches are known in previous and current research sponsored by the U.S. Department of Energy (DOE). Putting them together for a DMFC is a good idea.
- The project is in the startup phase, so the approach has not been tested yet. It is innovative to apply a PGM-free cathode to a DMFC system. If the project is successful, the impact will be high. There is good organization between the team members, who specialize in anodes, cathodes, and systems.
- This project integrates resident institutional expertise in PGM-free cathode catalysis (the University at Buffalo); supported anode catalysis (Kansas State University); electrode fabrication, characterization, and optimization (Carnegie Mellon University); and multiphase mass transfer (University of Kansas). The project includes an early go/no-go decision in fiscal year 2019.

- The team is taking a fairly systematic approach to developing a new fuel cell. One issue is that the motivation of the work does not seem to be clear, and what are suggested as the objectives do not quite match the deliverables. The stated project objectives are to reduce noble catalyst loading and cost, enhance cathode tolerance of methanol poisoning, and decrease methanol crossover. All objectives are using pure methanol, but the deliverable is for 3 M methanol or greater, 250 mW/cm^2, with a 4 mg/cm^2 catalyst loading. Some electrode characterization is also mentioned. Neither the objectives nor the deliverables are wrong, but they do not match. There is no measure of "tolerance to methanol poisoning" or "methanol crossover." There is a catalyst loading target, which is a start. The principal investigator (PI) should consider revising the objectives or the deliverables.
- The approach relies on replacing a Pt catalyst in the DMFC cathode with a PGM-free catalyst, which effectively makes this a PGM-free catalyst development project. From the electrocatalysis point of view, this is another DOE Electrocatalysis Consortium (ElectroCat) effort. The odds for this research to be successful are minimal, given the magnitude of the PGM-free catalyst development challenge clearly demonstrated in ElectroCat projects (several already involving the University of Buffalo group, which is responsible here for PGM-free catalyst development).
    - There are numerous fundamentally flawed assumptions in this project. The first one is the importance of reducing methanol crossover to make DMFCs viable; it is grossly exaggerated by the team. Controlling the feed concentration of methanol can minimize crossover losses (they are of concern only at the highest DMFC voltages anyway). Notwithstanding the ubiquitous lack of PGM-free catalyst stability, the proposed approach is almost certain to result in low PGM-free catalyst activity, which will dominate the overall cell performance. Lower performance than that of state-of-the-art DMFCs is likely going to be the outcome. The importance of methanol poisoning has been entirely misstated in the project. Methanol does not poison Pt at potentials (and temperatures) at DMFC cathode voltages that guarantee reasonable fuel conversion efficiency. The title of the project is misleading. In practice, most, possibly all, DMFC concepts assume operation on "pure methanol" in a water-balanced system, with water required for the anode process, and the same is true of this effort.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Although it is early in the project, key early elements have been met. PGM-free cathode catalysts are to be tolerant to methanol. Growth of vertical supports for vapor deposition is shown. Modeling has begun.
- The project just started. Early accomplishments include development of a fuel cell test platform, initial fabrication of anode and cathode electrodes, and rotating disk electrode (RDE) measurements.
- The team appears to be on track.
- It is too early to assess accomplishments and projects. More performance demonstration is needed at either electrode.
- The part of the effort devoted to the development of vertically aligned conical carbon nanofiber structure is interesting. The catalysis part has been derived largely from the University of Buffalo effort in ElectroCat-funded projects. Methanol tolerance of virtually all oxygen reduction reaction (ORR) PGM-free catalysts is a universal property, so methanol tolerance data are merely restating the obvious. All the data showing poor methanol tolerance of Pt catalysts once methanol concentration is made sufficiently high is also not novel; this has been demonstrated countless times before. Electrode characterization appears premature for as long as a promising PGM-free catalyst for the DMFC cathode has not been developed yet. DMFC performance demonstrated by the team to date has been very low, much below the DMFC state of the art. No advantage of high feed concentration of methanol has been demonstrated so far. It may prove to be an unattainable task, given zero-order kinetics of methanol oxidation at concentrations higher than 0.3 M or so.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- One strength of this team is a well-coordinated mix of specialists focusing on each subsystem of the MEA. The University of Kansas team is apparently responsible for MEA fabrication, which is also a strength. This part should be emphasized, as it will not be trivial to integrate two different electrode technologies.
- There are good collaborations among partners, with clearly defined roles. The University at Buffalo will develop a methanol-tolerant and low-cost PGM-free cathode catalyst. Kansas State University will develop vertically aligned carbon nanofibers with an ultralow-PGM-loaded anode catalyst. Carnegie Mellon University will fabricate and characterize electrodes. The University of Kansas will conduct modeling and system integration.
- The team members seem to be collaborating well. There are no external collaborations yet.
- The project has a good inter-institution collaboration.
- There are four partners. It is not 100% clear what each partner's role is, but there are results from each university partner. A summary of each partner's tasks and capability is suggested.

Question 4: Relevance/potential impact

This project was rated **2.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- A highly efficient and low-cost methanol fuel cell is an important component in the fuel cell technology portfolio.
- It is good to see methanol not forgotten as an intermediate green fuel on the way to a hydrogen economy. The project addresses key barriers to DMFCs: PGM loading and activity.
- The project has the objective of improving methanol fuel cell performance and reducing PGM loading for lower cost.
- The project is relevant to the development of DMFCs for portable power. However, none of the proposed pathways toward improvements to DMFC performance and cost promises to be successful.
- DMFCs have their uses, but this technology is not critically important for any sector. A comparison with the advantages of this approach to a reforming methanol fuel cell would be valuable, as would a suggested use case of the technology.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The future plans generally build on past progress and will contribute to overcoming identified barriers. The critical step is to synthesize high-performance, PGM-free ORR catalysts that are stable and durable.
- The team has a good unit of experimental and modeling efforts. The team should include benchmarking on standards.
- If the objectives matched the deliverables, it would be easier to comment more on the relevance of the future work. The team will likely achieve the milestones, but it is unclear whether this will mean that the project has met its objectives.
- There are a couple issues that the PIs need to address quickly. (1) Catalyzing vertically aligned carbon nanofiber has been previously investigated and presents a challenge. The PIs should review the literature more extensively to help their work. (2) A PGM-free catalyst, though more tolerant to CO/methanol poisoning, is not stable under polymer electrolyte membrane fuel cell operating condition. The stability issue needs to be addressed at an early stage.
- There is very little in the proposed future work that stands a good chance of overcoming known barriers of DMFC performance and helping to achieve the very ambitious goals of this project. The plan lacks new ideas, which may not be surprising given the maturity of the DMFC concept. Methanol tolerance aside, the ORR development part does not promise a breakthrough, which depends entirely on the progress in the

development of PGM-free catalysts in ElectroCat projects anyway. The correlation between RDE and fuel cell performance, while interesting, can be (and has been) performed in one of the University of Buffalo ElectroCat projects. The outcome should be just applicable to DMFCs as it is to hydrogen–air systems. Catalyst scale-up is unnecessary as long as an active and stable catalyst is not found. Sputtering a standard PtRu anode catalyst is unlikely to improve anode electrocatalysis, which requires new formulations to overcome an approximately 0.2 V gap between the thermodynamics and practical PtRu-based catalyst systems.

Project strengths:

- This project combines the strengths of PIs at four institutions, and there are clearly defined tasks.
- There is good teaming in integrating some of the previously developed catalyst technology.
- Project strengths include innovative anode and cathode approaches and the use of modeling to help guide critical system operation with pure methanol.
- The proposed milestones are SMART (Specific, Measurable Attainable, Relevant, and Timely).
- There are very few project accomplishments, but the team deserves the benefit of the doubt, given the limited time project has had to prove itself worthy. This project may need major re-scoping to stand any chance of meeting its very difficult targets.

Project weaknesses:

- Since water transport is critical, the team should add a membrane screening component—especially some of the new thin commercial membranes. There will be great pressure to have good cathode performance at ambient pressure, which could limit performance.
- There is uncertainty in developing stable and durable PGM-free catalysts in the presence of crossover methanol. Perhaps the team should wait for real progress in the much larger ElectroCat project.
- The team needs to address the anode catalyzing issue (low risk) and instability of the PGM-free cathode catalyst (high risk) as soon as possible.
- The main weakness of this project is that none of the proposed approaches stands a good chance of meeting the very challenging targets of this project. In particular, this concerns the unwarranted belief that introducing a methanol-tolerant but poorly performing catalyst is going to result in high power densities. At the DMFC current densities required to generate high power, crossover has no impact on DMFC cathode performance. However, a poorly performing PGM-free ORR catalyst, additionally requiring thick electrodes to reach the required catalyst loading, is certain to have a negative impact on the power output relative to any Pt/C catalyst. Overall, the team's biggest weakness appears to be a lack of DMFC expertise.
- It is unclear whether the researchers know why they are doing what they are doing. From a technical perspective, the researchers are fine, but there is no clear reason a direct methanol fuel cell is needed. There are many good reasons why one might want to develop a methanol fuel cell, but without an application, uncertainty will remain around the objectives, which will lead to milestones and targets that relate more to what can be achieved rather than what needs to be achieved. This may not be a problem at this stage, but the answer to the question "why?" needs to be addressed.

Recommendations for additions/deletions to project scope:

- If this project is to have a chance of meeting its goals, the team needs to concentrate on improvements to the anode, rather than ill-conceived reductions in methanol crossover and methanol tolerance and unsubstantiated benefits of the use of high methanol feed concentration (there are some benefits, but overall, they are quite minimal). Improving the anode is easier said than done, but it is the right primary focus of any research aimed at changing DMFC status in a major way. The way the PGM-free catalyst development has been carried out to date appears not to be DMFC-specific and is largely a duplication of the effort in other projects. Deletion should be considered.

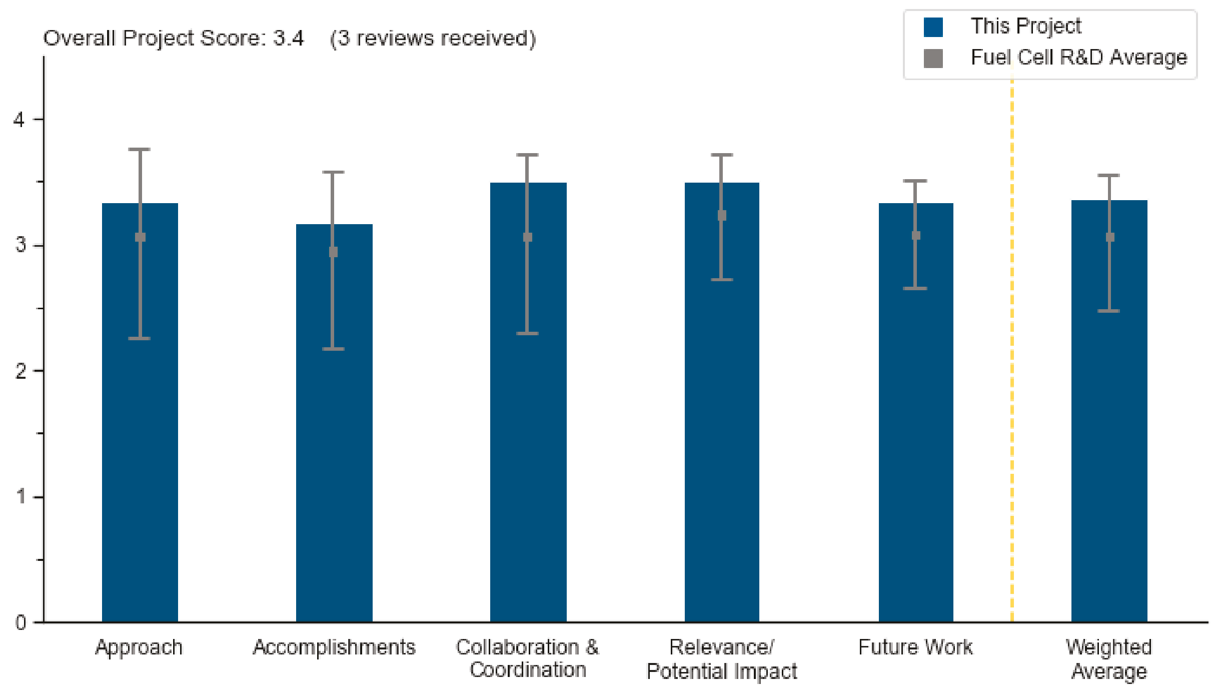
Project #FC-318: Lab Call Fiscal Year 2019: Accessible Platinum-Group-Metal-Free Catalysts and Electrodes: ElectroCat

Jacob Spendelow, Los Alamos National Laboratory

Brief Summary of Project

Platinum group metal (PGM)-free cathodes are much thicker and coarser than PGM cathodes. Model calculations suggest significant effects of electrode thickness on oxygen transport that, in turn, cause losses of several hundred millivolts at high currents. Similarly, H+ resistance for ~5 µm PGM-based cathode catalyst layer causes losses of ~20 millivolts, while a first approximation of the required ~100 µm PGM-free cathode catalyst layer results in losses of several hundred millivolts. The project targets improvements in electrode transport and catalysis of PGM-free catalysts to achieve U.S. Department of Energy target power densities. The project addresses the barriers of durability, cost, and performance.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an interesting approach to improving accessibility through electrode structure design. This is being tried for Pt-based catalysts, but it should be more effective here with thicker PGM-free electrodes.
- The focus on membrane electrode assembly (MEA) testing is appropriate. Robustness testing and operation of the full range of conditions will be important.
- This is an innovative approach to addressing the limitations of electrode design for PGM-free catalysts. The modeling portion will be important to guiding electrode structure development.
- The approach is based on catalyst and electrode structuring to improve transport in PGM-free electrodes. The project has little emphasis on catalyst synthesis.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has just started. There is good preliminary data on electrode structuring. There is some uncertainty as to what catalyst is going to be used in the project.
- This project is in the start-up phase, so it has only been a short period of time. The project team has started developing proton channels with encouraging utilization numbers.
- This project is just starting, so there are no accomplishments to date.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- There is a good assembly of collaborators to reduce project risk. Advanced characterization from the DOE Electrocatalysis Consortium (ElectroCat) will provide good analysis to support hypotheses.
- The project will be integrated with ElectroCat and likely leverage the PGM-free catalyst expertise at Los Alamos National Laboratory.
- The plans for collaboration are good and include collaborating with and taking advantage of ElectroCat's capabilities.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The proposed effort is highly relevant to the implementation of PGM-free catalysts in fuel cells. Succeeding in decreasing the mass transport barriers will have a high impact on the ultimate reduction of fuel cell MEA costs.
- The impact will be determined by the performance and durability of the catalyst used in electrode development.
- The project is relevant and related to Fuel Cell Technologies Office efforts in PGM-free catalysts and ElectroCat.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The effort is just beginning. The proposed plan is complete. It is suggested that the project team focus on one "best in class" PGM-free catalyst, versus the implied multiple catalysts.
- The project's proposed future work is directed toward improving the accessibility of PGM-free active sites.
- The proposed future work looks appropriate for the project goals.

Project strengths:

- The project concept should improve the accessibility and performance of thick catalyst layers. The proposed interactions with ElectroCat should leverage the consortium's capabilities in order to accelerate project accomplishments.
- The approach purports to address both proton and oxygen transport and the ability to change electrode architecture to maximize each. Similarly, the approach seems very flexible in being able to change the gas and proton channels.
- The strength of the project is in the principal investigator's experience in evaluating MEA performance and past accomplishments in microstructuring cathodes for PGM catalysts.

Project weaknesses:

- There is no major project weakness in reference to the electrode focus of the project, but there was a lack of consideration of the catalyst.
- No weaknesses are evident at this time.

Recommendations for additions/deletions to project scope:

- *Note: Reviewers did not provide comments in response to this question.*

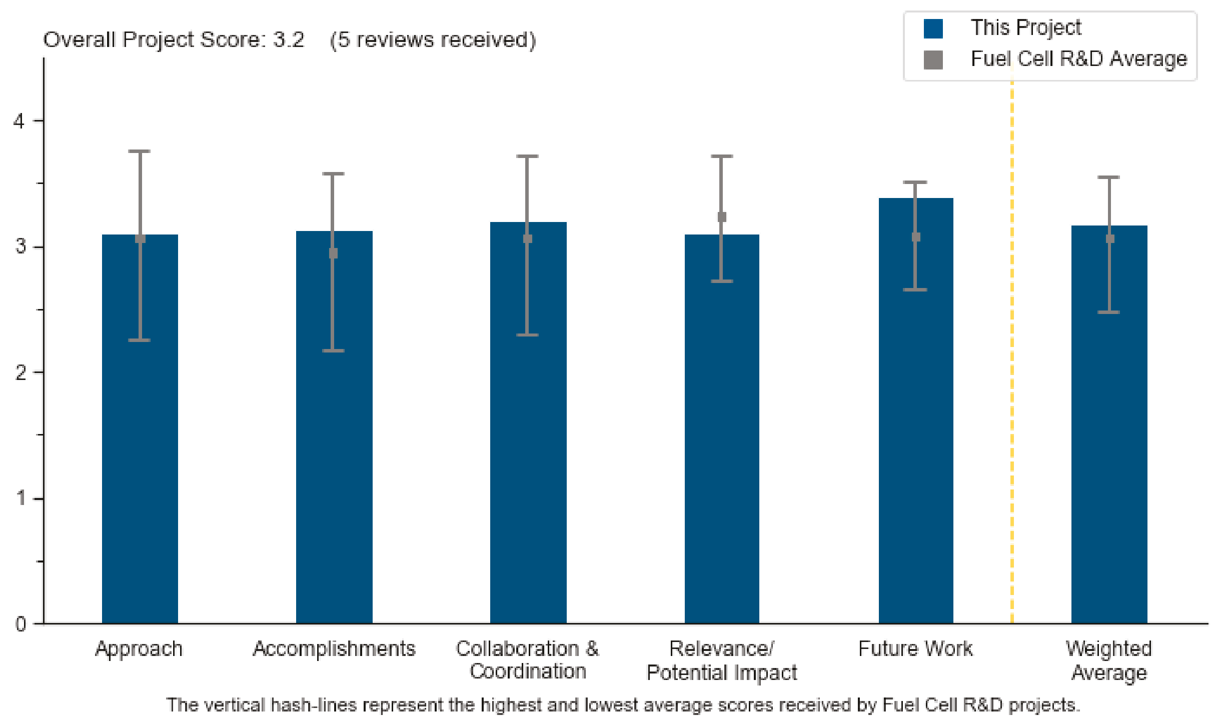
Project #FC-319: Lab Call Fiscal Year 2019: Low-Cost Gas Diffusion Layer Materials and Treatments for Durable High-Performance Polymer Electrolyte Membrane Fuel Cells

Rod Borup, Los Alamos National Laboratory

Brief Summary of Project

The objective of this project is to reduce the cost of gas diffusion layer (GDL) materials and improve GDL performance. To reduce GDL cost, the project will use low-cost fibers, use lower carbonization temperatures to reduce processing costs, and develop low-cost gas phase surface treatments to replace Teflon treatments, thereby lowering manufacturing costs. GDL performance will be enhanced through improved water management. The project will develop super-hydrophobicity coatings, which will prevent water flooding and transport losses, and incorporate hydrophilic pathways separate from hydrophobic domains to provide a pathway for water removal.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Reducing cost for GDLs and replacing the Teflon-coating process for GDLs is a good approach. If lower-temperature carbonization materials show improved performance over traditional GDL materials, then it is worth it.
- The proposed approach of concurrently considering materials and processing to reduce the GDL cost while raising the performance appears relevant. Durability aspects should not be forgotten.
- The critical barriers being addressed are cost and performance toward membrane electrode assemblies (MEAs) with a focus on the GDL; the aim is to decrease component cost by introducing new raw materials (i.e., natural fibers) or cheaper processes for post-treatments, while improving performance by better

controlling water- and gas-transport-related properties, thanks to the management of hydrophobicity and hydrophilicity within the structures. It is not clearly mentioned if the strategy is considering both cathode and anode sides. If only the cathode is being addressed, this should be clarified and justified. If both sides are being considered, this should also be clarified, as well as how their differences are being handled. The approach is GDL-based only, and it does not directly address durability. The cost reduction based on cheaper fibers seems clear, but it is not obvious how the treatments proposed to replace Teflon would reduce cost. It should be clarified what the cheaper processes might be. In addition, the cost reduction at the GDL level should be huge to have a strong impact on the stack cost; the expected decrease could be clarified.

- More detail would be appreciated on whether or how this approach is different from or builds on previous work done by partner Oak Ridge National Laboratory's Carbon Fiber Technology Facility. Some questions remain on the ability of low-temperature carbonization treatments to meet the electrical conductivity target (which is of growing relevance, with ever-higher current densities). Teflon is relatively inexpensive, so the gas phase treatment has to at least match the material cost. Gas phase treatments are usually reactive, so stability over time may be a concern.
- This is a new project that is just getting started. Some of the approaches could be more clearly delineated, such as the type of superhydrophobicity that is to be pursued, including the biomimetic approach. Several sources of low-cost fibers are being considered, but the approach to choosing and evaluating these materials could be more systematic, including evaluation of the chemical content (e.g., nitrogen and others).

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has just begun, so it is hard to judge the accomplishments. A few alternative materials have been synthesized, which is promising.
- It is very early in the project, so it is difficult to fairly assess the accomplishments and progress. The team has had some promising initial results.
- This is a new project, but some progress has already been made, including choosing and characterizing carbon precursors.
- The project has just started some months ago. The first results that were presented appear promising.
- The project is at too early a stage for ranking. The project's activities are going on as planned with the implementation, characterization, and testing of new fibers.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- Los Alamos National Laboratory is known as a leader in GDL and mass transport studies, Oak Ridge National Laboratory is a leader in imaging, and the National Renewable Energy Laboratory has good testing and synthesis capabilities. This is an excellent team to accomplish the work.
- The project team has a very good level of knowledge for investigating this topic. The team's contacts with GDL industry suppliers will be useful for investigating the processability of the most promising solution(s), as with Strategic Analysis, Inc. (SA) for evaluating the projected costs.
- The team's activity-sharing and coordination with three main laboratories is appropriate. A link with industry is planned in the next steps, and industrial products are being used as the baseline, which is consistent with the goal. Consulting manufacturers about upscaling the capability of the developments is planned but should be confirmed.
- There is good vertical collaboration with other Fuel Cell Consortium for Performance and Durability partners. Collaboration outside of the national laboratories would be beneficial.
- The team could benefit from interaction with a GDL supplier and/or original equipment manufacturer (OEM).

Question 4: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is of high relevance for achieving the cost, performance, and durability targets of the Fuel Cell Technologies Office, in particular with the current trend of producing MEAs from gas diffusion electrodes.
- Reducing GDL cost, primarily by reducing material cost and processing, is a significant enabler of fuel cell commercialization, and thus this work is relevant and potentially impactful.
- If the project's objectives are reached, the potential impact will be important in terms of MEA cost due to the GDL, but at the moment, the project has only just started. It is too early for any conclusions to be drawn about actual potential impact. However, it will naturally be limited to GDL cost and performance.
- Cost reduction at material (or GDL) level is a good approach only if the new low-cost material matches current GDL performance. If not, then the MEA and eventually the stack cost may be more with lower performance. An analysis of the cost and performance tradeoff will be helpful in directing this research.
- The potential cost reduction impact is high, but it is probably not critical to the success of fuel cell technology. The performance compromises from low-cost materials are a particular concern.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- This is a well-laid-out plan, but emphasis should be placed on the relationships between the structure and composition, function, and cost.
- Because of the very recent start, the planned future work corresponds mostly to the project's initial work plan. This is adequate.
- The proposed work is well in line with the project targets. Mechanical characterizations of the developed GDL could be explicitly added.
- The team needs to add a target for thermal conductivity and assess the performance against it. This is important for membrane and electrode durability at high current densities and grade-climb high temperatures. Assuming the beginning-of-life targets are met, the team should develop a plan to address coating stability.
- The proposed future work is good, but the project is aiming at developing low-cost GDL materials, and there are no tasks for estimating cost or understanding cost and performance tradeoffs.

Project strengths:

- The project brings to bear significant resources on an important cost and performance component for fuel cells. There is strong potential for the discovery of new, naturally resourced, low-cost materials and hopefully scientific understanding of material advantages and process optimization.
- The project's technical strength is in its clear approach, with several new materials already identified and tested as fibers for the preparation of carbon papers for their further study as possible GDL components. The team is also a positive, as it is conducting the developments proposed with good skills for manufacturing, characterizing and testing of new components.
- The project's strengths include its team and technical topic. This topic is important but somehow has been neglected for many years by the research community in general.
- The project appears well structured, with a high-level project team.
- The project's partners have strong diagnostic and testing capabilities.

Project weaknesses:

- Details are missing about the technical process and the justification for cost reduction of the new hydrophobic treatment that is planned. It should be clarified whether and how the strategy is addressing both cathode and anode sides. All GDL properties should be considered in the characterizations planned. It is not clear from the presentation how durability is being addressed by the developments planned;

information is also missing on how the selected routes will enable better stability, but this was not a major objective, and the project is only starting.
- There is relatively limited understanding of structure-and-composition–function–cost relationships in this area, and the project could be improved by introducing a framework for understanding these relationships.
- A cost estimation from a third party (SA or another group) is missing; an analysis of lower-cost materials versus a performance tradeoff is also missing.
- The project would benefit from collaboration with a GDL supplier and/or an OEM.
- No weakness is identified at this early stage of the project.

Recommendations for additions/deletions to project scope:

- The team should explain the reasons (based on technical evidence) for expecting cost reduction with the new hydrophobic treatments. More details should be given about how new, lower-cost component structures should lead to improved properties and/or performance. The team should clarify whether the strategy is addressing both cathode and anode sides, and how. The team should also clarify in more detail how durability is being addressed, including whether there is a possibility to maintain or improve water or gas transport properties and their stability, as well as what the risk is regarding the hydrophilicity/phobicity stability of the new materials.
- It is recommended that the team add a thermal conductivity target, something necessary to mitigate potential high-temperature, high-current-density MEA degradation. The researchers should pursue coating stability testing if they successfully identify a candidate that meets initial life targets.
- The team should add a task for cost analysis based on the final performance of the developed GDL. Otherwise, this whole activity is meaningless.
- The project could be improved by introducing a systematic framework for understanding, along with complete characterization.

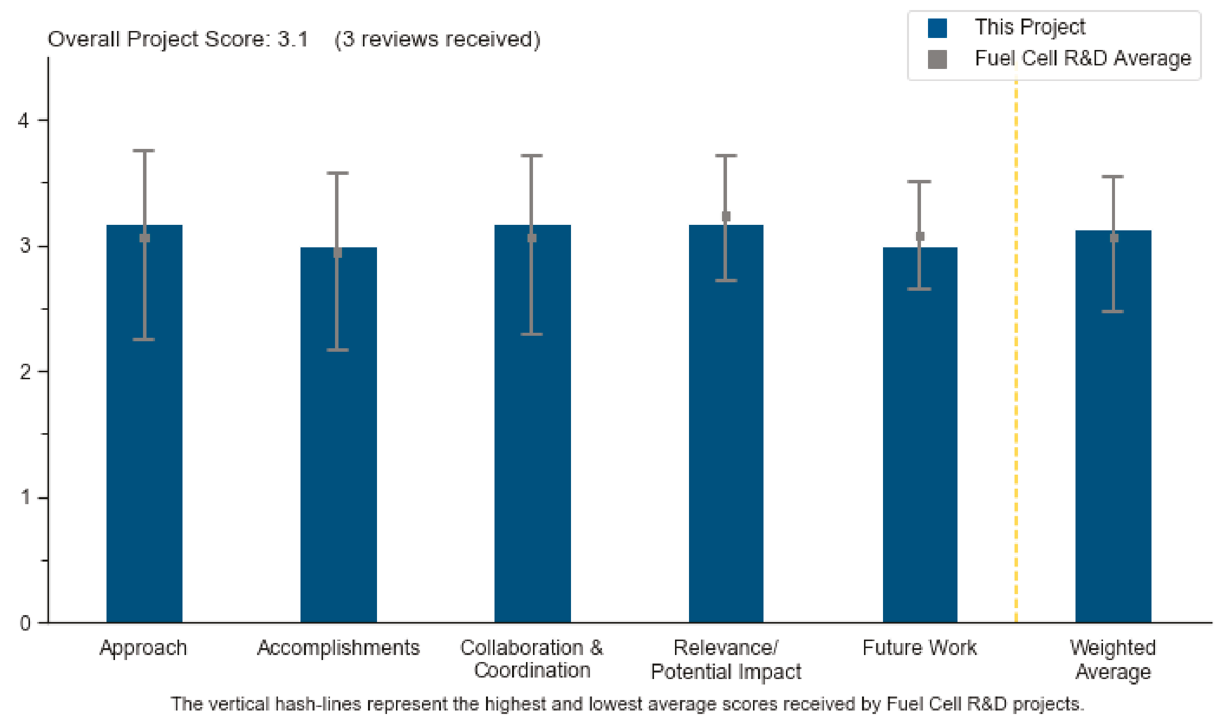
Project #FC-320: Lab Call Fiscal Year 2019: Electrode Ionomers for High-Temperature Fuel Cells

Michael Hibbs, Sandia National Laboratories

Brief Summary of Project

Sandia National Laboratories (SNL) seek to synthesize durable ionomers and demonstrate their use in fuel cells that can operate at temperatures of 200°C–300°C. These ionomers could reduce costs of future fuel cell technologies by enabling operation at high temperatures without humidification and at low-platinum-group-metal (low-PGM) loading. The project team plans to achieve >500 mW/cm^2 peak power density under hydrogen/air conditions, total PGM loading of <0.125 mg PGM/cm^2, and performance decrease of <5% after 1,000 hours of operation at 200°C.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This very early research and development (R&D) work is aimed at a relatively wide-open area, which is electrode function in intermediate-temperature fuel cells. It is forward-thinking to integrate the promise of phosphoric acid membranes in covalently functionalized polymers and their evaluation in electrodes, and the work addresses industry concerns about the next phase of fuel cell R&D.
- Phosphoric acid fuel cells (PAFCs) have had many challenges over the years. This approach offers a new perspective over the traditional or gel electrode (polybenzimidazole [PBI] or phosphoric acid [PA]) strategies. While the project is just starting, the team has some reasonable preliminary data that support the benefits of this type of membrane.
- The critical barriers being considered are cost, performance, and durability, focusing on the electrodes and high-temperature polymer electrolyte membrane (HT-PEM) operation only. The specific targets proposed

are low compared to low-temperature (LT)-PEM cases, but the targets are also lower than the state-of-the-art (SOA) HT-PEM cases with 500 W/cm² peak power and 5% performance loss after 1,000 hours of aging. Only the PGM loading that is being targeted is in the same range as that of LT-PEMs, with 0.125 mg/cm², which seems far too challenging for HT-PEM operation. The work is focused on the ionomer; hence the project team should consider linking with other projects that are focused on catalyst and membrane electrode assembly (MEA) development, at least for final implementation and assessment. The approach was initiated because of the general advantages of operating a fuel cell system at higher temperature, with lower costs thanks to humidification removal and easier heat management. However, at the highly innovative level of this work, it would be important to also mention the risks of getting performance at the targeted temperature that is too low or poor start-up management at ambient temperature. The approach aims at replacing the proton conductors within the catalyst layers with phosphonic groups that are less sensitive to the leaching issue. In the activities presented, the results are compared to previous innovative developments but not to the SOA components of the HT-PEM fuel cells, which should be part of the approach.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project is in very early stages, and while little tangible progress has been made, the team has started well and appears to be on the right track. Leveraging previous polymer chemistry probably gives the best chance for success.
- The project has just begun, and therefore, expectations for progress are minimal. However, the preliminary data look reasonable at this stage and show good progress toward the ultimate DOE Hydrogen and Fuel Cells Program goals.
- To assess the project's accomplishments toward DOE objectives, the results of the fuel cell tests that are planned for later will be needed. Regarding the project objectives, the progress is fair. The synthesis of at least one new material allowed for a comparative test to be performed with a previous material that was developed by Los Alamos National Laboratory (LANL) for HT-PEM operation as well. This material presents specific behaviors with better performance at 200°C compared to 160°C, but the performance is very low. More materials need to be prepared and tested to properly assess progress.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- It is a good idea to integrate directly with LANL and indirectly with Rensselaer Polytechnic Institute to leverage other polymer chemistries besides those poly(phenylene) polymers available at SNL. LANL will be a great partner for evaluating polymers in a fuel cell.
- Both SNL and LANL are well regarded; however, it would be best to have an academic or industrial partner with expertise in PAFCs. It is acknowledged that this is a lab call project, but engaging a researcher with PAFC capabilities at some point would go a long way in validating the concept.
- Two national laboratories are involved; this seems relevant for the actions planned. A link should be envisioned with other projects focused on other MEA components, at least for implementation and/or assessment purposes, including protocols. It will also be necessary to plan links with industry for further development and for relevance in regard to scalability.

Question 4: Relevance/potential impact

This project was rated **3.2** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Intermediate-temperature fuel cells potentially have much higher efficiency than PEM fuel cells, and their research is very promising. Few other laboratories are looking at this type of chemistry, and this project is potentially impactful far beyond its timeline. For such exploratory and high-risk work, this project is well designed.
- Fuel cell operation between 100°C–200°C could be very advantageous. If successful, this project has the potential to advance the phosphoric acid electrolyte field.
- At the system level, it should be clarified whether the gain that is expected thanks to temperature increase (>200°C) would still be valuable if performance loss is too high compared to conventional components. However, this analysis is hard to do at this stage in the project because more progress is needed. At the material level, evaluating the potential impact would require the team to get more data in actual fuel cell conditions.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The polymerization of new polymers with this functionality and testing them in an MEA is good initial work. Having several synthetic schemes reduces the risk of failure for synthesizing new polymers.
- The work proposed for both membrane and electrode–ionomer synthesis looks to be reasonable and well designed.
- The project's future work is still very open regarding the formulations that are to be synthetized; this is maybe not clear enough when considering very short-term objectives (sooner than June 2019). For longer-term plans, low-PGM durability is mentioned; this seems much too ambitious a goal and is maybe not so relevant. Performance with the usual PGM loadings should be strongly improved first. The possibility of bridging this new route with old PA-doped, PBI materials could be considered, as well as other baseline materials for membranes or catalysts to fill the gap with SOA for initial performance.

Project strengths:

- This project has the potential to advance the PAFC field. The idea of strongly binding the PA to a quaternary amine could solve one of the main issues of PAFCs: PA loss at high temperatures. The fully aromatic structures look to be stable in the preliminary tests that have been run to date.
- The main strength of this project is the initial idea of proposing a new molecule that is expected to compete against the weaknesses of previous materials due to acid leaching. The type of material proposed presents interesting conductivity properties and original behavior during fuel cell testing. The team has identified possible obstacles and proposed means for mitigation.
- The project's strengths include its broad polymer synthesis and its good leveraging of collaborators. This project is doing potentially high-impact work in an important area.

Project weaknesses:

- It is unclear how the team intends to overcome some of the traditional issues with PA or PBI/PA fuel cells. For example, there are issues with start-up/shut-down, liquid water, PA catalyst poisoning, etc. Even with the fully aromatic backbone polymer, there are still reservations about long-term operation at elevated temperatures (~150°C–200°C).
- The performance level is low. The gap with conventional HT-PEM fuel cells should be considered and discussed, major causes should be identified, and solutions should be proposed. No hydrogen/air data were presented. The stability target does not seem consistent with the current status of the project and may be too ambitious.

Recommendations for additions/deletions to project scope:

- Comparison and positioning should be done regarding the SOA components of HT-PEM fuel cells. The team should discuss and explain the justification for the performance difference with previously developed PA-ADAPP and PPFS when the temperature is increased from 160°C to 200°C, particularly when considering the limited differences seen in the conductivity data. Selecting one route and improving the initial performance with conventional PGM-loading electrodes should be prioritized.
- It would be helpful to include some start-up/shut-down and durability testing data, as well as a comparison with traditional PBI/PA systems. Even a comparison with literature results would help to show the differentiation of this approach in those areas.

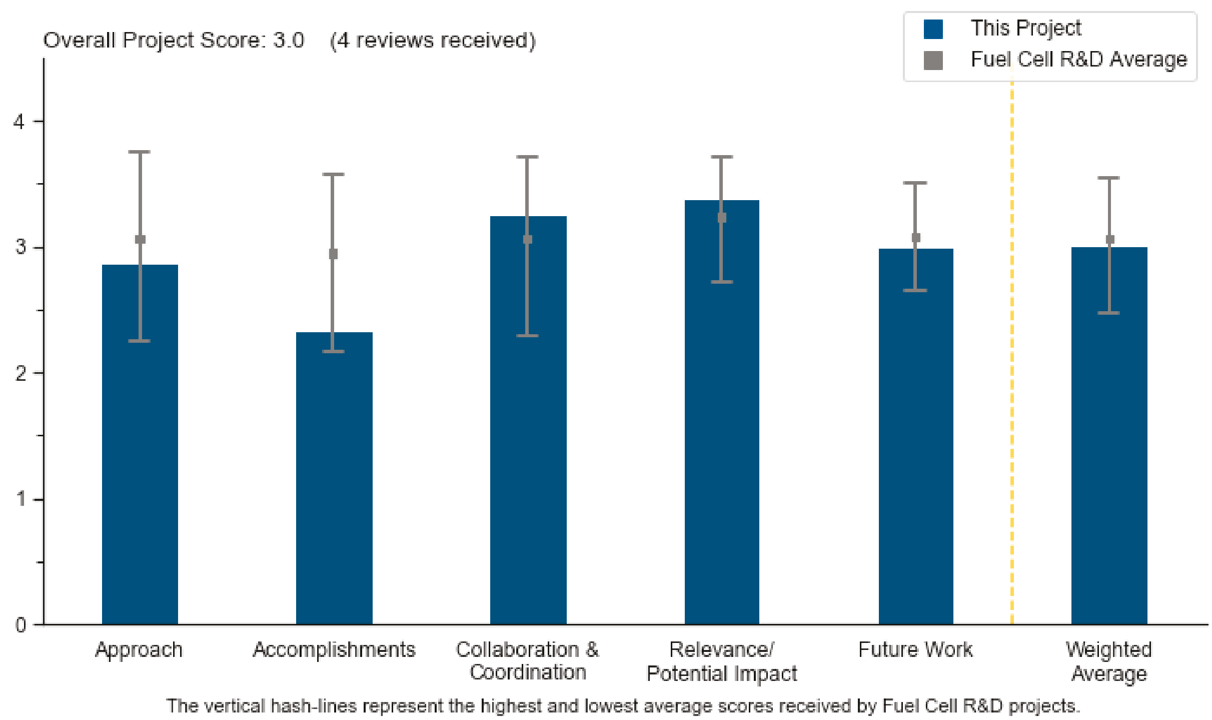
Project #FC-321: Lab Call Fiscal Year 2019: Solid Phase Processing for Reduced Cost and Improved Efficiency of Bipolar Plates

Ken Ross, Pacific Northwest National Laboratory

Brief Summary of Project

The goal of this project is to develop and demonstrate methods to fabricate bipolar plates (BPPs) to meet or surpass all 2020 U.S. Department of Energy (DOE) technical targets for BPPs, including a cost target of less than $3.00/kW$_{net}$. The fabrication concepts with the greatest potential to meet the technical targets will be identified and ranked using best practices of product design and development. Among the manufacturing approaches to be evaluated is high-velocity cold spray coating, which is orders of magnitude faster than currently used vapor deposition techniques. Top-ranked concepts will undergo process development, and coupons will be tested to validate performance. The project will fabricate and test full-scale prototypes and conduct economic analysis to validate achievement of cost and performance targets.

Project Scoring



Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **2.9** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The overall approach appears to be good since the team is utilizing cost models to help screen alternative concepts, which should help ensure that the project develops a BPP that meets both the challenging technical targets and the cost targets.
- The project has identified pathways to identify the problems with achieving BPP targets and the solutions to those problems. The project’s approach does not explain how the team will fabricate ribbed BPPs. The principal investigator said the method was proprietary, which makes it very difficult to evaluate.
- It would be beneficial to see more detail on the approach, but the general outline appears sound.

- It is unclear from this poster what is driving the cost of BPPs; it could be raw materials costs or processing. Knowing these details would help with evaluating whether the approach is well designed to meet the 2020 DOE targets. It would also be helpful if the slides presented how current, state-of-the-art BPP technical properties compare to technical targets; this information would help with understanding where improvements need to be made or what would be the most impactful. It is stated that cold spraying should be lower in cost than chemical vapor deposition (CVD). It would be beneficial to include some generic cost comparisons, even if not for the materials used here, to demonstrate that the approach used in this project should result in cost savings. Since Strategic Analysis, Inc. (SA) has participated in the project, it seems it would be possible to attain these data. However, since a breakdown of BPP manufacturing costs is not provided, it is not possible to determine whether improving production rates by "orders of magnitude" would reduce costs by orders of magnitude, 10%, or 1%. The presenter mentioned that cold spraying should result in fewer pinholes than CVD, but it is not clear why this would be the case or if there are any data to support this.

Question 2: Accomplishments and progress

This project was rated **2.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This ranking tool seems like it could be helpful, but it also seems like this analysis should have been done in the proposal stage to identify that the proposed strategy had merit. While the specifics of the fabrication categories may be proprietary, some generic data should be presentable, such as that Category 1 is expected to reduce cost by XX% or improve conductivity by YY%. The lack of any details makes it hard to know how much of an impact any of the concepts might have on cost or technical performance. Based on the milestone table, it appears that coupons should have been generated, but no data were presented, and the presenter stated these had not yet been prepared, so it is assumed that this milestone was not met on time.
- No details on results to date are provided, so it is hard to assess. It is also not clear how much work has been done since the only indication is that the project started in October 2018. The work to date appears to be the completion of a concept down-selection process, but the details are sparse.
- It is early in the project, so the accomplishments and progress are not easy to assess.
- This is a new project; the activities are just initiating.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project has identified important coating technology and a company with experience in fabricating coated BPPs. SA provides excellent guidance on cost.
- The project's collaboration and coordination is positive; the partner has experience in addressing BPP goals. The project could benefit from engagement with an original equipment manufacturer (OEM).
- The team has good partners with the right experience and interest in this project. It is too early to comment on the actual collaboration.
- The inclusion of industrial partners is beneficial for allowing researchers to better understand what processes may be feasible in a manufacturing setting. It seems that data from SA has not been used as well as it could be.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- A high-rate fabrication method for producing stable BPPs is needed, and this approach has the potential to meet that need.
- BPP cost and durability are significant enablers for the DOE Hydrogen and Fuel Cells Program.

- This project is definitely focused on a technology that still needs to be developed to meet the automotive targets.
- Given that current BPPs do not meet cost targets, it seems innovation is needed in this area. A higher score would have been given if it had been clear how well current BPP technologies address cost and performance targets.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed future work is light on details, but the approach seems sound. For Al to be viable, a perfect pore-free coating with good adhesion will be needed. The team should clarify what the surface pretreatment is, as well as how likely cold spray is to meet formability and pore-free requirements.
- The proposed development of three selected fabrication concepts provides multiple pathways to success. The team will need to demonstrate a method for forming BPPs without developing punctures in the plates.
- The go/no-go is missing one key metric, which is measuring the contact resistance between the BPPs and a typical gas diffusion layer (GDL). This interfacial resistance can be large with some materials and carbon GDLs, and it should be assessed early in the project to rule out surface coatings that have high contact resistance.
- The work seems to be following the project plan, but it is behind schedule. It is not clear from the slides if the project is on track to meet the go/no-go.

Project strengths:

- This is a good approach with a low-cost process and cost focus. The project has a good team with the right experience, capabilities, and background.
- Strengths include the potentially high throughput of cold-spray processing.
- The new approach to coating the BPP may give high-rate deposition.
- Given that the project was only six months old when the slides were due, it is not surprising that only initial results were available. Cold spraying is a novel approach to BPPs.

Project weaknesses:

- The team claims to have a proprietary method for forming BPPs that eliminates stamping and the high cost of processing equipment; however, the researchers will not discuss the method, so it is very difficult to evaluate. If DOE wants an evaluation of this proprietary forming method, they will have to find an alternative evaluation method.
- The presentation was light on details, so it is difficult to gauge. The team needs to clarify what the surface pretreatment is and how likely cold spray is to meet formability and defect-free requirements.
- The lack of any details presented in this poster makes it difficult to assess this project. Estimates of the potential of cold spraying were not presented.
- The technical milestones do not include all of the key technical targets.

Recommendations for additions/deletions to project scope:

- The project scope is acceptable.
- The team should measure all of the metrics established by DOE (i.e., the list shown on slide 3). In addition, the team should measure the contact resistance of BPPs and GDLs and compare that to the baseline BPP.
- The team should consider interacting with a stack developer or OEM.
- The team should discuss the forming method so it can be evaluated.

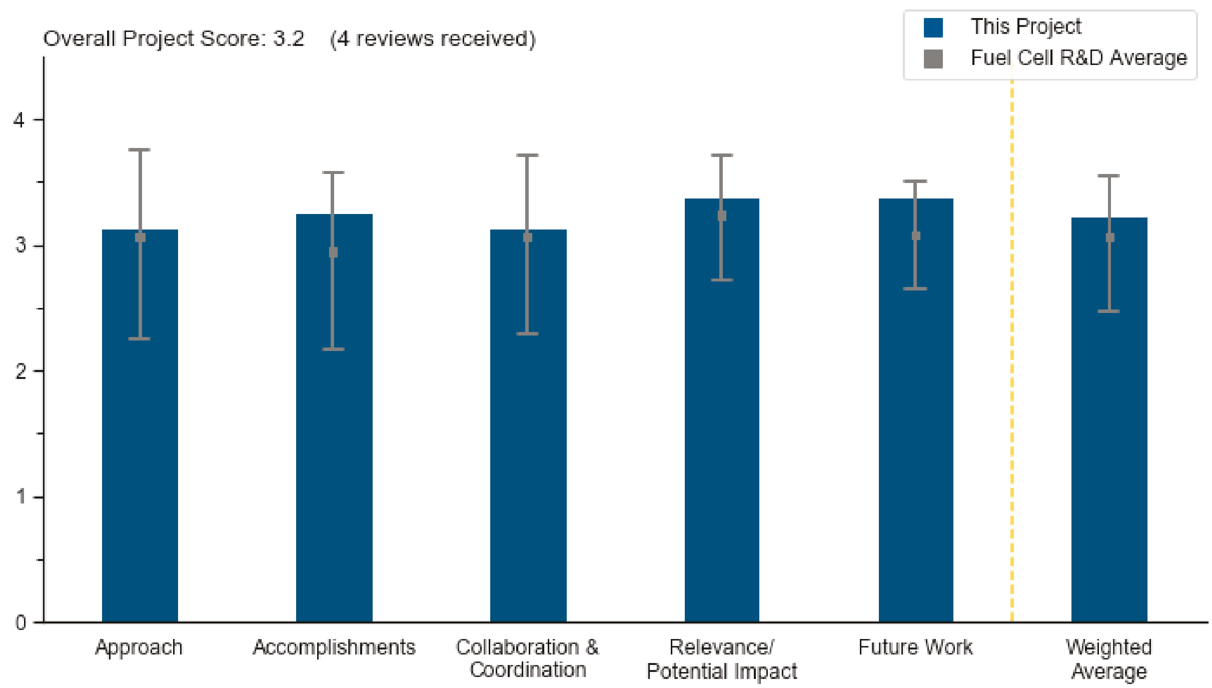
Project #FC-322: Lab Call Fiscal Year 2019: Polymer Electrolyte Fuel Cell Electrode Structures with Encased Catalysts to Eliminate Ionomer Adsorption on Catalytic Sites

Deborah Myers, Argonne National Laboratory

Brief Summary of Project

This project intends to address the lack of sufficient surface power density at rated power for an automotive polymer electrolyte fuel cell (PEFC) stack and the lack of sufficient performance durability due to direct contact between the proton-conducting and electron-conducting components of the PEFC cathode catalyst layer with the platinum catalyst surface. The approach is to protect Pt and Pt_xCo_{1-x} nanoparticle cathode catalysts from direct contact with the proton-conducting and electron-conducting phases while also maintaining sufficient oxygen, proton, and electron transport to the catalytic sites. This is achieved by encasing Pt and Pt alloy catalyst particles in the cages and pores of zeolites. The new catalyst powders will be synthesized and characterized, and membrane electrode assemblies (MEAs) using the catalysts will be fabricated and tested.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Fuel Cell R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an excellent, but very challenging, approach. If successful, it will boost the performance (areal power density) and durability too, as Pt nanoparticles are not in contact with the ionomer directly.
- The project has a logical approach to address key issues with low-platinum-group-metal (low-PGM) electrodes. The work started with some prior Argonne National Laboratory (ANL) results and learnings.
- The approach is very logical and focused. The project has spoken to and planned for key challenges.

- There are many questions or uncertainties that would have to work out for this approach to work. First, the zeolites have insufficient conductivity, and placing the catalyst within an insulating cage is a dubious start. The encaged catalyst's having electrical and ionic connectivity through the catalyst layer will be very difficult to achieve. Even for rotating disk electrode testing, the team needed to add carbon for electrical conductivity. Finally, if the team is able to achieve all of that, the question as to whether caging the catalyst will lead to decreased dissolution is completely open.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- It is impressive to see that 62 Pt catalysts were synthesized. However, getting Pt or PtCo in zeolite cages will be very challenging. Really good progress has been made so far, considering the project has just started.
- At this point, the researchers are just getting started; they have been able to make a number of catalysts, although they are quite far from demonstrating sufficient performance.
- It is six months into the project. Although struggling to get reasonable oxygen reduction reaction activity, the team is recognizing the problem and revising work accordingly.
- It is early, but there are materials in hand already. Many samples have been made.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- This is a relatively modest project that should not need multiple collaborators. Having said that, the other members of the Fuel Cell Consortium for Performance and Durability are doing what they do best: K.C. Neyerlin (National Renewable Energy Laboratory [NREL]) with MEA studies and Karren More (Oak Ridge National Laboratory [ORNL]) with microscopy.
- The team members cover all of the required tasks.
- This is a small but focused team.
- Between ANL, NREL, and ORNL, this is a good team, but communication with other or outside teams is not clear.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This is a critical and well-known issue; many different approaches, such as various types of ionomer and ionic liquid, have been tried without much success. If this works, it will be the ultimate solution to the problem.
- The impact could be high in reducing Pt dissolution and migration away from the catalyst. The key concerns would be processing cost and quality control.
- This project may improve the performance and durability of low-PGM electrodes. If successful, the cost reduction could be substantial.
- This is hard to judge without knowing if these can ever be made economically. They have so many challenges that it is hard to believe that they will be able to meet them all, certainly not in this first project.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The team's focus on electrical continuity and cycling stability is perfectly appropriate. The cycling stability is the entire *raison d'être* and should be shown first.
- The work is well laid out. More needs to be discussed about how electrical conductivity might be maintained. Carbon inclusion is laid out, but the seemingly random inclusion could still lead to significant metal deactivation. This seems to be a key risk in the project. Secondly, the impact of water management should be discussed.
- All proposed future work is targeted toward achieving the project goals. The most challenging thing will be to avoid Pt deposition outside or on the zeolite cage.
- There is a clear plan.

Project strengths:

- It is a unique idea. If, for some reason, caging a catalyst will stop it from dissolving, this will have broad applications for fuel cells, direct methanol fuel cells, and electrolyzers.
- The project has a novel idea that will offer significant learning and chance for improvement. The goals are focused.
- The approach to solve the issue is a major strength, along with the team players.
- This is a small and focused project. The challengers are understood.

Project weaknesses:

- Zeolite has a proton conductivity of around 0.1 S/cm, which may hamper the performance. Also, carbon needs to be integrated into the catalyst layer to provide electron conductivity. Additionally, Pt needs to be inside the cage, so it is a very complex system to make work. This is not really a weakness but a challenge.
- The synthesis team is not as experienced as other groups. This is a topic that would be better executed by industry.
- There is a risk with the carbon conductivity and water management. There is concern over the cost of the process.
- There are too many leaps of faith. It must be believed that placing the catalyst in a zeolite will stop dissolution. Then it must be believed that once it is in the cage, it will have heady access to ions, electrons, and reactants. Finally, it must be believed that it will be economical to manufacture. Any one of these is a fatal flaw.

Recommendations for additions/deletions to project scope:

- The team should down-select a few catalyst candidates and work with those only.
- Although the chances of these catalysts do not seem favorable, the go/no-go performance metric seems to be incorrect. The important thing to show would be the decrease in catalyst dissolution while being able to communicate with the catalyst. If the researchers can show this, they should be given the chance to try more effective catalyst blends.
- Considering the developmental stage of the project and similar development that has already been done in the industry, this stream of work will not add much value.

2019 – Infrastructure and Systems R&D
Summary of Annual Merit Review of the Infrastructure and Systems R&D Subprogram

The Infrastructure and Systems R&D subprogram aims to reduce the cost of hydrogen production, storage, use, and transport to enable H2@Scale. The subprogram includes three project categories: Hydrogen Infrastructure R&D, Technology Acceleration, and Systems Analysis. The Infrastructure and Systems R&D areas in 2019 included (1) low-cost, high-efficiency liquefaction, pipelines, chemical carriers, and tube trailers; (2) low-cost and reliable compressors, pumps, dispensers, and stationary storage; (3) grid integration of hydrogen production; (4) novel methods of manufacturing and improvements in durability of hydrogen technologies; and (5) heavy-duty fueling technologies. R&D priorities are informed by crosscutting systems analysis. The subprogram collaborates with state and local organizations and other federal offices and agencies (such as the U.S. Department of Defense, U.S. Department of Transportation, and the U.S. Department of Energy Offices of Science, Fossil Energy, Nuclear Energy, Wind Energy, Solar Energy, Geothermal Energy, and Advanced Manufacturing) to leverage outside activities, coordinate efforts, and build opportunities for new technology applications and deployment.

Summary of Infrastructure and Systems R&D Subprogram Reviewer Comments

The Hydrogen and Fuel Cells Program (the Program) reviewers commented positively on the level of industry and stakeholder engagement and participation within the Infrastructure and Systems R&D subprogram. Most notably, the subprogram was lauded for the progress and success of the H2@Scale initiative, though more work is needed. Suggestions for future H2@Scale research topics included further assessment of value chains, such as co-produced oxygen and renewable hydrogen for various applications, especially on a regional basis. There is also a need to identify near-term value propositions to support the transition to H2@Scale.

Program reviewers commended the increased emphasis on reliability and cycle life of infrastructure technologies. Specifically, the work on hydrogen dispenser hoses was called out as an example of successful technology transfer, which is needed to reduce the cost of dispensed hydrogen. In addition, the work on magnetocaloric liquefaction is recognized as having the potential to be high-impact. While Hydrogen Infrastructure R&D was considered to be well balanced, reviewers suggested that there be more research on hydrogen compression technologies. It was also recommended that Hydrogen Infrastructure R&D be expanded as a way to address the near-term priority of low-cost hydrogen.

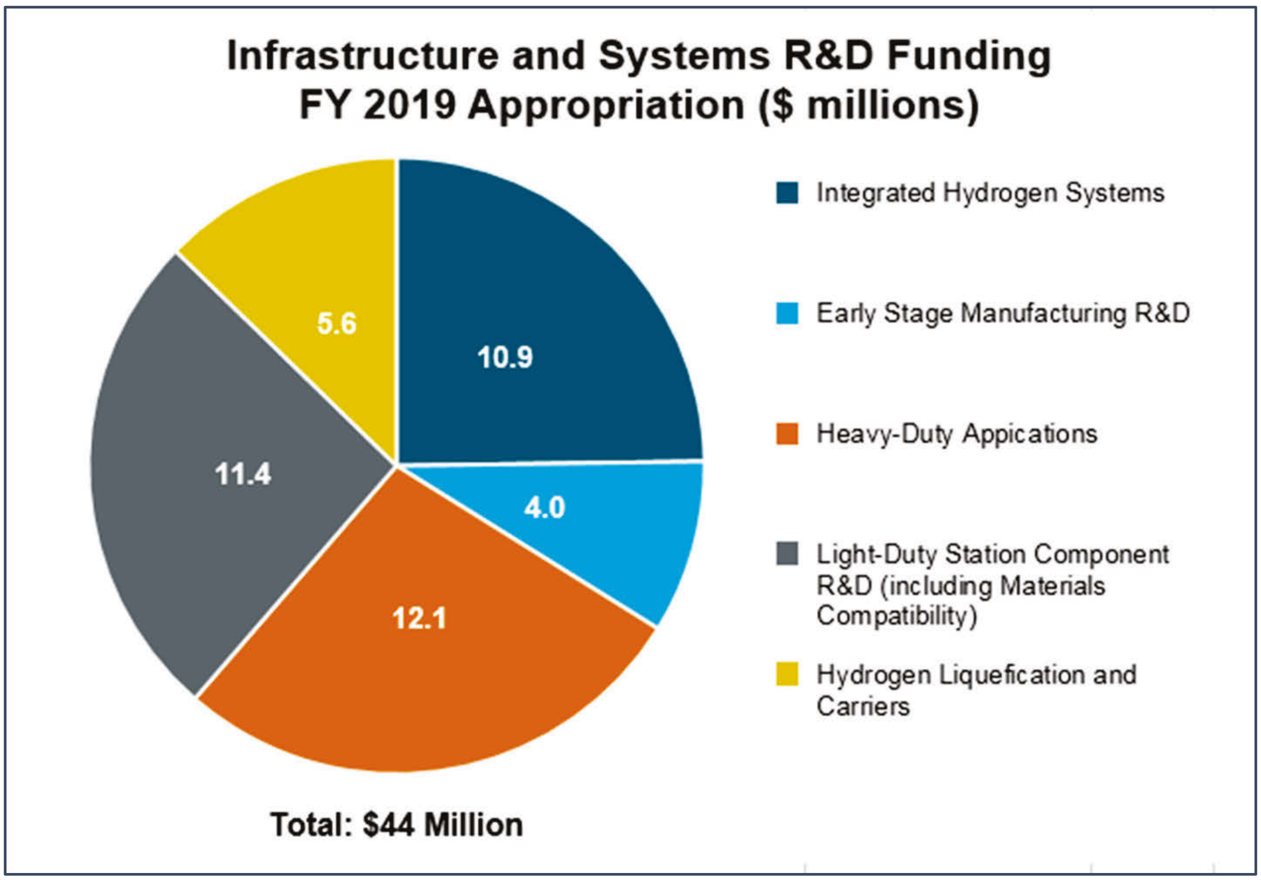
Within the Technology Acceleration activities, reviewers applauded interagency collaboration, as well as stakeholder engagement on new hydrogen and fuel cell applications, such as with the H2@Rail workshop. In addition, the Technology Acceleration project on advanced hydrogen refuelers was recognized for its high impact potential. Reviewers also pointed to the progress made on membrane electrode assembly (MEA) fabrication methods as one of the most significant accomplishments of the entire Program. Reviewers suggested that additional early-stage R&D be focused on manufacturing of hydrogen technologies, in particular low-temperature electrolyzers, to support cost reductions and value chain maturation.

Systems analysis, including technoeconomic analysis, on medium- and heavy-duty fuel cell applications was cited as a strength of the subprogram. Reviewers recommended that the technoeconomic analyses be expanded to assess renewable hydrogen production. The Systems Analysis activities were praised for providing a benchmark for business cases, a tool for measuring progress in market development, and guidelines to the global community. Suggestions for future research topics included life-cycle analysis of various e-fuels, analysis on reducing material consumption to support moving toward a circular hydrogen economy, and energy transition analysis.

Nine Hydrogen Infrastructure R&D projects were reviewed, receiving scores ranging from 2.8 to 3.7, with an average score of 3.3. Nineteen Technology Acceleration projects were reviewed, receiving scores ranging from 2.8 to 3.7, with an average score of 3.3. Under Systems Analysis, five projects were reviewed, receiving scores ranging from 3.0 to 3.6, with an average score of 3.4. The individual project reports in this section contain a summary of the project, the project's overall score and score by question, and the project-level reviewer comments.

Infrastructure and Systems R&D Funding

The fiscal year 2019 appropriation for the Infrastructure and Systems R&D subprogram totaled $44 million. The breakdown between Hydrogen Infrastructure R&D, Technology Acceleration, and Systems Analysis funding is shown in the figure below. The funding is expected to reduce the cost of hydrogen delivery and dispensing, support wide-scale hydrogen production and use, and enable resilience of power generation and transmission. Future work in the subprogram is expected to focus on applied and early-stage R&D for the H2@Scale initiative related to hydrogen production, integrated energy systems (including nuclear hybrid energy systems), advanced manufacturing, and hydrogen energy storage. For Systems Analysis, funding is focused on the hydrogen value proposition for H2@Scale, the levelized cost of hydrogen from renewable and nuclear hybrid-integrated hydrogen production pathways, the impacts of hydrogen delivery/onboard storage/fuel cells on R&D needs for onboard hydrogen storage options and associated costs, emissions from hydrogen pathways for fuel cell medium- and heavy-duty trucks, and hydrogen fueling station business assessments.



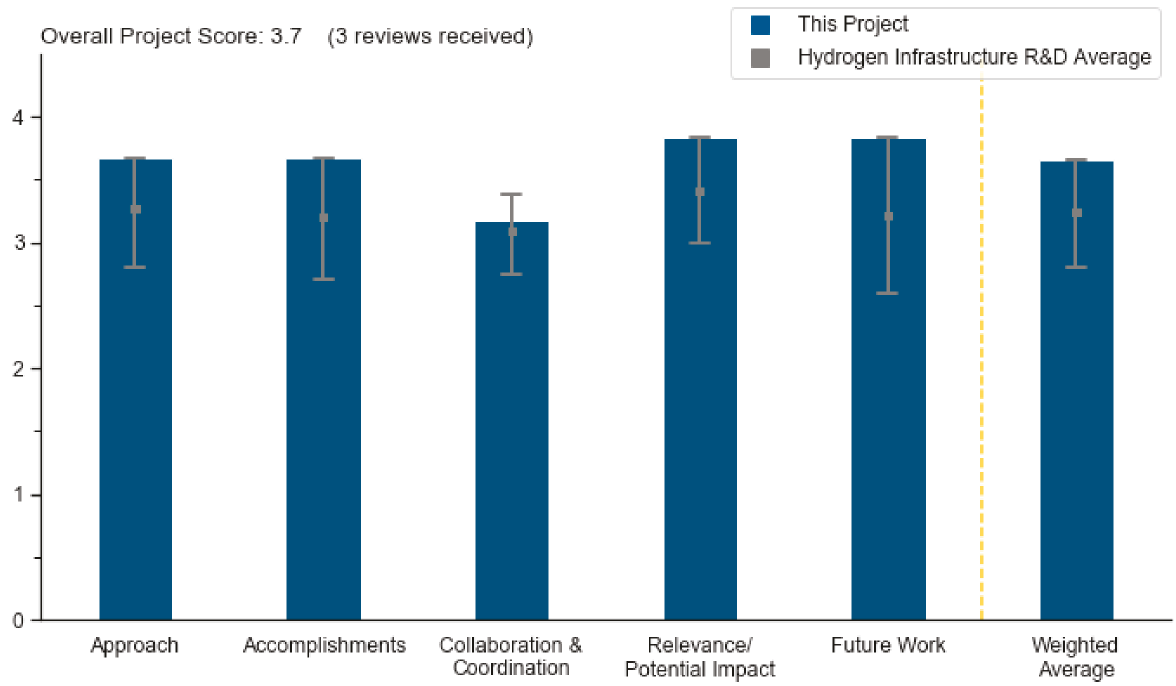
Project #IN-001: Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Steels

Chris San Marchi, Sandia National Laboratories

Brief Summary of Project

The primary objective of this project is to evaluate the potential for modern, high-strength steels to facilitate reductions in the cost of hydrogen pipelines. Specific goals are to (1) characterize fatigue performance of high-strength girth welds in the presence of hydrogen gas and compare performance to that of low-strength pipe welds, and (2) establish models that predict pipeline behavior as a function of microstructure in hydrogen to inform future development.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is very well founded: focusing on microstructure understanding and then bounding the project with focus on three specific materials and their behavior, with regard to specific behaviors (crack nucleation and cryogenic behavior). There is much to look at here, so this approach will, one hopes, keep it manageable. Also, the approach of defining each task with a “Science Question” provides a great metric to make sure that the work being done ties back to that question.
- This effort is addressing important aspects aimed at understanding the mechanisms controlling the hydrogen embrittlement (HE) degradation process. The project has selected a subset of issues that are critical to informing relevant problems of material capability for hydrogen storage and delivery. Generally, there are multi-scale modeling and experimental approaches that take advantage of some of the unique capabilities at Sandia National Laboratories (SNL). The project’s approach to high-strength ferritic steel microstructures aims to have a mechanistic understanding of fractures and further understanding to inform

resistance in >950 MPa strengths. Further elaboration on the Fe-C-H (density functional theory [DFT] and molecular dynamics [MD]) models is requested. If this is for ferritic stainless steels, then it is unclear how relevant these models are if Cr is not incorporated. The work on the Kelvin probe is very interesting; however, it is unclear what question this is answering, whether the models will be linked to the actual material, and whether the Kelvin probe will be used to try to validate the models. The project's approach to high-strength aluminum alloys aims to understand the mechanism of HE in high-strength Al as well as the role of moisture on surface interactions. The details surrounding the DFT modeling and MD modeling are unclear. It is also unclear if there are any plans to look at the uptake behavior independent of cracking in the hydrogen and H_2O environment; this would facilitate seeing the extent to which hydrogen uptake will occur. Additionally, it would be beneficial to couple some of the MD simulations at the crack tip to the focused ion beam milling (FIB) of **transmission electron microscopy (**TEM**)** results by Gangloff and Ro that quantified the structure. The project's approach to transferability of damage and crack nucleation aims to generate an HE-induced crack nucleation prediction capability framework for fatigue. This looks specifically at models to hydrogen-induced deformation and damage. It is unclear if the team has a means of quantifying the initiation lives or if there is strong evidence that the hydrogen will actually affect the initiation life. This is of particular importance if the project team wants to move toward engineering applications. Oftentimes, large-scale defects (much larger than the atomistic or dislocation processes) will lead to initiation on engineering components. It is not clear how the team is defining "initiation," which is a big problem in the field. The answer to this problem may be dependent on how initiation is defined. This may be defined as the first slip step on the surface, to 1 micron, or to 1 mm. This depends on what resolution is being defined as "initiation." Additionally, the project team's approach to the microstructure of austenitic stainless steels aims to understand the physical process of HE in austenitic stainless steel, which would inform materials design. It is unclear how the team is incorporating the hydrogen into the crystal plasticity model. It is also unclear what parameters the team is modifying, as well as how the boundaries are being handled. It is unknown whether the project team is tuning this via constitutive laws gathered from polycrystals that have been hydrogen-charged or from single crystals. Finally, the team's approach for materials for cryogenic hydrogen service aims to establish metrics and materials selection for cryo-compressed hydrogen storage on vehicles.

- The tasks and questions being answered in this project are well defined. Separating the "science questions" from the "engineering goals" in framing the approach for each task is well appreciated. It is not clear, however, how these five tasks were selected as the focus—whether these were specified in the call or chosen by the applicant.

Question 2: Accomplishments and progress

This project was rated **3.7** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This project started recently, so technical results to date are modest. Interatomic potentials have been added to the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), which is a big accomplishment. There is good progress on the "set-up" aspects of the tasks, and it seems like there should be many good results in the remainder of the year.
- Obtaining the stakeholder feedback and distilling that into a prioritized matrix of materials and failure conditions to test is a worthy accomplishment. It is recommended that the principal investigators do a sense-check on that matrix to make sure that they agree that no high-priority materials or failure modes have been omitted. Likewise, the initial tribology studies and the initial work on the test methods document represent significant accomplishments in the first year of the project.
- This is a new project, so there is not much progress; however, there are clear objectives that will be able to be tracked as progress is made.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- There may be more industry and/or supplier stakeholders that could be involved. The discussion in the presentation about contribution from NASA was helpful. Companies like Parker and others are a possibility. This is related to the issue of "validating" the materials and performance criteria that the project team has chosen.
- This is a new project, so the extent of collaboration is yet to be fully established. However, several collaborators were engaged, and these plans are solid and will reasonably improve the project. Such collaborations could and likely will be expanded as the project moves on.
- Multiple laboratories are working on each task; the accomplishments indicate that there is good collaboration between the laboratories thus far. There is no collaboration from industry or academia yet, but it is reported to be in the works—there is a funding opportunity announcement out for industry partners.

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Dedicating resources to the fundamental understanding of the materials interaction and degradation progress is very important. Such efforts will develop the data, understanding, and expertise needed to inform the design material selection and the ability to address or avoid issues in structural applications. These materials interaction issues will drive much of the economic consideration in transitioning and scaling hydrogen-based fuel economies. More specifically, by investigating traditional steel materials systems (with modifications) and candidate Al materials systems, this effort is addressing pertinent issues.
- This project is foundational for the goals of DOE and the industry, as it will underpin the design and deployment of safe hydrogen systems and also play a key role in improving the reliability of systems and equipment for hydrogen storage, dispensation, and compression.
- The presentation did not explicitly tie the materials challenges back to specific components in hydrogen storage infrastructure. While the relevance is clear generally, it could be more powerfully stated. The potential impact of this work on the field is demonstrated through the conscientious tying of microscale processes to engineering design. The project team works closely with codes and standards, and information will be disseminated to the industry through those channels. Additionally, advances in understanding of materials properties will be made available to the broader research community via Granta.

Question 5: Proposed future work

This project was rated **3.8** for effective and logical planning.

- The future work is well scoped for the resources of the project, and it would be pretty easy for the scope to grow too far, given the number of materials that could be considered and the daunting task of developing both models and test protocols for a wider range of failure modes. In particular, the focus on looking at the role of water in hydrogen on material degradation seems very valuable. There may be other likely impurities in hydrogen fuel that need to be studied.
- The project's future work directly addresses the challenges identified in each task and is aligned with answering the fundamental questions. It is worthwhile to note that at least two objectives of the project—the identification of a ferritic microstructure with sufficient hydrogen fracture resistance and the quantification of crack nucleation—may not be fully achievable within the scope of the project. However, these are important challenges that should be addressed, even if the ultimate research outcome is unsuccessful or incremental.
- The project team has a good plan; this project is just starting.

Project strengths:

- The project has an excellent technical plan addressing fundamental hydrogen material capability challenges. There is solid engagement in areas and materials systems that are relevant to engineering applications, excellent breadth in the different materials systems and issues, and multiscale modeling and an experimental setup that engages in many disciplines. The project takes advantage of unique experimental capabilities at SNL.
- The project approach is very strong and does a good job of focusing on different length scales and utilizing computational modeling in an impactful way. It also appears that the consortium is doing a good job of leveraging the strengths of various members and collaborating on tasks.
- This is a well-organized project with clear focus on issues critical to safety, reliability, and cost of hydrogen production, transport, and dispensation.

Project weaknesses:

- The project's collaborations are somewhat limited. It is likely that this limitation is a function of the new project and that collaboration is anticipated to grow. While each of the project tasks have finite and achievable goals, in aggregate, there is a good deal of proposed work. The total effort is ambitious.
- The project should have input from more industry collaborators to validate that the materials and impacts being researched are the most important to the industry.
- The broad nature of the tasks encompassed in the project make it somewhat difficult to quantify the impact of the overall effort.

Recommendations for additions/deletions to project scope:

- Specifics plans should be clarified for how the information and results will be disseminated and made available to industry working on component or system design and development. It is unclear whether the project team expects that the work will lead to any specific test protocol recommendations, similar to the polymers project.
- There are no recommendations, but this may change as results begin to be generated.

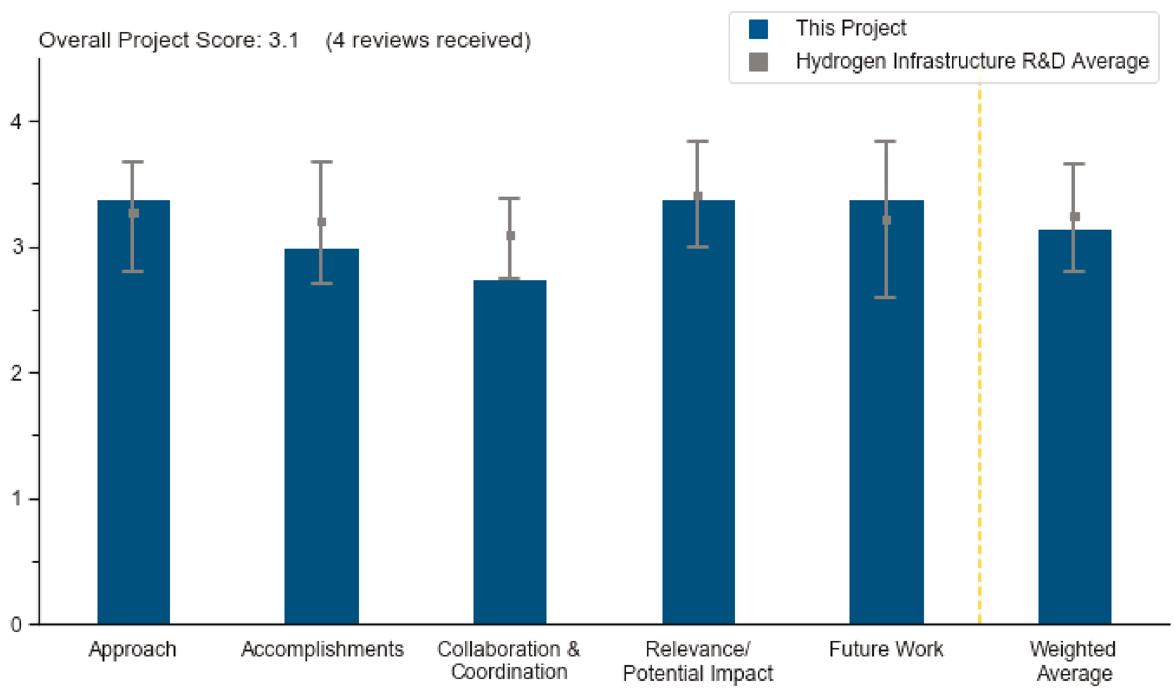
Project #IN-004: Magnetocaloric Hydrogen Liquefaction

Jamie Holladay, Pacific Northwest National Laboratory

Brief Summary of Project

The Pacific Northwest National Laboratory (PNNL) magnetocaloric hydrogen liquefaction system is expected to be considerably more energy-efficient than the Claude cycle. At 30 tons per day, the latter shows 40% efficiency, while the former is projected to be 70%–80% efficient. In this project, investigators will demonstrate the PNNL system liquefying ~25 kg/day. At industrial scales, the concept is expected to have a figure of merit (FOM) >0.5 (as compared to the Claude cycle system's FOM of <0.3). The project will also identify a pathway to a larger-scale system with an installed capital cost of less than $70 million.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has a methodical approach to developing individual aspects of the technology. The project team identified a weakness in the design and applied new innovations to overcome it (i.e., length of magnetic field). The material characterization work by Ames Laboratory is very impressive progress for this application and possibly others.
- The project's approach—to liquefy hydrogen by way of magnetocaloric refrigeration—is very sound. Utilizing the bypass approach is a great way to gain efficiencies by reducing the approach temperature in gaseous hydrogen.
- The project's approaches to increasing the FOM, reducing system cost, and meeting the U.S. Department of Energy's targets are correct. The only suggestions for improvement would be to try to use the system equations on slide 29 to see what other knowledge can be gained from a sensitivity analysis. Much effort

went into the theory and background discussion to justify needing to change the designs to increase the aspect ratio for length to distance (L/D) for an FOM equal to 0.65.

- The presentation focused more on the technology's "potential" than actual progress to prove that potential. This is a concern. The project update presentation jumped around, ran out of time, and did not necessarily focus on the challenges going forward. Two key aspects are recommended for the approach:
    - The project needs to narrow its focus on proving that liquid hydrogen (LH2) temperatures can actually be realized with this technology, and at the efficiency stated—in other words, whether the technology will actually function, and function at the power levels stated.
    - There may be gaps as to the expectations of both power efficiency and capital effectiveness. Both should be critically reviewed this year to have a balanced assessment when compared to reality of actual operation and competing technology. Ultimately, the project must determine the "spigot" cost for LH2 with the capital and operating costs, as well as whether it offers a meaningful reduction in overall cost. This is not stated in direct terms.

  It is encouraging to see that the stated approach is to focus on the lower-temperature regime based on last year's comments, but there does not seem to be actual progress to date, even at the warmer temperatures. Next year's report will be critical to understand if progress is being made on this approach. There are significant deviations from "theory" to "reality," and it is unclear that this project understands.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The principal investigator has mapped out a clear path demonstrating how his project is aligned with DOE's goal and how it is working toward meeting those objectives. Increasing the FOM from approximately 0.3 to >0.6 was clearly stated and communicated during his presentation. Progress was clearly demonstrated via the use of a "bypass" approach in the two-stage design, and the performance models were validated.
- The project has been able to make significant improvements to stage one of the process by reducing the layer count from eight to five. The presenter mentioned that stage one and stage two will continue developing as separate projects moving forward. It is unclear how the project will capitalize upon the accomplishments of stage one.
- Empirical testing is driving to the liquefaction goal. Understanding material characteristics is revealing the nuances of the magnetic technology. Recognizing the need to target and deliver the 20 K goal is prudent.
- Progress has been slow on actual demonstration of the technology. Even the higher-temperature work encountered issues preventing testing from being completed. There are significant hurdles to the technology, as well as commercializing into an actual industrial project. To a certain extent, the challenges that delayed progress this past year are indicative of the types of issues that will be encountered on a much larger scale as the project continues. There seems to be a "don't know what we don't know" aspect to the work when it comes to actual experience with LH2.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- The project has shown good progress with materials work from Ames Laboratory. Collaboration with Washington State to introduce supporting technology is important. Developing a relationship with an organization that can support commercialization efforts, particularly economics, would be a good step in 2019.
- The collaboration with PNNL and Ames Laboratory appears to be really strong. The project does list collaboration with the Hydrogen Delivery Technical Team (HDTT), which includes three energy companies, but it is not clear how or what value HDTT has brought to the project.
- While valuable partners are involved, there are no partners that can provide valuable feedback and input on the actual installation or operation of a LH2 plant. This collaboration is critical to getting the initial system

to work, getting it to scale up to an industrial level, and understanding some of the basic limitations of operating hardware, particularly cryogenic systems. Most important, it is unclear whether it would actually reduce the "all-in produced cost" of LH2 to an extent that warrants the technical risk.
    - There should be a review of competing technologies for capital and electrical efficiency. For example, the work published by Integrated Design for Efficient Advanced Liquefaction of Hydrogen (IDEALHY, a European Union program to develop hydrogen liquefaction capacity in and for Europe) in terms of efficiencies of existing facilities and other cycles (e.g., mixed refrigerants) can also substantially improve existing technologies.
    - The assumptions within the presentation could benefit from critical input from the existing operators of LH2 plants.
- It seems like it has been the same partners for several years working on this effort. The opportunity exists to reach out to others and see what additional partners could contribute to this very important effort.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Applying this technology, particularly for stranded hydrogen streams, has very high potential, assuming reasonable packaging. Large-scale applications might be attractive if the economics are more competitive than traditional liquefiers. International markets where demand is in isolated pockets may be a perfect fit for the technology.
- Alternative forms of hydrogen liquefaction are very relevant when considering the future hydrogen supply requirements for the fuel cell electric vehicle market. Such systems will be key for filling the hydrogen supply gap in areas where distribution is less reliable.
- The principal investigator has mapped out a clear path demonstrating how his project is aligned with DOE's goal and how he is working toward meeting the associated objectives and impacts.
- To the extent that hydrogen liquefaction can be improved from a capital and operating efficiency perspective, these new technologies offer a path to lower-cost production and distribution of hydrogen, which is critical to the success of the market. The challenge is whether this work truly will have a meaningful impact on overall cost. The material has not shown that. Stating unproven reductions in power from 10 kWh/kg to 5 kWh/kg (where 5–6 kWh is the theoretical limit based on exergy) does not provide the potential reduction in overall cost of produced LH2. It is unclear what percentage of overall cost that represents. Similarly, the capital cost numbers as presented are questionable.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The principal investigator has done an excellent job in documenting his past effort, and future work for this effort is based upon sound engineering and scientific approaches.
- It is great to see the focus on 20 K temperature. Credible economics are an important achievement before the next DOE Hydrogen and Fuel Cells Program Annual Merit Review. Proof of design and material changes recognized in 2018 are necessary.
- Future work for this project will focus on the design, build, and demonstration of stage two. The demonstration results from stage one will likely increase stage two development efficiencies. It would be good for the project to clarify the plans to align the stage one and stage two development activities.
- To the extent that the project is focusing on lower-temperature performance and testing, that is good. The project should, in parallel, better quantify the "produced" cost of LH2 to show overall potential of the technology based on what is known today.

Project strengths:

- The overall project strength is high. This technology challenges conventional, inefficient design. The technology may have multiple spinoff applications. Proof of 20 K is vital.
- The project has a strong accomplished principal investigator who is willing to push the FOM for hydrogen liquefaction by pursuing innovative system approaches: two-stage system and advanced technologies such as bypass, layered, and aspect ratios (L/D).
- The project's strengths lie in its ability to deliver a technologically advanced product that has the potential to support multiple markets.
- This is a substantially different technology to liquefy gases to cryogenic temperatures. This is a strength in that, if successful, this technology offers breakthrough potential.

Project weaknesses:

- No major weaknesses were identified, but the project could be strengthened by having more system modeling and a sensitivity analysis of the whole system and its major subsystems that could be optimized or further insights into the overall system performance that could increase the FOM, similar to the knowledge gained from the aspect ratio learning.
- There has been limited progress to demonstrate that the core technology can actually produce the desired temperatures needed to liquefy hydrogen. This will be a critical milestone. The next milestone would be whether the technology can be built to operate at an efficiency to justify its investment. The next milestone would be whether it can be built on an industrial scale, cost-effectively. None of these has been demonstrated yet.
    - There is a lack of actual operating and industrial experience that established companies can provide.
    - Counter to its stated intent, the project presented a cost estimate that does not show a decrease in capital cost. The estimate excludes critical cost elements that are usually included in other published costs. On an apples-to-apples basis, the equipment costs do not compare favorably to existing hardware. The cost estimate is missing costs for land, site infrastructure development, utility feed, hydrogen production, hydrogen pre-purification, equipment installation, truck loading facilities, and adequate product storage. Some portions such as "piping and valves" and "process controls" are substantially less than would be required to integrate a 30-tonne-per-day facility to modern, safe, industrial practice.
- The project's weakness rests in the complexity of the design and the product's reliance on the rare earth materials.
- The economic analysis seems weak and hard to defend. This needs more work by a credible partner.

Recommendations for additions/deletions to project scope:

- The expectations of both power efficiency and capital effectiveness should be critically reviewed this year to have a balanced assessment when compared to reality of actual operation and competing new/improved technology. Ultimately, the project must determine the "spigot" cost for LH2 with the capital and operating costs and whether it offers a meaningful reduction in overall cost. This spigot cost is not stated in direct terms. If a benchmark analysis has not been done with competing new technology as published by other work, such as IDEALHY, then that should be done in parallel with the above technology validation to understand the potential benefit.
- The project should focus on demonstrating that the core technology can work to 20 K temperatures and can approach the desired efficiency. This is a key "stage gate" to pass prior to proceeding further and should be accomplished as soon as possible, especially after four years of work so far.
- The project should maintain the course.
- No additions or deletions to the project scope are recommended.

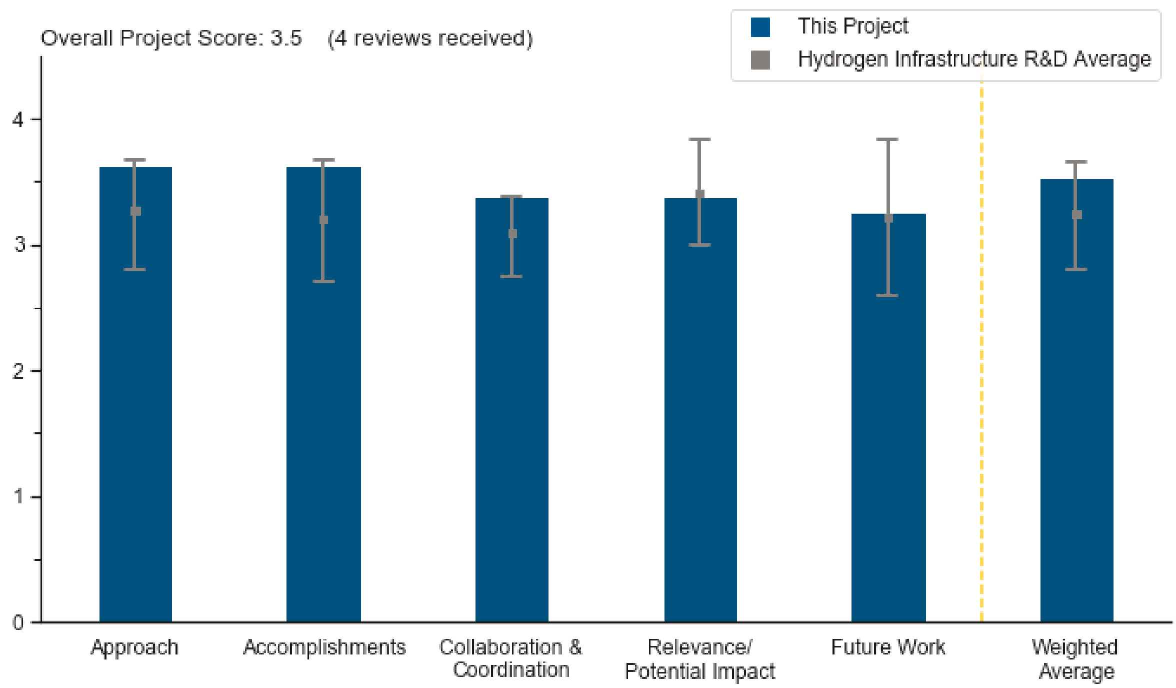
Project #IN-005: Electrochemical Compression

Monjid Hamdan, Giner ELX, Inc.

Brief Summary of Project

This project will develop and demonstrate an electrochemical hydrogen compressor (EHC) that is lower in cost, higher in efficiency, and more durable. Specifically, the project will (1) fabricate hydrocarbon membranes with enhanced properties for use in EHCs, (2) improve EHC water and thermal management, (3) optimize stack hardware and demonstrate cell performance, and (4) build a prototype system. Development of reliable and low-cost, high-pressure hydrogen systems is needed to enable market penetration of fuel cell electric vehicles.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The proposed approach is based on the use of electric potential in polymer electrolyte membrane (PEM) stacks, instead of mechanical compression to compress hydrogen to the pressure necessary to fill up fuel cell vehicle tanks. This technology potentially has higher reliability, lower maintenance, and smaller energy consumption compared to the incumbent technology. Two major differentiations of this project are using solid supported membrane that allows for much higher pressure difference and replacing Nafion-type perfluorosulfonic acid (PFSA) with an aromatic-based PEM that delivers lower cell voltage.
- The work is outstanding. It is very clear that the researcher has approached this work systematically. The project team first achieved 200 bar (compression ratio 10), then 360 bar, and then 875 bar, with a stepwise increase in performance. The team has solved core issues, demonstrated a working system, and increased the technology readiness level (TRL) sequentially, achieving project objectives.
- The team has scaled up the membrane size 6x, which is a good step toward overall scale-up of the EHC technology. The team has also developed a new membrane and a better membrane support (solid supported

membrane) that has demonstrated sealing up to 20,000 psi. Thus, the effort is well directed toward addressing the technical barriers and meeting U.S. Department of Energy targets.
- The project team had a clear presentation, a well-presented approach, and nice modeling work to quantify the performance gaps and tie them into the approach. The project has a good approach for overcoming challenges across various tasks and project elements.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- All of the project's major technical and design milestones have been met, and the project progresses well toward DOE goals. The project team demonstrated a scale-up to 300 cm^2 membrane electrode assemblies (MEAs), which gives confidence to the team's successful project outcome.
- The project team has made excellent progress with the development of a new support structure for the membrane, as well as a new chemistry for the membrane. These achievements have helped the team demonstrate both an increase in system efficiency and the EHC system operating at 875 bar.
- The project's approach and progress are sound. The 875 bar target was met. As the researcher indicated in his presentation, additional work clearly needs to be done to scale up the final system (which hit 875 bar) to a larger size and to lower operating voltage for the compression ratio indicated.
- It seems like milestones are being met and impressive performance is being demonstrated. The status of the project was well articulated for years 1 and 2.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- Although the collaborators and their roles have been listed, the overall presentation gave the impression that the work was mainly done by Giner ELX, Inc. (Giner). Perhaps this is an indication of a very tightly integrated team, but it may be useful also to elaborate upon the team members' respective roles in individual aspects of the work and how often the team met, interacted, held discussions, and teleconferenced.
- Giner worked well with outside partners such as Rensselaer Polytechnic Institute. The project's achievements included substantial coordination and involvement from other partners, which demonstrates excellent teamwork.
- From presented data, close cooperation between partners and interaction with collaborators are clearly seen.
- There is good integration among the team members.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project is making good progress toward the technical targets, but its operation seems to have been demonstrated mainly under steady-state operation and not start/stop or intermittent operation, which may create a different set of issues (e.g., thermal expansion and contraction, potential leaks). It would be useful to verify the suitability of the design—for example, with the 50 cm^2 system at 875 bar under intermittent operation—and fix any bugs; this will demonstrate the robustness of the project's EHC system under real-life operating conditions.
- Hydrogen compression is a critical issue that is very necessary in the development of the hydrogen energy infrastructure. Current mechanical compressors are unreliable and expensive. The potential benefits of electrochemical compressors make investment in this technology pathway compelling.
- The proposed electrochemical hydrogen compression could replace unreliable and expensive incumbent mechanical compression and reduce energy consumption. Though this is not critical in constructing

hydrogen fueling stations, this technology could substantially assist in the deployment of hydrogen infrastructure.

- There is a clear opportunity for electrochemical compression, and it is impressive how high the achieved pressures are. Cost may remain a challenge, but this work should be continued to see how far electrochemical compression can be pushed.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- Addressing how the system performs with "impure" hydrogen and under start/stop operation would be key to ensuring that the EHC can be a viable alternative to existing hydrogen compression technologies. If, for example, membrane robustness or sealing cannot be maintained, then the effort and labor to replace these, and the resulting downtime, may end up as the same issues that are listed as drawbacks for existing mechanical compressor technology.
- A substantial part of the project's future work is dedicated to stack optimization for 350 bar operation, while 875 bar operation was already demonstrated and is the final project goal. It seems logical to carry out the majority of optimization work for 875 bar. The durability of the stack pressurized operation, especially with the aromatic PEM, is not planned, though it could be one of the major selling points (or the showstopper) of the proposed technology.
- As the researcher indicated, the system needs to be scaled up. All "issues" related to scale-up need to be addressed. Larger active area, higher flow rates, cost reduction, etc. are all crucial to getting this system commercialized. The project needs to migrate to a higher TRL before commercial adoption.
- The project's next steps are clearly described and appropriate, given the current stage of development.

Project strengths:

- The EHC technology offers an attractive alternative to mechanical compression, owing to the lack of moving parts and therefore the promise of lower maintenance and possibly lower capital costs for station installations. The team has made good progress in scaling the system size and operating at high pressures. The team is solving the challenges associated with membrane development and sealing at high pressures.
- This is an important technology pathway and an excellent effort to lift the TRL of this technology. The work that was done in this project is excellent and has raised the bar for the technology. Units were built, tested, and validated, and good data was generated. This is a meaningful contribution to the advancement of this technology.
- The project has a good combination of component and stack/system technical work and technoeconomic analysis. The hydrogen compression data is compared with model work. The pace of the scale-up work is good.
- The project had a very nice presentation and slides, clear technical progress, and a clear plan for the next steps to advance this potentially promising approach to compression.

Project weaknesses:

- The system needs to be demonstrated under real-life conditions, even if at a low hydrogen flux rate of 0.5 kg/hr. With the design's current state of development, the team should be able to project how EHC costs may compare against those of competing technologies. With the estimated system endplate of 12-inch thickness (i.e., 1 ft.) for a 1000 cm^2 active area, a weight of several hundreds of pounds per plate with the additional weight of bolts, etc., is implied. Therefore, the system weight is likely going to be significantly high, which may complicate any potential field repairs. Thus, if the system is "down" because of issues with membrane or sealing that needs to be replaced, the time to bring it back up (unbolting, removing endplates, etc.) may require more than one person and thus increase maintenance costs.
- The durability of the EHC development is not addressed properly at either component or stack level. The reproducibility of large-size PEM and cells should be presented. The technoeconomic analysis lacks sensitivity analysis and comparison with the incumbent (mechanical compression) and emerging

(pressurized electrolysis) technologies on the basis of capital and maintenance costs, footprint, and safety. It is desirable to consider the effect of stack weight (i.e., endplates) on the capital and maintenance costs.
- Additional work needs to be done to increase the size and scope of the system. It needs further advancement before it can be commercialized.

Recommendations for additions/deletions to project scope:

- Rather than focus on embrittlement of the components, a focus on the effect of impurities on membrane operation may be more impactful and relevant to operation in the field.
- Ultimately, this technology will have value only if it is integrated into a commercial arena. The project needs to be supported with that goal in mind.
- A study of durability should be added to the work plan.

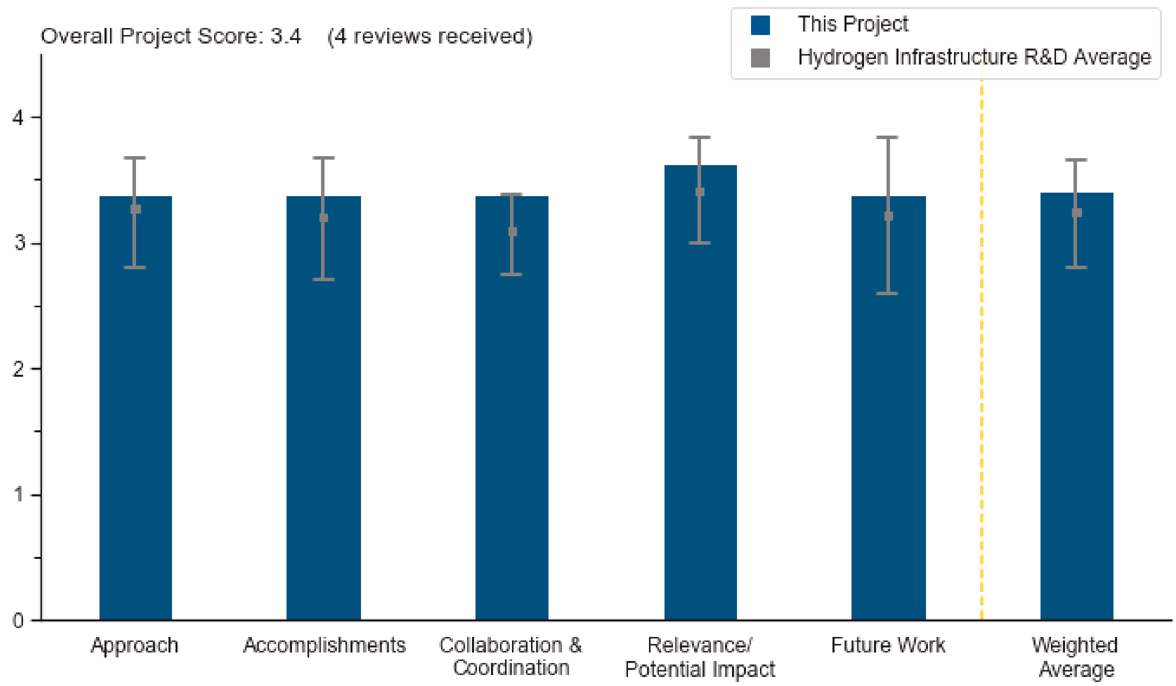
Project #IN-007: Metal Hydride Compression

Terry Johnson, Sandia National Laboratories

Brief Summary of Project

The project seeks to overcome barriers to improve the reliability and costs of gaseous hydrogen compression. The hydrogen compressors available dominate station costs (48%) and downtime (24%); metal hydride compression has the potential to improve the reliability of 700 bar refueling. The project's main objective is to develop and demonstrate a two-stage metal hydride compressor (moving from technology readiness level [TRL] 2 to TRL 5) with a feed pressure of 150 bar that delivers high-purity hydrogen gas at an outlet pressure of >875 bar. Each stage consists of 2–3 hydride beds with materials optimized for that stage. The experiments will be designed to demonstrate a scalable system with a pathway to meet U.S. Department of Energy (DOE) targets. The project will collaborate with synergistic project Hybrid Electrochemical–Metal Hydride Compression (PD-137) because both include a high-pressure metal hydride stage.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Note: This is a new project in 2019. Reviewers were given the option not to evaluate Accomplishments. In such instances, the other criteria were re-weighted to total 100% (see the Introduction section for details).

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project team's approach is excellent in terms of compressor bed design; alloy material selection, characterization, and testing; and prototype demonstration. The principal investigator's (PI's) leveraging of the expertise of Greenway Energy (GWE), in terms of hydride materials selection and costing, is a very good idea. It ensures that the project progresses in a timely way and meets its intended goals.
- The work is good. State-of-the-art metal hydride systems cycle at a faster rate and hold smaller total volumes of metal hydride materials that are crucial for meeting industry cost targets. Most of the work done

was based on materials from literature review, rather than fundamental understanding of the materials and developing more advanced alloys that can more optimally meet targets. There is scope for this project to do much more, and there are exciting opportunities for the researchers to consider more advanced approaches.

- The project closely integrates system modeling, testing, prototyping, and cost estimation in a way that promises to make tangible progress toward DOE metrics. The barriers and objectives are clearly identified.
- The project's approach to developing a metal hydride compressor is sound and logical. It appears that it solves one problem but introduces other problems. Analysis is needed on how much maintenance the metal hydride compressor needs and on what the cost and frequency are versus conventional technology. The project team needs to investigate what level of conventional compressor improvements would be necessary to meet the hydride compressor, as well as whether that is feasible. Comparison also needs to be done over 10 years of full system operation, including energy inputs. The team needs to know if this would lower the required conventional compressor improvement required to hit break-even. Waste-heat scavenging is a good option, but it limits application of the technology.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The PI is on track to meet the project milestones, despite the challenges usually associated with managing multiple teams with varying tasks and timelines that are interdependent. The project has managed to complete milestone 7.1 in a timely way. This is very encouraging, considering that the intelligent selection of hydride alloys for use with the compressor is one of the most critical steps for the success of the prototype demonstration. The project has developed a method at Ames Laboratory (Ames) and Hawaii Hydrogen Carriers (HHC) to produce about 4 kg of AB2 alloy for use on the compressor beds. This reproducible method of making the activated AB2 alloy will likely ensure easy scaling of the process at commercial scale. One can envision contracted commercial vendors using this method to make high-quality alloys for hydride compressors. Consequently, there will be fewer issues with variability in the quality of alloys bought from the selected commercial vendors.
- The team has done great work on solving the technical issues of getting a metal hydride compressor to work. This is excellent analysis and predictive work.
- The project has made excellent progress on components and prototype design. Delays from suppliers have led to late completion of milestones, but the project should not be held accountable for these delays. Still, it is a bit concerning that there is no target delivery date for the high-pressure vessels.
- To the extent the project has met its work plan, it has accomplished the tasks as provided. Therefore, it is on track with the goals it has set out. For DOE goals to be met, however, the project course needs to be adjusted to bring it to par with state-of-the-art systems.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- There appears to be effective collaboration between the three groups (Sandia National Laboratories [SNL], HHC and Oak Ridge National Laboratory [ORNL]), as well as with Ames and GWE's project (PD-137). The project team is made up of companies that are world experts in the fields of hydride technology and prototype design and fabrication. These companies have previously performed related projects, potentially making it easier to conduct project communication, time management, cost estimation, and materials sourcing. All the project partners are fulfilling their objectives; for instance, SNL is on track to accomplishing the design and fabrication of compressor system components, and HHC and ORNL are completing the sourcing, ball milling, and characterization of the hydrogen storage properties of the alloys for use on the laboratory prototype.
- The collaboration within the team is very strong, and the project's close interactions with GWE appear to have been helpful, particularly for selecting high-pressure candidates. However, the team could benefit from stronger interactions with other DOE and university efforts on the materials side. The team has

excellent expertise in metal hydrides, and discovery of a better high-pressure candidate is outside of the project's specific scope. This is not in dispute, but there could be opportunities for broadening the selection efforts beyond literature reviews by partnering with other institutions.
- It appears the work is well coordinated within this area of expertise. Stepping up to a higher level through targeted use cases would be beneficial to bolstering those cases and providing justification for the energy inputs required.
- There is clear evidence that the researcher has worked well with outside partners.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project will enable reliable and cost-competitive hydrogen refueling at 700 bar, if successful. High-pressure mechanical compressors are available; however, they require huge capital investments and maintenance costs. Therefore, metal hydride compression could provide an economical, reliable alternative with longer life expectancy. Through this project, new metal hydride alloys for the high-pressure stage could be identified and tested under practical conditions, paving the way for the future discovery of alloys for two-stage 700 bar compression.
- Hydrogen compression is a critical issue within hydrogen energy infrastructure. Current mechanical compressors are unreliable and expensive. Alternate approaches are a must. Metal hydride systems offer an excellent pathway for hydrogen compression and should be explored as part of the overall technology portfolio.
- The project is very innovative and important for the Hydrogen and Fuel Cells Program. It has the potential to revolutionize the current compression technology, which remains one of the biggest cost drivers in hydrogen.
- The technical relevance helps solve issues related to conventional compressor durability and maintenance; however, it is difficult to see the relevance outside certain applications with excess heat available. General mechanics can service conventional compressors, but it is not clear how a hydride compressor is serviced (on the rare occasion it needs service).

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The project places high emphasis on prototype integration and testing of the complete compressor, which are logical next steps. Since performance and cost are ultimately related to the choice of materials, it is unlikely that high-efficiency targets will be achieved. However, demonstration of the compressor should still be considered a significant advance, and the plan for future work is well positioned for this.
- The proposed future work is a logical development from the previous year's work. Future work is aligned with the project's objective of demonstrating metal hydride compression at 700 bar to increase the TRL of this technology from TRL 2 to TRL 5.
- To the extent that the project has been mapped out, the researchers' proposed future work is consistent with the proposal. However, it is suggested that the researcher review other work in this field and channel his future work toward meeting state-of-the-art standards in this field.
- All future work is logical and relevant to demonstrating this technology.

Project strengths:

- The project is made up of teams who are experts in the field and who have performed similar types of projects. The project has managed to make significant progress in design and fabrication of components for the hydride compressor and in the selection, characterization, and testing of the hydride materials. The team has managed to make their own alloy combination for the laboratory-scale prototype, which is a significant step, given that the development of alloys was not a core activity of the project. The project has also managed to stay on track, even though it has been challenged by material quality issues from commercial vendors prior to deciding to make the material in-house. There are no issues envisioned with the team's completing the remaining milestones. However, to achieve milestone 10.0 and be on track to meet DOE 2020 targets, the team should devote more time to prototype assembly, integration, and testing, as it usually involves dealing with unknown unknowns and requires numerous iterations to perfect the system.

- This is a very strong and innovative project with excellent expertise, a clear work plan, and potentially high technological reward. The team deserves credit for its focus on prototyping and demonstration, as well as its consideration of cost projections in the system analysis. The combination of system modeling, design, and technoeconomic analysis is an asset.
- The project team has done excellent technical work in identifying materials and characterizing performance. There are great models of performance.
- The researcher has good fundamental knowledge of this field. The work has been competently done, and the engineering effort is solid.

Project weaknesses:

- An inherent challenge of the project is its lack of focus on the development of a high-pressure stage material (250 to 875 bar). Materials development is outside the scope of the project, and the project is focused on the selection of literature-based materials, which in most instances would be extrapolations for the high-pressure stage; therefore, it is hard to fault the project when the literature materials do not practically behave as predicted. Ideally, separate and complementary efforts should be made to develop high-pressure hydride alloy materials that can be tested under practical conditions in this project. To ensure the project does not end because of lack of funds, better predictions or projections of the costs of materials and components are needed, as well as sensitivity analyses to mitigate cost overruns, especially when planning for future phases. The practical scalability and reproducibility of the Ames alloy synthesis method at large scale needs to be determined.
- Ultimately, the compressor technology's viability depends on the availability of a suitable high-pressure hydride material (which was also identified as a key challenge by the project team). Although the project rightfully focuses on technology demonstration rather than materials development, tighter connections could be made with external DOE and university projects (including international efforts) that are focused on materials discovery and optimization. The team should consider expanding their collaboration network to include researchers who could provide these materials solutions within the compressor design.
- For this technology to be economical, the researcher needs to improve thermal transfer rates, reduce material use, and improve cycling time. This is crucial to the success of the project.
- The project needs a fundamental justification or plan for reducing the energy inputs.

Recommendations for additions/deletions to project scope:

- There needs to be a comparison of metal hydride compressors to electrochemical compressors; a detailed analysis of the full system operational costs, including energy; and a break-even analysis on the required conventional compressor improvements needed to meet metal hydride operational cost.
- This project needs more aggressive targets to bring the work to industry state of the art.
- The project scope is good and attainable.

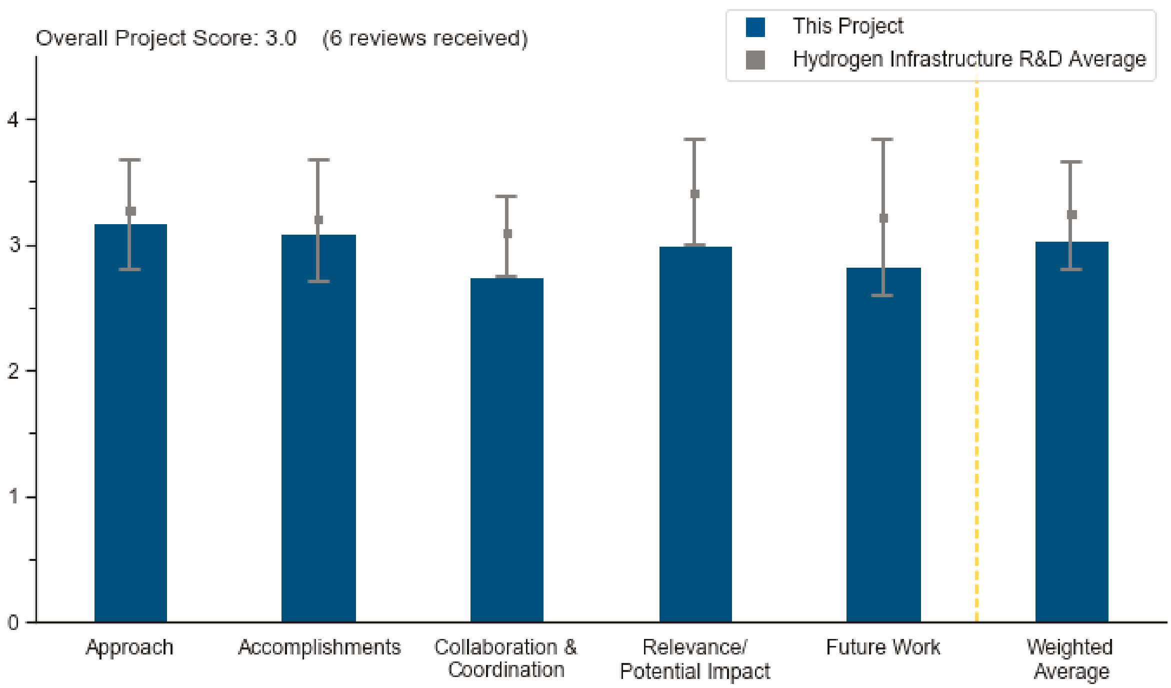
Project #IN-008: Dispenser Reliability

Michael Peters, National Renewable Energy Laboratory

Brief Summary of Project

Hydrogen fuel dispensers are a top cause of maintenance events and labor time at hydrogen fueling stations. This project seeks to identify the proper balance between dispenser costs—both capital and operations and maintenance (O&M) costs—and performance. The project consists of three major tasks: (1) a technoeconomic analysis of capital and O&M improvements to the chiller/heat exchanger, (2) reliability testing of dispenser components, and (3) development of an open-source and free hydrogen fueling model.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The work represents an important step in the development of hardware and methods for testing component failures under simulated operating conditions. This is an important research topic, and the data generated will be important.
- The approach of using a device with consistent and realistic conditions (i.e., in low temperature and at pressure) is a great way to evaluate dispenser components.
- The project's approach to testing dispenser reliability is sound. Utilizing multiple dispenser subassemblies (i.e., valve panels) is a very sharp approach that will optimize the time and cost for testing and data evaluation. Of the 40 test samples or subassemblies, it appears that some of the components used may not be true representations of the components used at current stations. It would be closer to ideal to test components that are representative of the current market.
- The approach to evaluating dispenser reliability is sound, and, per the presentation and supporting information, the principal investigator (PI) went to lengths to drill down into the root cause of failures and

the causes of shutdowns in the dispensers. One piece of the approach that may be lacking is whether the project is actually using valves, for example, that are being used in the field and are having issues. The presentation was not totally clear as to this point. The high-cycling test setup and leak detection method are very good.

- The use of a fill profile similar to the National Fuel Cell Technology Evaluation Center's fill and the use of a Kaplan–Meier analysis seem to be an appropriate approach. However, it is impossible to operate and analyze the systems in all permutations and combinations of temperature, humidity, etc. Therefore, the approach of testing a few dispensers with a limited range of variables seems to have limited value. The materials testing effort, pre- and post-hydrogen exposure, will produce valuable scientific output. Perhaps such materials work could be performed under the Hydrogen Materials Compatibility Consortium umbrella instead.
- The project appears to cover all the bases that can be covered based on the funding available.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has successfully simulated numerous test fills that are aligned with the SAE International J2601 fueling protocol. This is key for establishing a quality batch of data. Additional progress has been made in identifying that the equipment installation requirements were also significant contributors to the failure life of the components (i.e., valve stem torque). These are both great accomplishments. Understanding the results of Sandia National Laboratories' (SNL's) material analysis for the failed components is what is missing for this presentation. It is understood that SNL has a separate poster presentation for this effort. It would have been nice to include SNL's general conclusion of the findings in this presentation.
- The researchers have accomplished a good amount during this time and found key areas of failure. The way to address this is less apparent, as they do not have a good closed feedback loop with the valve manufacturers specifically to find out why things fail as they do (beyond their own hypothesis). Closing this loop would provide invaluable feedback to industry. The team does have a good close collaboration with the makers of nozzles and breakaways. It appears from the data that the bulk of the issues are with valves specifically; after 800 cycles, it appears there is a 100% chance of a failure of some sort. The statistical analysis of the predictive failures of the valves is reasonable and correlates with the project data. Further testing would provide this, but with valves from a different manufacturer, it is not clear that this would still be predictive. It should also be determined whether the data would be the same and whether the predictive calculation would give the same results if the valve stem torques were checked out of the box.
- Leaks and dispenser downtime are costly and affect customer experience and the safety and integrity of the station near the user. By simulating the fill profile, conditions, and indicative component failure, the components that need to be improved can be identified. This is a good step in the right direction. The project team should be able to evaluate the types of valves and determine which ones are more robust under operating conditions. The reseal effect should be used to understand what properties may be permanently changing as the components heat up to cause a reseal and when they return to operating low-temperature conditions.
- The project's progress and accomplishments are good overall. However, it is not clear what serves as the benchmark for each of these individual component failure rates; it may be equipment experience from compressed natural gas or industry operator expectations for a certain failure rate. This should be clarified. As far as the difference for actual torque compared to the torque manufacturing set point, it is not clear what the industry experience is for any other valves or valve stems with a torque manufacturing set point (for any fluid and/or pressurized gas). Observations and claims mostly indicate that those that integrate components into full systems (such as dispensers) should adopt a practice of always verifying the torque of newly received components. It is also unclear how much leakage is realistically acceptable.
- The quantity of data is low, mostly owing to the extended time that is required by the testing, rather than to any lack of effort on the team's part. Perhaps it would be possible to add additional test bays or to create duplicate test stands to increase the rate of data generation. This is probably outside of the project budget, but it is worth considering for future testing.

- The team detected and recorded leaks and failures, but the project has not shown the entire range of data, e.g., what components failed (other than the leaks due to the valve stem torque). It is not clear what value the present form of the leak and failure data that was presented will provide to the community, other than the fact that the team has quantified the number of leaks and failures of a limited set of systems and concluded that low temperature and high humidity are "bad." Materials analysis is a good start.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- Working with the valve manufacturer is a necessary and good step in the project. By providing the manufacturer with access to the test apparatus and data, the team is allowing for the validation of the testing methods and providing valuable feedback to the manufacturer on both the test standards and the field operation conditions; these may provide insights for future design and materials selections.
- The collaboration between SNL and the National Renewable Energy Laboratory (NREL) is well managed. The delegation of the hardware testing and the material analysis is a great way to ensure quality effort is being invested on each side. With the exception of Weh Technologies, Inc., and Walther–Präzision, additional collaboration with other component suppliers would have been ideal for comparing previous failure results. Overall, the collaboration is excellent.
- Although there seems to be good collaboration with certain manufacturers, there should be an opportunity to bring more component manufacturers into the mix as the industry grows. There may be an opportunity to bring third-party testing organizations into the project to help develop certification standards for critical components.
- It is good to have the main (current) stakeholders involved and engaged. However, including large valve and component manufacturers would help benchmark feedback for test observations; both current partners are boutique manufacturers compared to the market of conventional fuel component suppliers.
- Dispensers are made up of different parts: valves, instruments, nozzles, hoses, and breakaways. There is good collaboration for nozzles and breakaways. For the valves—which make up the bulk of maintenance needs and failures on this test setup—the project does not have a good feedback loop. Valves were chosen mainly for cost and, according to the PI, not necessarily because of their usage in the field. It is to be determined how the data will be made useful when it is non-attributable to industry. A good approach would be to work with willing participants (e.g., manufacturers) who want to improve their products and reliability in this specific market.
- Some coordination seems to exist between the two national laboratories in terms of failed components from testing that are being provided for materials analysis. Collaboration between the dispenser system provider and NREL did not seem to go beyond setting up their dispensing system for evaluation. It is not clear that the discussions with the system provider led to any meaningful progress in system design or material selection.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- System reliability is and will remain one of the key issues facing station operators. Customers expect stations to be operating 24–7–365, without exception. Data like those being generated here can help in designing and maintaining components and systems to meet these targets.
- This project satisfies the targets for relevance and potential impact very well. Station reliability is a key driver for market stability. The results and findings of this project will help improve station reliability and, ultimately, customer satisfaction within the market as a whole.
- The project shows the challenges the industry faces as car deployment ramps up and the stations become fully utilized. Many of these issues were not readily apparent in the demonstration period with low station utilization. Having testing devices that simulate high-volume throughput is a good way to put components to test as the market matures.

- The relevance would be much better if the poor reliability of the valves could be tied to feedback to the manufacturer to improve the manufacturer's product and, if that was then included in retesting, to see whether there was improvement. It is not certain that this is a good baseline of understanding (1) when the manufacturer may not be representative of what is in dispensers and (2) when the chosen manufacturer does not care about the results, as was more or less expressed. This may be more the fault of the valve makers than the PI.
- The relevance of the statistical population for dispenser failures is barely acceptable when compared to the typical minimum population requirement used for scientifically acceptable conclusions. Because of the impact of heavy-duty (HD) hydrogen fueling stations on hydrogen cost reduction, it would be good to extrapolate the lessons learned for HD H70 high-flow fueling.
- The potential impact is not very clear.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The project does a good job at identifying areas of concern for future work (e.g., the impact of humidity and ambient temperature changes). It is not clear that the project plans to address any of the identified concerns during future testing. The approach of conducting statistical analysis is a really great way to capitalize on the testing result and provide the industry with some tangible information that can be applied to existing stations.
- While the data for specific components will be an important deliverable from this project, a more impactful deliverable could be establishing a standard for the equipment and methodology used for component testing. The team should consider using this equipment and methodology to establish a testing standard, if they have not considered it already. The number of components needing testing will go well beyond what is covered in this study, and the methodology could become a service provided to component manufacturers, or it could provide a basis for a component certification process or design standard for the industry.
- It would be good for this project to continue and to integrate with the valve manufacturer to make either material or design changes themselves. A non-disclosure agreement with these companies would be invaluable. Feeding this information into the development of codes and standards for valves and fittings would also be supportive to providing a framework to allow the industry to follow some guidelines.
- The proposed future work should include hoses since these are a large cause of leaks and failures both at the fittings and at the hose itself. There could an opportunity to develop a test standard for hoses as well.
- This project should not spend time on a station operator's costs when a leak or failure occurs, as this is already part of project TA-014: Hydrogen Station Data Collection and Analysis. The project should stay focused on generating empirical and test data, not doing cost analysis and modeling. The team should consider including more details in the project report on specifics of where leaks occur and the potential observations of environmental factors' influence on leaks (even though this specifically would take much more time, possibly years).
- The proposed future work appears to be unfocused and very generic; it does not seem very impactful.

Project strengths:

- The strengths of the project include (1) that it recognizes how important it is to test components under operating conditions in hydrogen and (2) that it provides a consistent approach for testing and comparing alternative valve designs (e.g., plunger versus rotating) and the same component from different manufacturers.
- This is a very good and solid approach, with rigorous testing and modeling of predictive failures. The project has a great test setup; there is great potential if the team continues to provide valuable feedback to industry and standards developers.
- The project's strengths include the initial effort to generate data that can provide early indicators of failure rates for hydrogen dispenser components and information about where failures appear to occur first. This motivates the industry to put effort into designing and building robust dispensers with lower maintenance needs.

- The project's strength is the test bench. The test bench is closely representative of what hydrogen stations are experiencing every day, and therefore the resulting data has an extremely high factor of reliability.
- The project has generated valuable data by quantifying and statistically analyzing failures to provide real data for design improvements.
- The mathematical analysis of failures is a useful aspect of this project.

Project weaknesses:

- The number of cycles and data sets is relatively small. Also, the leak detection methodology may be overly sensitive in comparison with the way some leaks are actually discovered (i.e., a pressure leak test during fill). This could drive impractical solutions for small leaks that might be tolerable under normal operating conditions. Zero leakage from all valves and fittings would be preferred, but as long as the leaks are below lower explosive limits, zero leakage may or may not be practical.
- There is a lack of feedback channels with valve manufacturers. The actual use of these manufacturers in the broad hydrogen dispenser market seems uncertain. Better feedback from industry would be helpful to make sure that NREL is testing what is broadly used in the field. Going by the pictures, one of the manufacturers is not used by anyone.
- The project's weaknesses include the small number of project partners. It is easy to get distracted by topics other than generating failure testing results and data. Also, this project covers only light-duty dispensers; because of the low throughput, this effort may have a marginal impact on reducing the cost of fuel.
- The project's weakness is that not all of the components tested are truly representative of what is in stations today. The presenter mentioned that the project is using a "low-cost" valve instead of the more popular, more expensive option.
- The project is frustratingly slow in gathering sufficient data for a meaningful statistical analysis.
- The primary approach seems to be "try and see," which is not impactful.

Recommendations for additions/deletions to project scope:

- The project team should not include cost analysis efforts as part of this project; this is distracting and should be left up to the dispensers and station operators that are responsible for cost and economics. NREL labor hours should not be used for this. The team needs to assess when leaks are realistically unacceptable and redefine what is acceptable. The team should also provide dispenser integrators and operators with recommendations related to torque manufacturing set points for newly used dispenser components. The project team should also develop and/or research industry benchmarks for the failure rates of components, based on conventional failure rates.
- It is recommended that the project team create a feedback channel with codes and standards bodies based on data sets, and test other manufacturers in the set-up to correlate data among a broad set. There are currently at least six big players, with others trying to enter the valve market. These include Tescom Corporation (part of Emerson Process Management), Nova Swiss, GSR Ventiltechnik, Eugen Seitz AG, and Swagelok, none of whom are represented in this testing set.
- It would be nice for the project to test the unit under varying ambient temperature and differing dew points, something identified as a concern.
- The project should bring in hose manufacturers. The team should consider bringing in a third-party test organization in an effort to develop a certification standard for critical components to which manufacturers would need to conform.
- The project team should consider expanding the test apparatus to test more data and components.

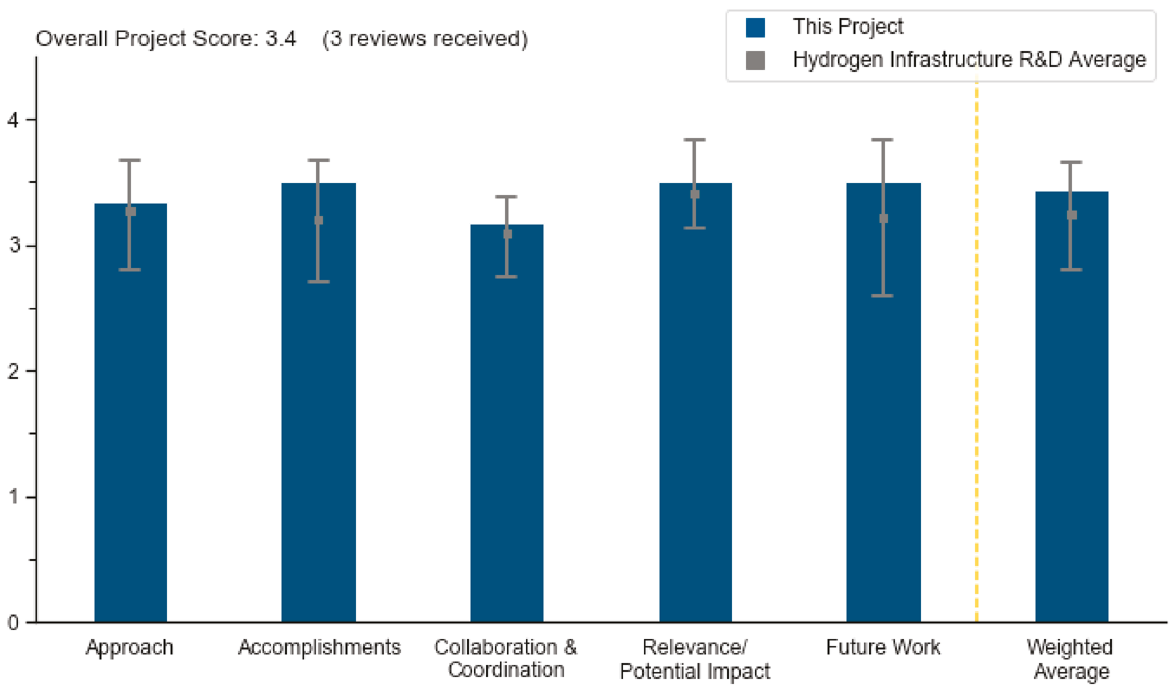
Project #IN-009: Advancing Hydrogen Dispenser Technology by Using Innovative Intelligent Networks

Darryl Pollica, Ivys Inc.

Brief Summary of Project

The primary objective of this project is to develop a robust and cost-effective system for dispensing and measuring hydrogen; the system is meant to further enable widespread commercialization of fuel cell electric vehicle (FCEV) technology. Key project activities include (1) development of robust sensor hardware and algorithms that improve accuracy based on empirical testing and enhanced meter temperature measurement; (2) development, testing, and demonstration of the use of dedicated short-range communications (DSRC) for use in vehicle refueling; and (3) simplification and cost reduction of flow control and hydrogen pre-cooling systems.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project's approach is excellent. The team has a clear plan to improve multiple systems within the dispenser. The systems they plan to improve consist of the Coriolis meter and the standard Infrared Data Association communication protocol.
- The approach to this work has been laid appropriately on foundations of safety, accuracy, and practicality. The effort has followed an appropriate plan to produce new results for applied technology in the hydrogen dispenser domain. Collaboration with industry and the National Renewable Energy Laboratory (NREL) has been beneficial. Field trials are being implemented.
- The project used an integrated approach, combining DSRC and an improved Coriolis meter, and built a dispenser system with a cooling system as well. The team used existing DSRC technology for this project

and claimed that it would be compatible with 5G standards in the future. The approach was to validate the work via a bench test prior to moving to field testing, which seems reasonable.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The accomplishments achieved so far are great. The project has completed the manufacturing of the dispenser assembly, which included the high-accuracy flow meter. Additionally, the project has integrated a high-accuracy servo flow control valve in place of the standard pressure control valve that is utilized in stations today.
- The applied use of the DSRC system and the improved design of the Coriolis flow meter and heat exchanger have comprised advancement in accurate and safe hydrogen-dispensing design. The potential positive market impacts can be identified based on increased accuracy and benefits in cost and design. The field trial, when completed, will help support the validity of the concept.
- The team has been able to achieve metering accuracy of 2% at bench scale and has made progress toward a lower-cost heat exchanger. The team has also completed installation of the system at NREL's Hydrogen Infrastructure Testing and Research Facility, and it remains to be seen if the metering accuracy can also be achieved during field testing or if the heat exchanger performs as well as simulations indicate.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The project's collaboration and coordination with other institutions are very sound. The combination of leading institutions with knowledge in both hydrogen station system design and hydrogen metering technology is very advantageous.
- There is clear demonstration of coordination between the solution developer, the key suppliers of the specialized technology, the user community, and the national laboratory community. Opportunities for direct collaboration with the automotive industry for the on-board communication solution are ongoing, and the additional expansion, which is necessary, will need to be accomplished outside of the project.
- The presentation lists the areas in which the team is collaborating with other partners. Details of such collaborative activities would have been useful, such as those pertaining to the design of the dispenser enclosure (and an explanation for why it is the largest-cost component of the prototype) and the integration of the Coriolis meter.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The scope of this project has great relevance and impact for the FCEV market. All accompaniments will bring great efficiencies and improvements in terms of both cost and reliability.
- The benefit of the improved accuracy of hydrogen dispensing, with reasonable cost, supports advances toward DOE Hydrogen and Fuel Cells Program goals and objectives.
- The project has made progress toward improving the meter accuracy, using a DSRC system for communication, and developing a lower-cost heat exchanger. It seems that the improved accuracy is based on empirical testing to some extent, so it is uncertain how the algorithms (based on empirical testing) hold up during field tests. The adoption of the DSRC system by automotive original equipment manufacturers (OEMs) is uncertain, although the team claims that it will be transferrable to 5G systems. The practical implementation of the brine-based heat exchanger is yet to be seen, but it appears to have lowered the cost somewhat.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- A significant portion of the proposed future work is related mainly to the validation of the dispenser. Although challenges are likely to arise, the project has shown that these challenges can be overcome.
- Completion of the field trial, which is being implemented in the coming weeks under an extension, is quite important. Future work beyond that trial is not contemplated, as the project is scheduled to end in June 2019.
- The proposed future work matches the team's work plan, although they appear to have lost the field demonstration site, which will directly affect their ability to complete their work scope.

Project strengths:

- The project has integrated collaborative industry and national laboratory partners to advance design concepts for more accurate and cost-effective dispensing technology. This demonstrates that safety, accuracy, and practical deployment have been prioritized. The use of several innovative approaches to metering, cooling, and communications using practically grounded principles can be impactful for the industry (pending the outcomes of the field trial proof of concept).
- The strength of this project is the approach to improve existing dispenser features with more innovative solutions that station developers can implement into their designs.
- The work seems focused on addressing specific challenges, and the project has addressed them (e.g., metering accuracy, communication, lower-cost heat exchanger).

Project weaknesses:

- The field trial is critical and has not yet been completed (although it is being implemented). The practical scale and impact of the project will depend, to a degree, on support from the automotive sector in taking up the communication solution. This highlights the need for continuing the expansion into the automotive sector and amplifying awareness of the benefits.
- The details of what is novel about this project's dispenser system are not clear. The details of "cost-optimized hydrogen safety system" are not given. The use of brine may, over time, lead to scaling (e.g., salt deposit) that could lower the system's heat-transfer efficiency. There is a big risk as to whether the DSRC technology will be accepted by automotive OEMs.
- A weakness for this project is in the reliance on the OEMs' acceptance of the proposed DSRC hardware. There is no clear plan or strategy that has been shown to ensure an acceptable level of confidence to overcome this issue.

Recommendations for additions/deletions to project scope:

- Unless it was already shown in prior years via bench-scale testing, the team may consider tests to demonstrate the purported advantage of the DSRC system, i.e., that only one roadside unit is needed to communicate with multiple nozzles.
- During testing of the DSRC technology, it is recommended that the project request early participation from the OEMs. Presenting only a findings report may not suffice for their full acceptance.
- Additions to the project scope are not applicable, as it is concluding in June 2019. No deletions are needed.

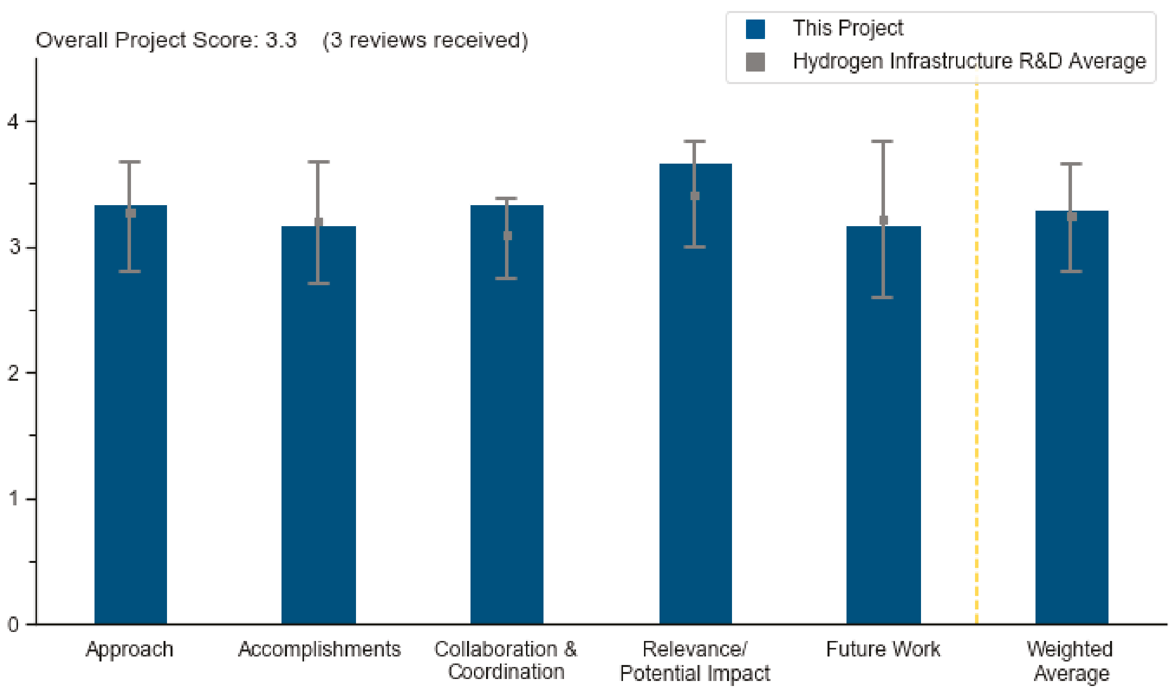
Project #IN-010: Cryogenically Flexible, Low-Permeability Hydrogen Delivery Hose

Jennifer Lalli, NanoSonic

Brief Summary of Project

This project aims to develop a hydrogen hose for fuel cell electric vehicles (FCEVs) that is (1) engineered to be flexible and enable hydrogen delivery at less than $2/gge, (2) durable in conditions of roughly -50°C and 875 bar for H70 (70 MPa) service, and (3) reliable and safe for conducting approximately 70 fills per day for more than two years. NanoSonic, Inc. (NanoSonic) is partnering with two national laboratories, a standards development organization, a local government, and industry to implement and test a cost-effective, metal-free, high-pressure hydrogen hose design that meets the above criteria, resists hydrogen embrittlement and contaminant leaching, and endures mechanical fatigue.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project is following a good, logical process to improve the design of the fitting/hose system.
- The project has a sound approach to the work, including well-developed ideas for overcoming obstacles.
- The approach seems fine, although the approach to finding an acceptable fitting to swage on the end seems problematic. NanoSonic states they do not design fittings, so they work with machine shops to come up with some to connect to the end. This is a large reason that a high mark cannot be given, as without this there is no dispenser hose.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Everyone would like to see the fitting–tube interface problem solved, and in spite of the ongoing difficulties, there is confidence that the team is on a good path. Results are never guaranteed in research and development projects, but the knowledge that is being developed by the team and the potential for a step-change improvement in cost or performance calls for continued support and potentially even extension of the project.
- The accomplishments in the materials science of the hose are good and well done. One of the keys to ensuring proper applicability is to have the hose tested on hydrogen gas. Until now, all testing has been done on hydraulic fluid and nitrogen, which are not indicative of how well it will react with hydrogen.
- Some obstacles were identified, including significant fitting failures that could hamper the work. However, alternate solutions were provided.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project is well connected to collaborators who will ensure project success, including the National Renewable Energy Laboratory (NREL) and CSA Group (CSA). CSA could also potentially support future certification efforts for NanoSonic.
- NanoSonic has a great array of collaborators on this project who will be able to provide integral feedback to project outcomes. Beyond Cardinal Rubber & Seal, Inc., though, it is not totally clear who is doing exactly what.
- Given the ongoing challenges with the tube–fitting interface, it would be good to get a fitting manufacturer on the project, as the design, materials, and function of the metal fittings are not in the project team's expertise.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The development of alternative choices for high-pressure fueling hoses for FCEVs is critical to the success of the FCEV industry. Current products are not suitable for the mass market, and this technology is necessary to get us there.
- The development of a low-cost and long-life hose would work to address one of the biggest failure modes of current station operation. If the design and cost targets of the project can be met, this would be significant.
- Hose lifetime and cost are critical areas for dispenser reliability and cost; through this work, it appears the project can produce a hose at a very attractive cost point. Testing with hydrogen will be critical.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The future work at Pacific Northwest National Laboratory and NREL is appropriate. Hydrogen testing is the critical path, but solving the fitting slippage will of course come first.
- There are good next steps planned in getting the laboratories involved in analysis of the failure modes.
- One minor weakness of future planning is the lack of direction related to actual tests using hydrogen gas. Much of the development efforts are using hydraulic fluid, and it is important that leakage, permeation, and gas-cycle testing be performed with hydrogen gas.

Project strengths:

- The project's overall strengths include the development of a critical piece of the fueling puzzle, which is currently a barrier to the commercial success of hydrogen as a vehicle fuel. Furthermore, this is a well-managed project that is poised for success.
- The project has a good, strong team with obvious expertise in flexible hose design. This is an important topic with directly impactful results, if successful.
- The project has strong materials science accomplishments and data. Other strengths include the strong reduction of permeation with special filaments and the project's methodical approach.

Project weaknesses:

- NanoSonic would benefit from seeking out a partner with deep experience in hose-crimp technology. There are countless companies with which to engage, not the least of which would be Swagelok or Parker Hannifin, among others. These companies would see the value this work provides to their business and would therefore make for a strong partnership that would push NanoSonic over the top.
- The overall project weakness is a lack of planning for testing with hydrogen gas, including leak, permeation, and impulse/pressure cycling.
- There is a weakness in expertise for fitting design and metallurgy.

Recommendations for additions/deletions to project scope:

- The team should add hydrogen-specific tests to validate the project: leakage, permeation, impulse/pressure cycling. The team should also examine the American National Standards Institute/CSA Heavy Goods Vehicles 4.2 standard and choose key performance tests to further validate the product.
- The team is on a good path and has shown great strength in working to solve the interface problems.

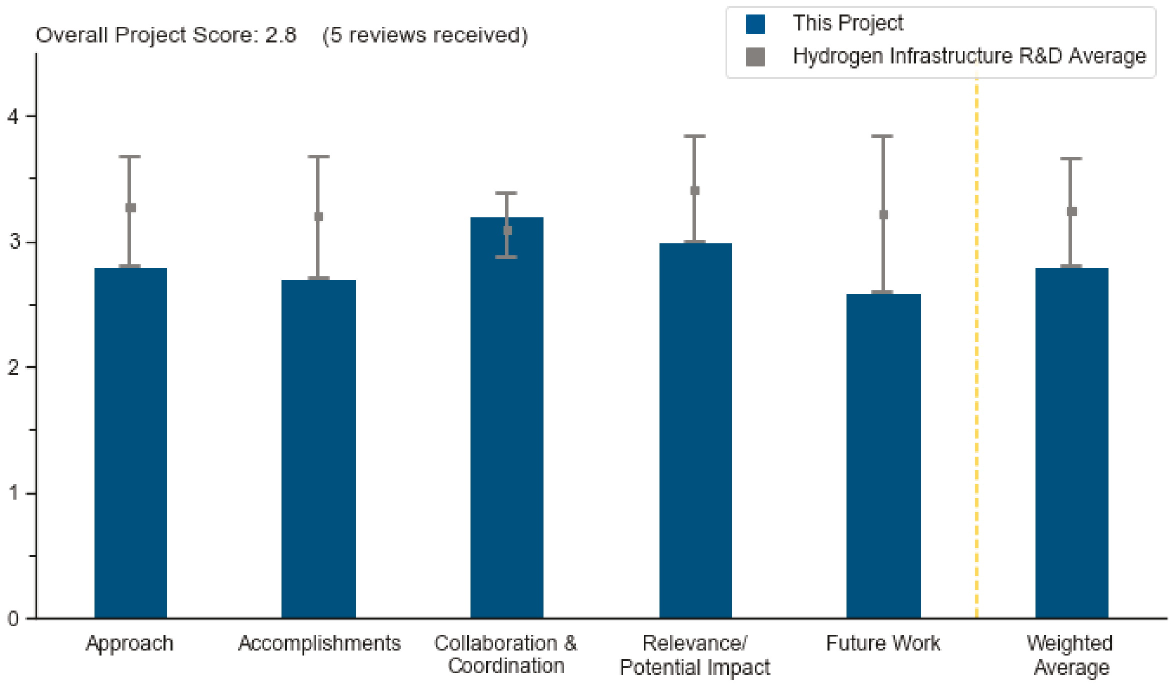
Project #IN-011: Coatings for Compressor Seals

Shannan O'Shaughnessy, GVD Corporation

Brief Summary of Project

Seal failure is a major contributor to hydrogen compressor maintenance, adding significant downtime and cost to compressor operation. The goal of this project is to improve seal life in hydrogen compressor systems by three to five times. The work focuses on two different types of coatings. For static seals, the project will develop barrier coatings that mitigate hydrogen ingress into the seals, which prevents premature failure. For dynamic seals, low-friction coatings that reduce wear and extend seal life will be developed. A room-temperature polymer vapor deposition process will be utilized to produce thin polymer coatings for both types of seals.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Hydrogen station reliability is a critical topic regarding the future success of the fuel cell market. This project’s objective is to make tangible improvements to seal life with vapor-deposited coatings. The approach taken constitutes two types of coatings, targeting both static and dynamic seals. Existing station reliability data were used to determine the strategy. The plan is dynamic and provides a high probability for success.
- Seal wear and hydrogen leakage are important problems that need to be solved, and the barrier coatings and lubricious coatings approach has merit. The team seems to have started addressing production issues (e.g., inclusions, uniformity) but did not provide data to support the statements on success in solving these issues. The work to test the coated seals in a compressor is a good start. The work scope seems very similar to prior years, and the presentation did not provide specific milestones or stage gates against which project progress could be evaluated.

- The approach of the project is interesting—to apply thin vapor-deposited coatings on O-rings to create a barrier and lubricious surface—but it is unclear that this effort has any chance of improving the critical issues with elastomeric seals. The barrier coating has a high likelihood of capturing the hydrogen in the elastomer, which would result in explosive decompression. The lubricious coating could be helpful, although there could be other options for the design, such as the surface finish specification.
- The approach is sound but could use some improvement. The justification of the helium results as a surrogate for hydrogen was not clear. More time should have been spent rationalizing this. There were some data that indicated the hydrogen permeability data did not correlate with the helium permeability data; more time should have been spent discussing this discrepancy.
- This talk and presentation were a little hard to follow. It sounds like the hydrogen barrier coatings work has not gone well, and the project is shifting to the low-friction seals for piston heads. A good deal of background material was included, but the specific relevance to this project was hard to follow. It sounds like the work on hydrogen barrier coatings is still on helium, and hydrogen testing has not yet started. Improved clarity on what exactly the project's approach is would be helpful.

Question 2: Accomplishments and progress

This project was rated **2.7** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made significant progress in regard to the overall objective to improve seal life by three to five times. The coatings have demonstrated the reduction of helium permeation and mass loss for dynamic seals. Although helium is a comparable gas to hydrogen for testing, it will be interesting to understand the coating's true ability to reduce permeation in high-pressure hydrogen applications. Nevertheless, the results show that successful high-pressure hydrogen testing is achievable.
- The work with a national laboratory to demonstrate the usefulness of the coated seals during compressor operation is good progress. Likewise, the connection with additional industry customers is a step in the right direction. It would have been useful if the team had presented data that supported the claims that the project increased the deposition zone by 10x through changes in chamber geometry. Likewise, the results of the permeation tests would have been useful to support the team's claims of success in solving inclusion-related problems.
- The accomplishments are well-defined, but the discrepancies with the test data need more explanation.
- Progress toward the overall project and DOE goals appears to be slow. In fact, the hydrogen permeability function of the coating did not provide positive results because of issues with applying the coating. Because of these results, the project has decided to stop effort with the barrier coating evaluation and focus on the lubricious coating. This change in direction seems to acknowledge the coating's lack of ability to provide the barrier function, which is more important to the DOE goals than the lubricous function.
- From the presentation, it sounds like the hydrogen barrier coating work has failed. It does sound like there is some promise for the low-friction coatings, although apparently only 50 hours of testing have been done so far. Specific quantitative metrics for the low-friction coatings were not seen in the presentation, nor was how well GVD Corporation (GVD) is doing in meeting those metrics.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The team has a good balance of original equipment manufacturers and testing facilities. This will allow for quality test specimens and data validation. Overall, the collaboration and coordination is well covered. Additional collaboration with active station owners would be an added benefit.
- It sounds like testing is taking place at NREL, which is a good partnership.
- The team has a good list of collaborators that will support the success of the project.
- The collaboration with the national laboratories (e.g., National Renewable Energy Laboratory [NREL] and Oak Ridge National Laboratory) is good. Additional collaboration with industry partners beyond Takaishi Industry Co., Ltd., would have been useful for obtaining feedback regarding the application and failure

modes. In addition, the project should have contacted Pacific Northwest National Laboratory (PNNL), which is leading the Hydrogen Materials Consortium effort on polymer compatibility with hydrogen.
- Various partners seem to be providing support, mainly through testing the coated products rather than participating in an integrated effort. It was not clear how the total funding was distributed across the partners or how to evaluate the level of support that each provided. One of the tests that was being run at the national laboratory was cut short because of equipment failure, but no plan was presented regarding whether the testing will resume or what the schedule might be.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- DOE's objectives are in support of systems that are both "reliable and affordable." This project is aligned in both aspects. As stated in the project's objectives, the goal is to improve maintenance frequency and decrease hydrogen cost per gasoline gallon equivalent (gge). This is excellent.
- Compressor reliability is significant weak link in the fueling station system. Any improvements to minimize down time and increase reliability and durability are critical to the success of the fuel cell electric vehicle industry.
- Hydrogen permeation and the lubricity and wear of the seals are important aspects to preventing equipment down time in hydrogen infrastructure. However, the properties of the polymer of the base component (e.g., the O-ring or a gasket) also play a role, and it is possible that the O-ring/gasket performance is not mitigated (or mitigated to only a limited extent) by utilizing the project's coatings. Although the project's coating technique could theoretically be applied to a large number of components simultaneously and for components of shapes other than O-rings/gaskets, the project has not shown data supporting these potential attributes.
- The need to evaluate hydrogen compatibility with polymers is important. The project appears to significantly overstate the relationship of seal failures with the cost of hydrogen. It is not clear how improved seal performance would ever reduce hydrogen compression, storage, and dispensing costs from $3.50/gge to $2.00/gge. The project makes statements about the impact of seal failures without any evidence or other supporting information.
- Because there were not clearly defined metrics in the presentation, it is hard to determine the impact. Clearly, there could be a benefit, but the potential for this approach to provide the full benefit for compression was hard to follow.

Question 5: Proposed future work

This project was rated **2.6** for effective and logical planning.

- The project has achieved an acceptable level of success during testing, and it plans to expand the testing soon. Additionally, the project has already begun to supply the product to industry stakeholders for testing and plans to increase that effort in the future.
- There is a definite need to pursue hydrogen permeation testing and other performance tests using hydrogen gas. It is unclear whether the team has considered explosive decompression in hydrogen environments.
- The team is focused on field trials and building commercial partnerships, which overall are good and reasonable steps. However, a significantly greater scope of technical work than just partnership-type activities was expected, based on the level of funding for the team's Phase IIA work.
- There were not many specifics in the future work.
- The proposed future work for this project indicates dropping the barrier coating effort and focusing only on the lubricious coating. This change of direction will further reduce the relevance of this project. The wear of O-rings has not been identified as a critical barrier for the industry. Certain suppliers may have issues with the wear of O-rings, but this may be due to their design or incorrect selection of O-ring material.

Project strengths:

- A key strength of the project is that it is addressing a major low-reliability component in the fueling station system: compressors. The technology offers promising results, as shown with the data from Powertech Labs, Inc., and HydroPac, Inc.
- The project's strength is having multiple approaches to improving seal failures (i.e., barrier coating and lubricious coatings).
- The company is leveraging barrier-layer technology to mitigate down-time issues in hydrogen infrastructure equipment.
- The project's strength is thinking "outside of the box" to improve the failure modes of elastomers in hydrogen applications by using a coating.
- It sounds like NREL will do testing of the low-friction seals, which is a good step.

Project weaknesses:

- The project activities, milestones, and stage gates are somewhat poorly defined. Although the team seems capable, the work presented is missing the scientific depth and understanding relative to other projects within the Fuel Cell Technologies Office.
- It is concerning that there is little supporting data showing that the improved seals are actually effective in hydrogen environments. There is a need to explore testing at higher temperatures and higher pressure (1000 bar).
- The weakness for the project is the fragility of the barrier coating application. As mentioned during the presentation, "Hydrogen permeability did not match the helium permeability due to particulate inclusion in films caused by modification of deposition chamber." If this application can be improved to withstand minor defects, the barrier coating application will be considered excellent.
- The project weakness is the focus and overstatement regarding the impact of seal failures. The lack of data indicating the improvement of the barrier coating and the sensitivity of the application process are weaknesses of this project. In addition, the test conditions to evaluate the permeation were only at ambient conditions and low pressure. The project has notable weaknesses in the approach and execution of developing a robust seal to address the seal failures. A response was also provided during the presentation that this coating is intended for applications that are not in constant exposure to hydrogen, which is a weakness because of the limited application of this project effort.
- This presentation and set of slides were hard to follow. It is unclear what the metrics are, how far along GVD is toward achieving them, or what the specific approaches are to improvement.

Recommendations for additions/deletions to project scope:

- The project should consider analyzing coating efficacy on different polymer systems, since vendors may use a variety of different formulations for their respective seals and O-rings. Such data could possibly show the efficacy and/or generality of the approach for different polymer systems and may help guide manufacturers in polymer selection. The team could consider verifying the uniformity of coatings when a large number of components are coated simultaneously (for higher throughput), as well as when coating components with more complicated geometries.
- A recommendation is that the project use failure mode tools (e.g., failure mode and effects analysis) to examine the potential of the coating to provide the necessary functions in the application. The project team should contact PNNL regarding evaluating polymers in hydrogen applications. The project should not dismiss the barrier application, even though it will be difficult because the lubricious coating is less interesting and less impactful.
- It is recommended that the team conduct sample-level permeation testing using hydrogen, evaluation of explosive decompression, and evaluation of the material's resistance to higher temperatures (operating) and pressure (up to 1000 bar).
- The project should evaluate the possibilities of modifying the barrier and lubricious coating application methods for other materials and surfaces (e.g., sliding surfaces of compressor piston chambers).

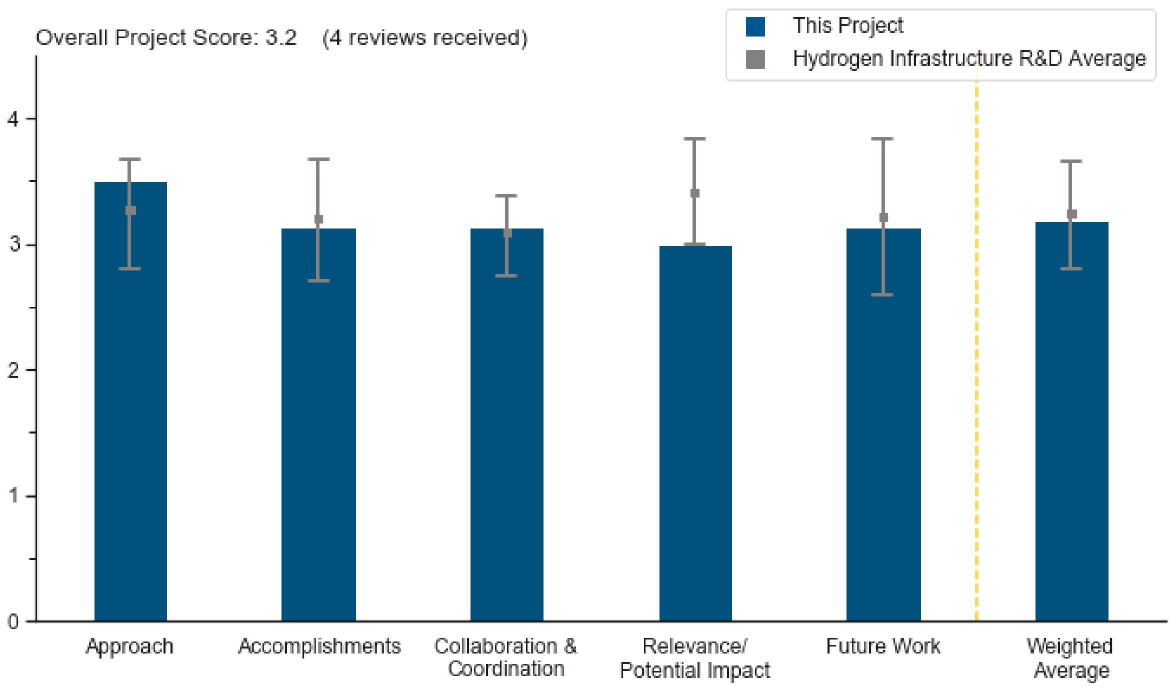
Project #IN-012: Low-Cost Magnetocaloric Materials Discovery

Robin Ihnfeldt, General Engineering & Research

Brief Summary of Project

Hydrogen is less expensive and safer to transport and store in liquid form. However, converting hydrogen and keeping it in liquid form is not easy. The energy required for hydrogen liquefaction at the point of production is high, and hydrogen boil-off from cryogenic liquid storage tanks needs to be minimized. This project seeks to address the high cost and low energy efficiency of hydrogen liquefaction. To overcome these barriers, this project is developing a low-cost, energy-efficient magnetic refrigeration technology for hydrogen liquefaction. The project objective is to discover, develop, and commercialize low-cost, high-performance magnetocaloric effect (MCE) alloys to enable magnetic refrigeration to move from prototype to production.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure R&D projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The principal investigator's (PI's) approach is strong and sound. The approach of focusing on a low-cost and small-scale hydrogen liquefaction system has many merits overall. The focus on MCE material cost versus magnetic field cost is nothing new to the field, so there was a need for some additional insight into why the approach, which focuses only on materials with a second-order-only response and uses low-cost rare-earth materials, is going to maximize the search for better MCE materials. Overall, there is confidence in the approach and the PI's ability to deliver a few promising MCE materials.
- The characterization of the materials and the application of the doping solution to enhance performance are impressive. The development of casting techniques is important work for materials development. Achieving high stability for MCE materials is vital for the development of magnetic liquefaction.

- The project's approach of avoiding rare-earth materials is a good strategy to narrow options and improve efficiency. The project also does a good job defining the material requirements for conducting the research, much of which is based on what exists in the commercial market today.
- The approach to date seems good and is focused on material research. However, task 2.4, to develop a "small-scale" hydrogen liquefier, seems to be a significant deviation from the objective of discovering and commercializing MCE alloys. The "materials" skills to evaluate and discover MCE alloys are significantly different from those for producing an operating refrigeration system that utilizes those materials as only a part of the device. This step does not seem to fit with the stated objective and should be part of a redefined project with a different purpose and potentially different or additional skills.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The progress on the stated objectives appears good, as shown by the presentation materials and the "percent complete." The true evaluation of the project's success would be implementation by the magnetocaloric hydrogen liquefaction (MCHL) project led by Jamie Holladay (IN-004).
- The materials development and characterization are impressive. Material functionality is vital work.
- The material synthesis was successful, allowing the project to commercialize a product in small quantities.
- The accomplishments for this effort are strong. The team demonstrated the performance of several low-cost second-order MCE compositions for a wide temperature range (9 K–325 K) and showed that anneals are required to achieve good MCE properties. More was expected from the material discovery at this stage of the project. It is too early to comment on DOE's targets since the project does not have a prototype yet or a system model based on the material's performance.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- The team presented a long list of partners and their roles. As part of a small business, the team understands the importance of leveraging resources and knowledge from others.
- The project has exhibited great collaboration with universities and other related DOE projects.
- It is not clear how closely this project has worked with the MCHL project led by Jamie Holladay. Presumably, that project is the logical beneficiary of this work, but that project is not listed as a collaborator. The team should clarify whether connections have been made such that these are the materials that will be used by that project. Also, in terms of the next step for developing a "small-scale" hydrogen liquefier, performing this seems better suited for the MCHL project as a first step to validating the technology, not by the project that was tasked with materials development. The partners listed will not have meaningful input into the technology needed or the ability to integrate into an actual system. During the presentation, there was a comment that some potential future partners have been "engaged," but until they are formally part of the project, it is a risk that there will be no meaningful technology input for handling liquid hydrogen (LH2), nor input to commercial application. For example, a 300 kg liquefier is small-scale from the perspective of "production," but it would be very large from a perspective of "boil-off" recovery.
- It was good to see a diverse set of partners, but this technology needs more exposure to a wider variety of applications to secure help with further funding. The project lead needs to expand potential applications in the energy field to underpin development support.

Question 4: Relevance/potential impact

This project was rated **3.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The materials being developed within this project have a strong relevance to the application of liquefying hydrogen. For the fuel cell industry, the use of LH2 in transportation minimizes cost and logistics. It would be advantageous for the project to identify other direct or indirect applications to utilize the materials.
- This is a blended score. The relevance is high (3.5) with respect to developing adequate materials to validate the MCHL technology, although its value is predicated on successful results that prove it to be substantially better than existing LH2 production. The relevance is low with regard to the "boil-off recovery" extension of the project. It is not clear how the boil-off recovery advances the DOE targets for 30 tons per day (tpd) and 300 tpd production of LH2, nor how it achieves a production cost of $3/kg. Boil-off recovery is an after-the-fact "system improvement" tool for a fueling station and has no impact on production cost or efficiency. Its process parameters would be different, and the economics are substantially different from production. Boil-off efficiency can also be (and has been) approached via other existing technical approaches. It is not clear this would have any benefit until a preliminary economic evaluation is completed.
- Addressing the high cost and low energy efficiency of hydrogen liquefaction is critical to the DOE Hydrogen and Fuel Cells Program goals and objectives. This performer brings some uniqueness to the DOE's research and development portfolio by focusing on small-scale systems. The researchers claim that the modeling results for their small system look promising and their system could be used as a low-cost solution at fuel stations for preventing boil-off losses, but few details were presented, and what was presented was presumably preliminary findings. There is much anticipation for next year's presentation, in which the team might elaborate on these modeling results and the approach.
- Striving to achieve high-efficiency hydrogen liquefaction is an important goal; however, there must be other applications that can utilize this technology.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The proposed future work is strong. There is much anticipation for the prototype activities, focusing on having an optimal design determined from the team's model efforts this fiscal year (FY). The potential Phase IIa and IIb will be based heavily on the outcomes from the FY 2019 activities, but building a small-scale system is a natural progression if the project is successful with the FY 2019 activities.
- The project has a clear strategy for scaling up the MCE materials production line.
- The focus on driving for lower-cost materials is appreciated. Improving low-temperature performance is good. The project needs to identify new sponsors in liquefied natural gas, cryogenics for super colliders, and space or satellite applications.
- This is a blended answer. The future work proposed to complete material evaluation is good. The proposed future work for item 2.4 needs significant evaluation as to scope, need, and technology prior to being included in this project.

Project strengths:

- Their biggest strength is that the project is focusing on a low-cost and small-scale hydrogen liquefaction system. Hopefully, the team is not biased too much from larger systems and instead learns from them and approaches this challenge with an innovative solution that leverages the fact that the system is small; this could be a game-changer if the project is successful.
- The identification of materials to enable magnetic refrigeration is core to that technology. This project seems to have made progress in that area and has been successful. The project can likely be closed when this work is completed.
- The project's strength rests in its support from the project collaborators, such as the hydrogen liquefaction design team.

- The project is high in strengths.

Project weaknesses:

- There was hope that this material discovery approach might have been broader in techniques and results, but overall, this is a strong project.
- It is not clear that the MCHL project is benefiting from this work; it might be, but it is not clearly stated. Transitioning from a “materials expertise” project to a “system” project is a significant change that does not align with the original objective. It is recommended that this work be done as a separate project or integrated into the MCHL project since it requires substantially different expertise and experience from the materials work. It is also not clear that any evaluation has been completed that would indicate that developing a “boil-off recovery” unit is economically justified or technically possible.
- The project’s weaknesses are in expanding potentially high-value applications.
- The project’s weakness is the lack of access to equipment for larger-scale processing of materials.

Recommendations for additions/deletions to project scope:

- The scope is strong.
- It is recommended that the team complete the materials work. For the boil-off work, it is recommend that it be deleted since it does not fit the original objective and is of substantially different scope and expertise. If there is desire or intent to proceed, then it should be separated into its own project to be evaluated on its merit. If the boil-off recovery work continues, then the team should (1) perform an economic analysis of the capital and operating costs of such a unit, (2) evaluate the optimal size of such a unit (i.e., whether 300 kg is the right size; it is probably not), (3) evaluate its benefit relative to DOE objectives, (4) evaluate existing technologies (e.g., cold heads and recovery compression) that are commonly used today for comparable applications to see whether a magnetic refrigeration system offers any benefits, and (5) develop partnerships that can meaningfully help with the technology evaluation, economics, and technology development needs and provide input into the potential deployment strategy.
- The team should maintain the focus on technology and expand the focus on applications.
- There are no recommendations for additions or deletions to this project.

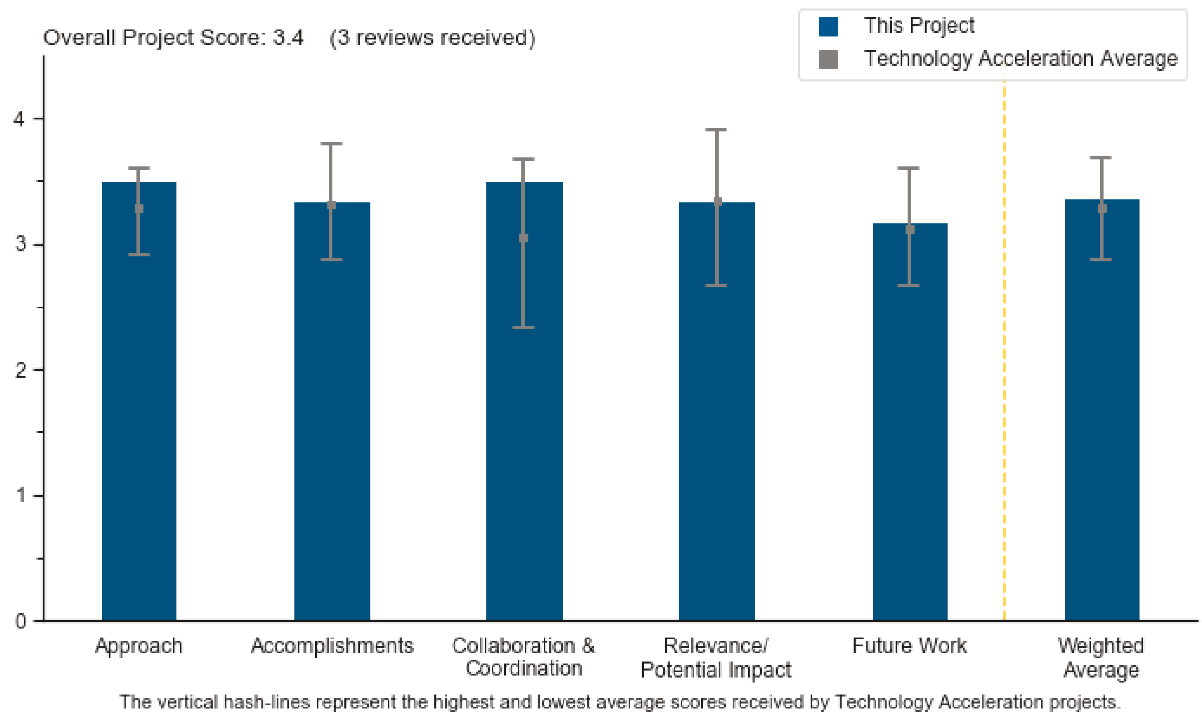
Project #TA-001: Membrane Electrode Assembly Manufacturing Research and Development

Michael Ulsh, National Renewable Energy Laboratory

Brief Summary of Project

The objectives of this project are to (1) understand quality control (QC) needs from industry partners and forums, (2) develop diagnostics by using modeling to guide development and in situ testing to understand the effects of defects, (3) validate diagnostics in-line, and (4) transfer technology to industry partners.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an excellent project. A systematic approach is being pursued to determine the capabilities of various diagnostic tools for quality control/quality assurance (QC/QA) of membrane electrode assemblies. The team is working to understand industry needs fully and is designing project activities in response to those needs.
- Advanced on-line QC tests are a critical need. The use of optical methods is innovative. Efforts to measure impacts of defects from a quantitative perspective are strongly endorsed.
- The techniques are useful, particularly in looking for deviations in catalyst coatings. The pinhole characterization is not clear. Clearly, these are a problem, but the effort to find what size of a pinhole is acceptable is not likely to bear much fruit. Once there is a pinhole, it quickly propagates, so if the minimum acceptable size is unknown, it is hard to know whether the detection is good enough.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The availability of QC/QA tools for full-scale manufacturing of polymer electrolyte membrane (PEM) fuel cell and low-temperature electrolysis membranes will be essential for achieving processing yields required for ultimate cost reduction. The team appears to be making steady progress toward the project goals.
- Optical methods for platinum loading are impressive. The use of membranes that are kilometer lengths allows NREL to establish a strong baseline database with respect to defect measurements. The goal for optical measurement was down to 0.05 mg/cm^2; however, the smallest step-size goal seemed to be 0.1 mg/cm^2, so it is unclear whether the technique can adequately cover the low end.
- The post-mortem work is good, but it seems many investigators have already published these techniques. For those techniques that might occur during processing, this would be helpful, but it is uncertain whether they can detect at relevant sizes. The catalyst monitoring is of more interest; however, here the correlations are not yet strong enough, though the team will likely close in and make this better.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The collaborative approach to working with end users is a major strength of this project. This is essential for this project to ensure that the team is developing characterization tools that industry will use. The team has also expanded to leverage capabilities of other national laboratories and universities.
- This is an outstanding assortment of industrial and association collaboration. The team has a very organized outreach campaign to understand what is needed.
- The team has an excellent team of collaborators, but it is unclear what the team is doing with General Motors. The work with Proton and Gore should maintain the focus on what is important to manufacturers.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- A sign of a product's maturity is its level of QC and QC understanding. Thus, this work is critical to implementation of fuel cell electrolyzers for the hydrogen economy.
- This project supports the goal of reducing cost at full-scale production of membranes for PEM fuel cells and low-temperature electrolyzers.
- It is not certain that Gore or other PEM manufacturers currently have a problem with thickness mapping. Clearly, the thin-film industry has methods to measure this already. The catalyst loading is of interest, and the team is closing in on methods.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- Finding out what variances exist in the catalyst layer, membrane thickness, and pinhole size probably should have come before finding out if they need to be, or can be, measured. It is good that the team was able and allowed to adapt mid-project to address low-temperature electrolysis needs.
- The proposed project efforts are well aligned with the needs of the community. The team endorsed linking quantitative defects to accelerated stress tests and lifetime prediction.
- The proposed work is fine, but there does not appear to be a budget allocated for the work.

Project strengths:

- The use of "whole material" optical or heat methods that have 100% inspection is a project strength. Demonstration of on-line measurement and the ability to build up a library of defects are also project strengths.
- Collaboration is the strength of this project, as end users define needs and guide project activities, and other organizations expand the "toolbox."
- This is a good team with very appropriate collaborations that should steer the project toward the most important characterizations.

Project weaknesses:

- The team should have worked to define what size variations were acceptable before determining methods to find them. For example, if a pinhole of any size is unacceptable, the project will need to find methods that can find much smaller pinholes than the optical techniques now being developed. Without knowing this, the team might spend a lot of time developing a technique that is not relevant.
- The low end of optical platinum loading detection may not be sufficient for typical anode loading.

Recommendations for additions/deletions to project scope:

- There should be a pause on the detection techniques until the researchers have established the resolution that they need.
- At some point, it may be worth expanding the scope to other types of fuel cells (e.g., solid oxide fuel cells).

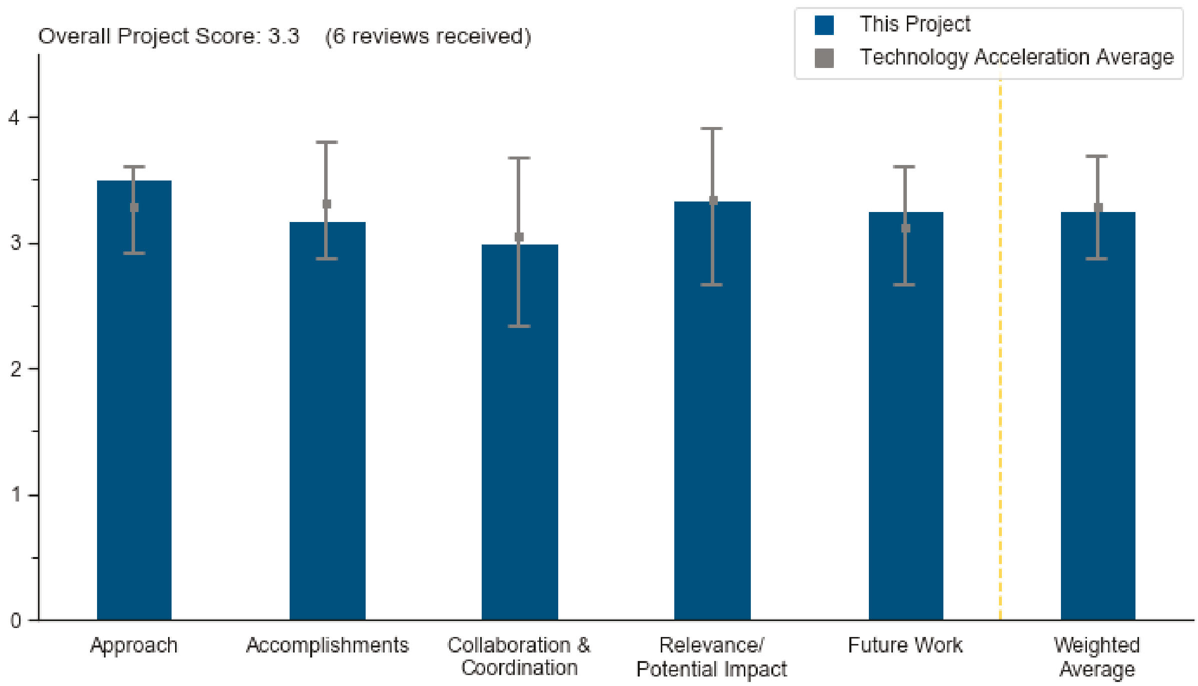
Project #TA-005: In-Line Quality Control of Polymer Electrolyte Membrane Materials

Paul Yelvington, Mainstream

Brief Summary of Project

With the goal of improving the reliability and reducing the cost of automotive fuel cell stacks, Mainstream seeks to improve in-line quality control (QC) technologies that are used in the manufacture of polymer electrolyte membrane (PEM) materials. To achieve this goal, the project team will build a prototype system capable of simultaneously measuring defects in a moving membrane web and membrane thickness over the full web width. The developed system will scan the manufactured membrane with 100% coverage, marking and logging defective regions.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach develops the methodology to identify defects in the major components of PEM cells. The approach includes transition of the analytical approach from small-scale offline to roll-to-roll (R2R) manufacturing. The team anticipates the development of a prototype system for industrial applications.
- The approach is a needed first step, which represents a significant advance vs. visual inspection of components, in both feature size and speed. This still requires some definition around data analysis to track back to defects, but the technique seems applicable to multiple substrates and components.
- The approach is valid. The team wants to see what the relevant defect size is, then find methods to detect it. The team is doing this for multiple categories, including membranes, gas diffusion layers (GDLs), and catalyst-coated membranes (CCMs).
- The project is not a "research" project but rather a development project based on compiling existing technologies into a system that can detect defects in a moving web. Thus, barriers and targets are not as

relevant in this project as compared to others. In fact, resolution on the cameras was reduced so that the quantity of data was reasonable.
- The goal of the project is to transfer a national-laboratory-developed non-destructive inspection technology into a commercial product. This objective is being met. The question is whether it is a product if no one buys it.
- The investigated approach is appropriate to address the main barriers and to reach technical targets.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- There is very good progress regarding defect detection and the evaluation of the catalyst loading. Results on the impact of defect size on durability would have been appreciated, as some cost elements have an impact when moving from today 100 µm detection to the next step of 25 µm, and the ultimate to 10 µm.
- Good progress has been made toward the stated goals of the project. Reduction of false positive and false negative rates at 100 ft/min speeds is fairly impressive. Identification of catalyst layer thickness to within the error bars is probably sufficient. The more pressing issue is detection of voids or large agglomerates that could cause hot spots or high creep areas.
- Demonstrating measurement of defects in membranes, GDLs, and CCMs, the team is able to measure catalyst thickness and distinguish between a false positive and a true positive. The team is developing techniques to measure catalyst loading on CCMs and GDLs. The testing of industrial materials has been initiated.
- The project has made good progress and has a commercial system available for install at customer sites.
- The QC thickness measurement and defect detection system developed by Mainstream appears to be suitable for its intended purpose. The only real question is whether this product will find commercial acceptance. Developed without active involvement by commercial membrane manufacturers, the company pursued an "if you build it they will come" approach.
- Although the team stated that it wanted first to determine what defects and defect magnitudes were relevant, then find methods to detect these, the researchers are in fact operating in the opposite fashion: they are determining what their current system can accomplish while waiting to find out relevant defect size from the National Renewable Energy Laboratory (NREL). This can possibly lead to a large amount of wasted effort. There is a very weak correlation between catalyst loading and pixel intensity, which is disappointing and brings the methods into question.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- Collaboration between Mainstream and NREL appears excellent. The involvement of more industrial entities as membrane electrode assembly (MEA) producers is appreciated.
- Collaboration with NREL is excellent, with coordination on defect creation and detection. However, this is to be expected, as this project originated from a technology transfer/licensing based on a Small Business Innovation Research topic. It would be good to see more interaction with potential end users to demonstrate the method on production or prototype components and work collaboratively on customer needs.
- The team reports collaboration with NREL, a leader in identifying defects in MEA materials and identifying the impacts of defects on fuel cell performance. The team identifies testing of industry samples. Industry interaction should be increased to get a greater variety of membranes, CCMs, and GDLs.
- The team is using NREL to determine the relevant defect size, which should have occurred as early as possible in the process but does not seem to have been started. As for the process development, the Mainstream researchers should be able to do this themselves, so extensive collaboration is not necessarily needed.
- There is minimal collaboration with other research institutions; however, the nature of this project does not require such elaborate collaborations.

- Although it appears that input from commercial manufacturers was solicited at the project onset, and commercial collaborations were pursued during the project, no commercial collaborations were established. This is a huge weakness of the project. By the end of the project, DOE will have invested $2.15 million dollars, and Mainstream will have developed a product that may or may not have a market.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The system will have the ability to eliminate defects in PEM fuel cell stack components prior to assembly of the stack or construction of individual fuel cells. The results of the analysis would be to discard faulty MEA components or MEAs prior to stack assembly, which should greatly reduce costs and increase durability of fuel cell systems. The methodology can lead to improved manufacturing processes and a reduction in scrap rate.
- Aside from NREL's work, this is the only project in the DOE portfolio focusing on automated defect detection in fuel cell/electrolyzer components. As these technologies are deployed in the market at larger quantities, QC is both a bottleneck and a larger expense, and this project addresses a key need.
- The project is relevant to the DOE Fuel Cell Technologies Office. In-line defect detection is critical for R2R processing to ensure concurrently lower scrap rates and thus lower membrane and MEA costs.
- There is apparent value of this QC product for MEA manufacturing. However, MEA manufacturers are apparently not showing interest. It would be helpful to know where the disconnect is.
- It is not convincing that a new method for determining membrane thickness is needed. Similarly, though QC methods are needed for online R2R fabrication of electrodes and MEAs, it is not certain that this method will be able to discern this. In addition, the team does not appear to have a "Plan B" if the camera does not work.
- It is unclear whether the industry is ready for such equipment.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed work appears appropriate to achieve the project targets. Quantified results of defect size on durability and a cost analysis should be presented.
- Clear direction for the development of a commercial product is the focus of this small company.
- The plan for future work is fine. The project needs commercial demonstrations, if not in the fuel cell industry then in other industries. There is a huge risk that Mainstream is developing a product that no one will buy.
- Future work addresses increasing sensitivity to observing smaller defects on a moving R2R system and scaling up the system to larger-size (commercial-size) components. Moving the prototype system to industry and finding manufacturing partners are important aspects of this emerging QC system.
- Transitioning to validation of the QC method (through performance testing) is a critical next step, as is working directly with customers and manufacturers.
- All of the future work is concentrated on improving the resolution and fidelity of the current process. There is no reference to establishing the actual guidelines or when the project will have this. The team has a goal of reaching a 10 µm defect resolution, which sounds very good; but perhaps the critical dimension is 100 µm, and anything smaller is fine. In that case, the researchers are wasting their time trying to improve. If the critical dimension is 1 µm, then the team clearly needs a new method. The researchers give a goal for web speed, but there is no basis to judge whether this is good or bad if they do not state how web speed adds to the cost of the process they are monitoring, and how this translates to total dollars per square meter of active area. If cost of the material is already down to $0.01/m^2, the researchers likely do not need to focus on this area.

Project strengths:

- An important strength is ability to work with NREL to get materials with known defects and to optimize the NREL QC technology to a prototype for demonstration on industrial R2R manufacturing. The organization's experience in developing turnkey systems is a definite strength.
- Strengths include the approach to creating controlled defect sizes and catalyst loadings for quantification of detection limits and demonstration of method. Another strength is looking at the different electrode configurations and how different pinhole types would interact with the catalyst-layer configuration.
- The Mainstream/NREL team's efforts to speed up development and demonstration of this kind of technology are of high value.
- The team has clear focus and concrete results with commercialization efforts.
- The team has good capabilities and a good approach to face a relevant problem.
- This is a nice product being developed to meet an apparent need.

Project weaknesses:

- The cost of the equipment and the cost of using the QC process in a manufacturing process needs to be determined.
- Data analysis, given very large datasets, was a stated challenge that did not have a fully defined solution yet. It would also be interesting to expand the range of catalyst loadings/types analyzed for better relevance to electrolyzers, which are not platinum on both sides and are still at high loading.
- Project focus to date has been entirely on making it better and faster. This is, of course, admirable, but there is no basis to back critical parameters of needed defect size and cost. Without this, it is unclear how anyone can judge what is "good enough" or "fast enough."
- It is not certain that the industry is ready for this. The principal investigator has identified that the commercialization may be better directed at more mature manufacturing industries. No commercial interest is demonstrated.

Recommendations for additions/deletions to project scope:

- It would be helpful to see some cost information. Presumably the cost will be well within acceptability, but this information is needed. The team needs to accelerate the work with NREL to determine the critical parameters or tolerable defect sizes.
- The team should include the effect of the defect size on performance and durability. The team should also investigate the two-dimensional spatial mapping, in particular for the loading mapping.
- The team should expand the project and funding to install equipment on an industrial production line and add a large-scale (3M or W.L. Gore) manufacturer to project.
- It would be good to add a range of catalyst thicknesses and types for electrolyzers.
- The team should explore alternative markets for the product.

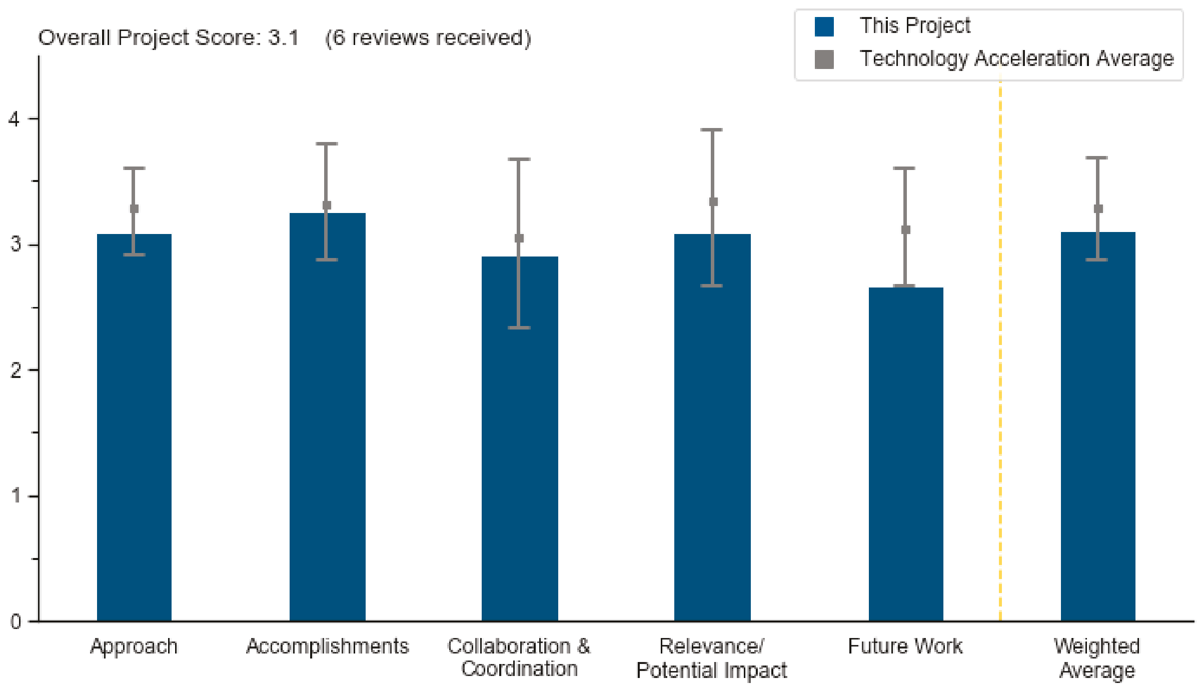
Project #TA-007: Roll-to-Roll Advanced Materials Manufacturing Lab Consortium

Claus Daniel, Oak Ridge National Laboratory

Brief Summary of Project

All U.S. Department of Energy-sponsored cost analyses for high-volume production of membrane electrode assemblies (MEAs)/cells assume roll-to-roll (R2R) processing will be used. The project objective is to develop R2R manufacturing techniques to reduce the cost of automotive fuel cell stacks at high volume (500,000 units/year) from the 2008 value of $38/kW to $20/kW by 2025. The project goals (depending on technology area) are to (1) increase throughput by 5x and reduce production footprint, (2) reduce energy consumption by 2x, (3) increase production yield by 2x, and (4) enable a substantial shift of manufacturing to the United States by assisting in the development of a domestic supply chain.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has an excellent approach in the demonstration (and performance verification) of the R2R techniques that are required for high-volume, low-cost fabrication of membrane electrode assemblies and that have not yet been demonstrated by industry. Performance validation of the ensuing R2R products is essential.
- It appears that Oak Ridge National Laboratory established an extremely qualified team of national laboratory scientists and engineers to perform this work, and there is value to performing research aimed at reducing manufacturing costs. The only concern for the approach is how it will be broadly transitioned to industry when there appears to be only a single industrial partner.
- Although this project focuses on manufacturing, which should normally be left up to industry, some good and promising results have come from it. Most notable is that a significant amount of material

was used, allowing for good process control of the materials being made. This allows for low sample-to-sample variability when comparing the impact of different processing parameters on fuel cell performance.

- The basic approach of using the R2R manufacturing process is appropriate and has projected cost savings of 63%. One area that seems to be missing is an on-line quality assurance strategy. R2R could have savings only if the process is running near defect-free, with minimal scrap.
- The project team is putting a good deal of effort toward eliminating the ionomer overspray layer, and it is not clear that eliminating this layer is at all necessary. The researchers wrongly assume that adding this layer will double the cost of their R2R process. That assumes a full rolling and unrolling. In reality, it could easily be done in the same winding as a separate layer, adding only a small fraction to the cost. In R2R, the cost is generally proportional to how many times you have to roll and unroll, while extra processes are minimal.
    - The source of the cost reductions is unclear, but \$0.013/mile for a fuel cell or an electrolyzer MEA seems unlikely. An assumed 12" web of >6000 m^2 is enough for 300 MW of electrolysis. The cost of 300 MW of electrolysis is ~\$120 million. This project is an attempt to drop \$120 million from costs by lowering a process cost by \$0.47. The reasoning behind this is unclear. Over their lifetime, those 300 MW of electrolyzers should generate 300,000,000 kg of hydrogen, so this achievement will lower the cost of hydrogen by \$0.0000000016/kg. Automotive fuel cells require about 10 m^2 of MEA, so one mile can generate enough MEA for 600 vehicles. If the researchers reach their target, they will only drop the cost of each vehicle by \$0.0008. Clearly, any increase in performance with an ionomer layer or slower processing will be well worth it. Clearly R2R will be, and is, the method of choice, but the focus on increasing speed may be misplaced.
- The approach charts describe negatives for catalyst-coated membranes (CCMs) and identify some of the projected benefits of the R2R gas diffusion electrode (GDE) method of fabricating electrodes and MEAs. Not a lot of detail on experimental approach is given. The composition of the slurry for deposition of the catalyst layer (CL) was not discussed. It should be made clear whether the slurry had Nafion in it, as well as how the slurry was cured on the CL and substrate material. Several critical parameters were not discussed in the approach.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The work on roughness was insightful and very helpful. The progress toward stated goals is good, but the metrics are in question. Adding an ionomer layer should not significantly increase costs.
- The team systematically evaluated key parameters relating to the R2R process; the performance achieved was better than that of the baseline spray-coated CCMs or GDEs, achieving the project goal.
- The coating and fuel cell performance shown is excellent progress. However, it is not clear how this is related to DOE goals, as these should be the industry's goals. It does show that the R2R coating technology does not have a significant impact on the cost of the MEA; it is mostly material costs. Also, this project team has made contributions to the state-of-the-art understanding of parameters for fuel cell electrode construction.
- The team has made substantial progress in better understanding and demonstrating GDEs with and without ionomer over-layers. The team has also established that smoother gas diffusion layers (GDLs) and hot-pressing are key to a good interface and good performance.
- The project team demonstrated improved performance with modification of CL surface roughness, and the work is predicted to improve GDEs made by R2R. The team demonstrated the use of slot-die coating with a smooth microporous layer. The team also eliminated the ionomer over-layer. It was not clear why the project was successful in eliminating the over-layer.
- It seems like much work has been performed, but a huge investment was made with minimal industrial involvement. If the objective was to establish a national-laboratory-wide capability in R2R manufacturing, then the objective was met. If the objective was to develop technology that will ultimately be practiced by industry, there is a long way to go.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- The project team has the correct partners on the processing and characterization side. The addition of Proton OnSite should help the team focus on the requirement needs, but this is for low-temperature electrolysis (LTE) applications, which will be lower in volume than those of fuel cell electric vehicles (FCEVs). The project needs to add an automotive original equipment manufacturer (OEM) to help guide priorities.
- The project seems to have a very solid DOE laboratory collaborative team. With the notable exception of the industry cooperative research and development agreement with Proton OnSite (which is not yet implemented), there appears to be a lack of industry involvement. Collaboration would be stronger with more industry input.
- The project has strong collaboration with other national laboratories but is limited to one industrial partner that works with electrolysis, not fuel cells. A majority of R2R processes are meant for fuel cell catalysts or membranes consistent with fuel cells, but not with electrolysis. The project should find a fuel cell collaborator.
- This project, by its very nature, is a laboratory collaboration, with five partner laboratories and two companies involved. The laboratory partners' roles are well defined. It is not apparent from the presentation if the number of collaborators is a source of delay or management complexity.
- The project appears to be an entirely DOE laboratory effort; an industry partner in the water electrolyzer marketplace has been added to the project.
- Large-scale MEA manufacturers need to be involved in this project if any value is to be derived from it.

Question 4: Relevance/potential impact

This project was rated **3.1** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- As stated in the presentation, R2R processing is required to achieve high volume and low cost. Therefore, it is highly relevant for the project team to pursue basic advancement and increased understanding of specific R2R applications that are not otherwise being conducted.
- The project has met its performance goal using the R2R process and may very well meet the eventual cost reduction targets of 63%. The ability to control the process and attain high product yield will be a critical next step.
- Defining the parameters and better understanding the processes during R2R formation would be much more important than trying to increase throughput. In general, the latter is more easily achieved. Understanding the structure, property, and performance issues as a function of the drying rate and solvents used would be a better use of effort.
- The project very quickly down-selected one particular manufacturing process and then went on to study how to optimize MEA performance using that manufacturing approach. Industry standards are done with the CCM approach, not the GDE approach. The project team could do a better analysis of different CCM manufacturing approaches.
- The description of the slot-die coating process is not adequate to fully understand how a 63% cost reduction is achieved. The $1.30 for the slot-die coating process should be broken out into individual stages (coating, drying, and bonding) and their respective costs.
- It is hard to get over the level of investment made in this project without industry involvement. There can be no impact unless the technology is transferred to a manufacturer.

Question 5: Proposed future work

This project was rated **2.7** for effective and logical planning.

- Examining multilayer coatings is a particular focus area worthy for future work. It is key to integrate drying and curing into both the procedure and performance research, as well as the cost computations.
- The proposed work is broadly defined to include multilayer coating, ink formulation, drying and curing, and flow modeling. The areas to be added should include the effects and causes of defects, strategies for defect detection and process control, and leveraging other ongoing projects' technologies where available.
- The team may continue some work for Proton OnSite, but roll speed is far less important with LTE than it is for FCEVs.
- The project focused in on one process (direct coat catalyst on GDL) and excluded another (coating catalyst on membrane). The basis for this was a flawed processing cost analysis, assuming single-use expensive (Kapton) transfer liners and discrete transfer liner hot-pressing steps. One could envision a CCM decal transfer manufacturing process that would not consume the "liner" but simply re-use it. Also, the transfer process of the catalyst to the membrane could be in an R2R heated laminator, again eliminating the discrete hot-pressing cost step. The point is that the project eliminated one approach for MEA manufacturing over the other too quickly, and with a shaky foundation.
    - Instead, the project team could focus on the question of the CCM versus GDE approach. The Pt catalyst utilization was long ago (in the 1990s) determined to be worse for the GDE approach versus the CCM approach. This is why the industry shifted away from the 1990s GDE approach in favor of the CCM approach. This could be different with today's new GDL materials, as alluded to in the presentation. However, that would be a valid factor for determining the outcome between the GDE versus CCM approach.
    - Also important would be an entire supply-chain-wide manufacturing cost analysis. It needs to be understood where the supply chain breaks between different types of companies. The team should consider whether it makes sense for a membrane manufacturer to make, package, and ship a 10-micron membrane, just for an MEA manufacturing company to unpack that membrane and use a similar coating machine to apply catalyst, and then repack it for a stack manufacturer to cut and assemble it as discrete components into a stack. On the other hand, the team should consider whether a fuel cell system OEM has access to the know-how and best materials needed to manufacture MEAs from bulk raw materials. Industry-wide common breaks in the supply chain would yield the best results, along with pricing competition at each supply chain break.
    - In summary, it appears that this project has transformed itself from one focused on issues and trade-offs surrounding manufacturing MEAs into a project focused on optimizing the performance of a fuel cell MEA by changing its construction parameters. However, credit is due to the team, as they have a done an above-average job at the latter.
- The proposed work is not descriptive enough. It appears to be a shopping list of topic areas with no description of the approach to solving or defining future tasks. For example, it is not clear what the project is going to flow-model.
- More industrial involvement is essential for this project to have any value.

Project strengths:

- The DOE laboratories are uniquely positioned to perform this work, as they have the resources and expertise, the work is not being done elsewhere, and the topics are pre-competitive and beneficial to multiple vendors. The cost impact of the various processes is key to their evaluation. The cost projections are very much appreciated and should be included even more in future work.
- The project team has five national laboratories with broad, comprehensive capabilities. The R2R approach seems to be technically successful thus far. The cost model shows a potential of 63% cost savings; it would be beneficial to see the cost breakdown or savings realization based on the current project status.
- Good progress has been made on improving MEA performance and understanding of the mechanism.

- The project team has good capabilities in processing and characterization.
- The project's strengths include the talent and capabilities of the team.
- The cooperation of all the national laboratories is a strength of this project.

Project weaknesses:

- The cost of the over-layer may be overstated in that (1) its net additional equipment cost may be low if the coating station is added to an existing process train, rather than being a stand-alone process, and (2) it may be desirable to lay down the membrane on a wet over-layer rather than a dried overlay (and this may eliminate the hot-pressing operation).
- A weakness of this project is that there are no fuel cell MEA manufacturers participating in the project. Proton OnSite is a manufacturer of electrolysis equipment.
- The overall objective of how the project advances the DOE Fuel Cell Technologies Office mission is a bit unclear.
- The team's goals do not seem to make economic sense. The current roll-speed costs are not significant, and neither is the cost of adding an ionomer overspray.
- The project's weaknesses include a lack of industrial involvement.
- The future work should address defect detection and process control.

Recommendations for additions/deletions to project scope:

- The project team should include specific cost analysis for each examined process. The team should explore the upper speed of each process, recognizing that the optimal line speed may be determined by economics (as high line speed may lead to long dryers and high capital cost).
- The project should add in-line process control and defect detection. The team should update the cost model based on the current process and set priorities based on future savings potential.
- The project would have a greater impact if a fuel cell manufacturer would participate in the effort.
- Broader participation by industry is needed.

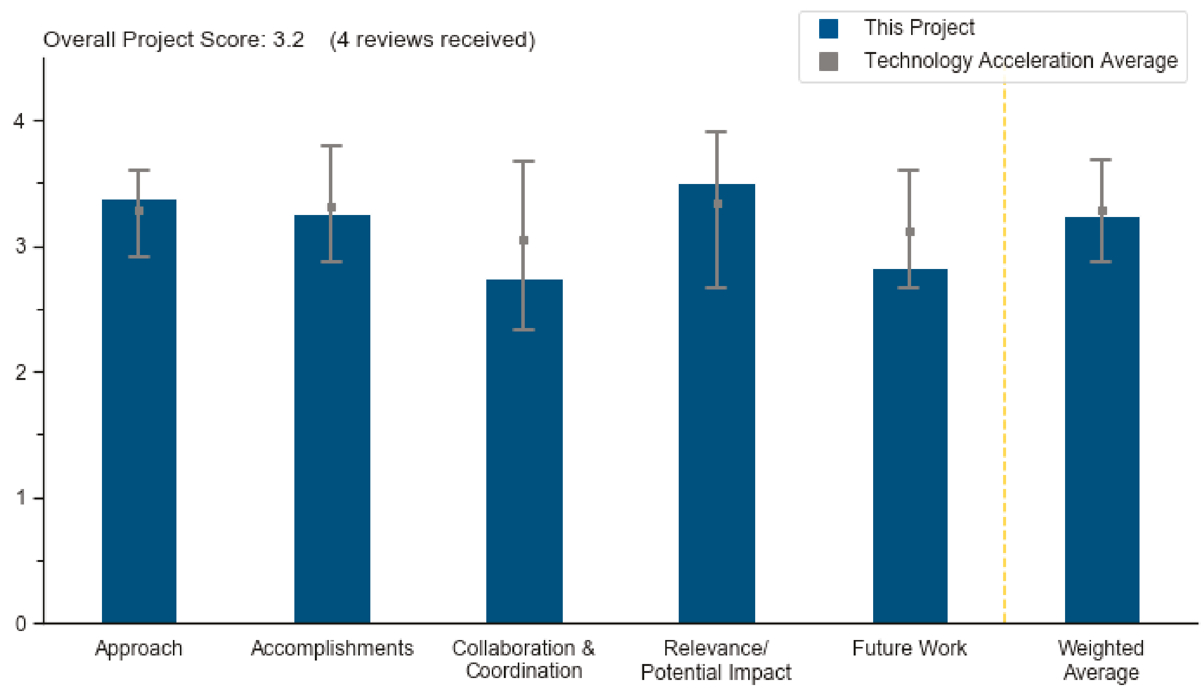
Project #TA-008: Material–Process–Performance Relationships in Polymer Electrolyte Membrane Catalyst Inks and Coated Layers

Michael Ulsh, National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to study the material–process–performance relationships for roll-to-roll (R2R) polymer electrolyte membrane fuel cell (PEMFC)/electrolysis cell materials to understand the coupling between process science and material properties and performance. The project team seeks to understand the impacts of ink formulation, coating and drying physics on ink microstructure, coatability, film morphology, electrochemistry, proton conduction, and mass transport. The project team accomplished the following tasks: (1) determined that slot-die coating results in higher-performance membrane electrode assemblies (MEAs) than gravure coating, (2) related catalyst ink microstructure to electrode microstructure, (3) improved methods for dynamic light scattering and zeta potential to better understand catalyst–ionomer interactions, and (4) initiated work on electrode cracking, showing that microporous layer cracks can induce catalyst layer cracks.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- A systematic approach is being used to assess different ink formulations and coating processes, with a good mix of materials and coatings characterization and electrochemical performance testing.
- The project's approach is good: to study how ink behavior relates to manufacturing processes and ultimate fuel cell performance.
- The individual pieces and the approach to quantifying and improving ink and electrode methods are promising.

- The approach is solid and instructive to the community. It would have been good if the team had done some fairly simple experiments to determine the amount of ionomer coating on the catalyst. Determining whether the isotherms change based on the solvent system will really give insight into what is leading to performance differences.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Given the limited amount of funding, it seems like this project has made much progress. Good correlations are being made between coating process, coating morphology, and electrochemical performance. What seems to be missing is research into explaining the "whys." For example, it was observed that electrochemical performance was better with slot-die coatings compared to gravure coatings, and this was correlated to morphology differences. It should be made clear whether these are differences that are intrinsic to the coating process or whether they are due to coating inks being more or less optimized for one process compared to another process.
- The project did not have any targets or go/no-go decision points, so it is more of a supporting analysis of the catalyst inks project.
- The project progress is good, but the need is less clear. The original equipment manufacturers and electrode manufacturers have excellent electrode knowledge; it is not clear that the national laboratories should be trying to develop this knowledge.
- The project's progress is impressive compared to the budget but not at all impressive compared to the start date; it is hard to see how this took two years.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- The level of collaboration on this project is exemplary, especially given the limited funding.
- There is not much industry interaction. The team could use more industry interaction on the inks; however, this could be an intellectual property issue.
- It is not completely clear what the other organizations did. It is also unclear how $200,000 was divided among the partners, or that it was very effective.
- It was not clear what, if any, of the work presented was in support of projects.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project supports the development of low-cost, high-yield manufacturing processes that will be essential to the long-term commercialization of PEMFCs.
- This is good, practical work that many groups will find useful. To make it more useful, more characterization to understand the differences the team is seeing will be needed.
- The project showed how important the ink parameters are to fuel cell performance, and also how unexpected simple adjustments on ink deposition techniques can have a large impact on performance. More study should be done here.
- Since improving electrodes and manufacturing is a goal for DOE, this project is well aligned and effective, especially considering the small funding level.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- While the approach is great, the performance is still so much lower than fuel cell state of the art that relevance is hard to judge. However, for electrolysis and platinum-group-metal (PGM)-free fuel cells, this seems to be a more valuable effort.
- The proposed work makes sense, but no additional funding appears to be planned for this project.
- It appears that the proposed work on PGM-free inks would be taking place too early to study any of the manufacturing aspects of these catalysts, as they are not at the technology readiness level needed for manufacturing.
- The team talks about working with K.C. Neyerlin to help understand the differences in performance. It is not clear how this work would be funded.

Project strengths:

- The project's strengths include the quality of the work, the connection of measurable characteristics to observed and measured performance, good higher-level analysis, and consideration of R2R issues.
- There is a focus on process and property relationships, with appropriate materials characterization being used to support interpretation of the results. The team is also collaborating with other national laboratories that have unique capabilities and with end-user companies that can benefit from the results of the project.
- The team shows good characterization of several different ink systems.
- The project demonstrates the large impact of the interaction of ink properties and application methods on performance.

Project weaknesses:

- The project's weaknesses include the lack of scope or follow-through. In all honesty, the work is quite good, considering the budget, but much more could have been done. It is not clear how the team worked together. There are many MEA characterization methods that are readily available to this group and that could have been used to try to discern the differences in performance from the various inks.
- The poor fuel cell electrode performance casts doubts on the conclusion's relevance to fuel cells. The project's connection to other efforts is unclear.
- Better industry interaction would be useful.
- The project has insufficient funding.

Recommendations for additions/deletions to project scope:

- It would be great to see the isotherm work on the catalyst inks as a function of ionomer loading and how that varies with the solvent system. It would also be good to see MEA characterization, especially mass transfer analysis and impedance, to determine what is going on with the different inks and methods.
- Focusing on electrolysis and PGM-free catalyst systems seems like a proposition with higher added value, as the electrode structures for those are less well developed and the need is there. Better integration with existing projects may be helpful. The integration is in progress but was not reported.
- This project should be continued, or a similar scope should be added to future projects.
- The project team should add more industry interactions.

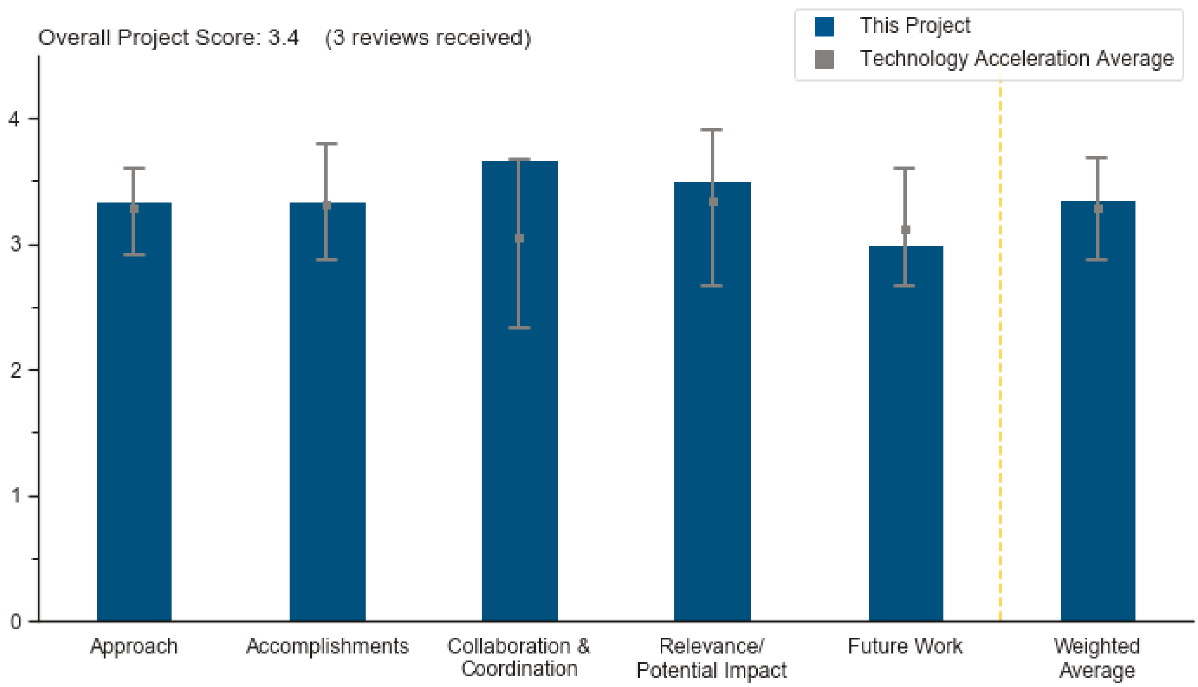
Project #TA-009: Maritime Fuel Cell Generator Project

Lennie Klebanoff, Sandia National Laboratories

Brief Summary of Project

The overall objectives of this project are to (1) lower the technology risk of future maritime fuel cell deployments by providing performance data on hydrogen polymer electrolyte membrane fuel cell technology in this environment, (2) lower the investment risk by providing a validated business case assessment for this and future potential projects, (3) enable easier permitting and acceptance of hydrogen fuel cell technology in maritime applications by assisting the U.S. Coast Guard and the American Bureau of Shipping with developing hydrogen and fuel cell codes and standards, (4) act as a stepping stone for more widespread shipboard fuel cell auxiliary power unit deployments, and (5) reduce port emissions with this and future deployments.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is very sound, including upgrading the unit to provide 480 VAC to meet Scripps Institution of Oceanography (SIO) requirements and ensuring that the unit and its operation meets all other local requirements.
- The approach identifies the objectives and barriers, is well designed, and appears feasible.
- The project's strategy shifted from reefers to ships at dock. It is unclear how power requirements break down, how many reefers can be powered from one fuel cell container, or what the limitations are for a ship at dock.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has significant accomplishments and appears to be able to demonstrate the use of fuel cells to power the SIO vessel. However, it is not clear what concrete steps are being taken to lower investment risk and to enable permitting. Perhaps certain stakeholders are on board and willing to move forward with regulatory documentation.
- Progress included exploring the Curtin Maritime site at the Port of Long Beach and the SIO site in San Diego for test deployment, as well as upgrading the unit to meet deployment needs at the SIO.
- It is not clear how the project is addressing the identified objectives from slide four: lowering technology risk and investment risk and improving permitting acceptance.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- The project has good partners for the execution. Although it did not work out, having Curtin Maritime and the Port of Long Beach on the team is a good partnership to better understand issues and site requirements. The SIO partnership will provide a good collaboration.
- Collaboration and coordination among the existing partners is outstanding, as seen in the progress discussed at the Annual Merit Review.
- It is apparent that the project is coordinating with other institutions.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- It is important to show that fuel cells and hydrogen can compete in a few stationary applications to maintain the overall Hydrogen and Fuel Cells Program’s momentum. Mobile refueling with hydrogen will be part of the planned test deployment. The benefit of gaining experience and engaging technology providers, regulators, and a real ship-docking site will be very valuable.
- Using the fuel cells in this application will help advance use in onshore power applications.
- The project clearly addresses a need.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- At this stage, it is very good that the project is also geared toward exploring the possibility of future host sites because test deployment needs to continue to accelerate user acceptance.
- There might be applications for the U.S. Navy for offshore power, or perhaps there are other research vessels or similar stakeholders that might need something like this.
- The future seems unclear. It would be good to know what the possible user demand for this technology is and how rules and regulations might impede its use.

Project strengths:

- This project requires understanding the host site's needs and a good deal of coordination. There is very good collaboration seen among partners, which resulted in timely upgrading to meet the host site's needs and the timely evaluation of potential showstoppers that could delay the deployment.
- The project's strengths include the team's flexibility to find the SIO after it was found that site requirements for Curtin Maritime setback regulations do not work. Using a 20-ft Container Express (CONEX) for these purposes is modular and a good fit.
- The project provides a solution to a specific need. The project addresses energy concerns both onboard a ship at sea and at dock.

Project weaknesses:

- This is an observation and not a weakness because the cost of hydrogen is not within the project scope: it would be good to develop a plan to secure lower-cost hydrogen supplies over a number of years, if this is possible at all.
- It would be good to show data statistics and/or a summary that highlights the effectiveness of the fuel cell, whether it has been running for one day or one week.
- The project was originally targeting reefer containers onboard ships. There are several questions, including whether there are different rules and regulations aboard ships that might interfere with technology adoption, how many reefer containers one of these units can power, what the lifespan of the unit is, whether there is an ideal type of ship that this unit might serve while at dock, and how scalable the technology is.

Recommendations for additions/deletions to project scope:

- It would be nice to know how many of these units might be needed to power reefers on a container ship, as well as what the ideal ship to be powered while at dock is. A better understanding of where the technology fits would help with understanding the potential range of application.
- Until results are available from this hoped-for host site, there is not really a need to modify the scope.

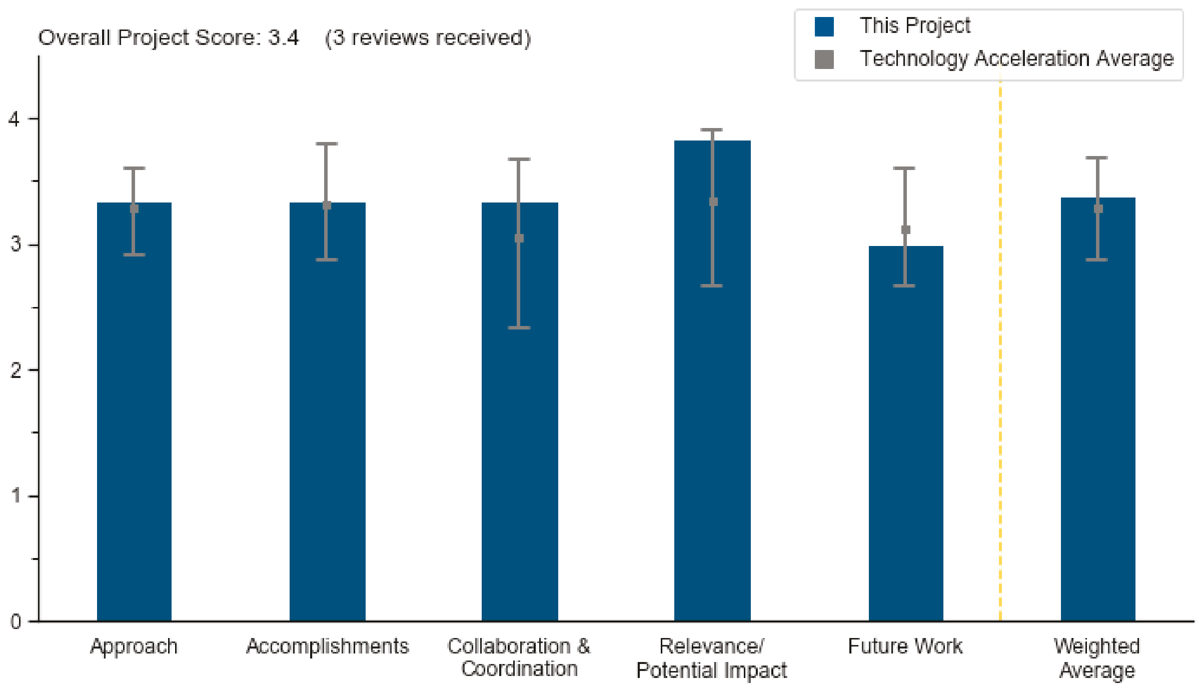
Project #TA-011: FedEx Express Hydrogen Fuel Cell Extended-Range Battery Electric Vehicles

Phillip Galbach, FedEx Express

Brief Summary of Project

This project will demonstrate hydrogen and fuel cell technologies in real-world environments. Fuel cells are being integrated into 20 battery electric pickup and delivery vehicles. Those trucks will operate 10-hour shifts, 260 days annually, amounting to at least 5,000 hours per truck for a total of 100,000 hours over 1.92 years. The project is expected to reduce diesel consumption by 100,000 gallons and prevent 270 metric tons of carbon dioxide.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach was a green, renewable, and sustainable technology, but it is a bit hidden in the presentation (see chart 3).
- The approach was identified at a very high level. How the efforts are going to be accomplished and who is responsible for accomplishments is not obvious.
- The project objectives are clearly identified. The critical barriers may not have been adequately addressed. Non-fuel cell maintenance issues have had a significant impact, and planning for maintenance facilities for 20 vehicles appears to be a late consideration.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The systematic demonstration of modification of delivery trucks, training of personnel, and testing of vehicle and power train requirements were achieved. The problems with the fuel cell system observed during testing and the impact on availability were addressed and resolved. The initial design issues with direct current (DC)-DC-convertor placement were resolved.
- All that was done was useful in meeting the goal of fleet experience with a fuel cell battery combination.
- The project is slipping its timelines, and there does not appear to be ample time to build and deploy the remaining 19 vehicles to meet the 2021 deadline.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The interaction with Plug Power was reported to be outstanding. The data release to the National Renewable Energy Laboratory was reported with no problems identified. There appears to be a problem within FedEx regarding the responsibility of using delivery trucks at longer distances from home base.
- There appears to be good coordination between partners, with the exception of the battery/electrical system provider.
- There appears to be little coordination between the plug and truck manufacturer with regard to the convertor.

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The commercial demonstrations are critical, and the FedEx and Plug Power effort is outstanding.
- If the project team is able to address maintenance and reliability issues to support the build-out of the remaining 19 vehicles, there could be a great benefit to the DOE Hydrogen and Fuel Cells Program (the Program).
- The project includes real delivery routes driven by actual users.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed future work is fine, but there was no indication of how the project team would solve the critical issues.
- The presenter gave a shopping list of future work with no discussion of approach, potential difficulties, or means to resolve future issues.
- The maintenance issues seem to have put the future plans in jeopardy. Without the demonstration of the remaining vehicles, the project's overall value and impact on the Program are greatly reduced.

Project strengths:

- Both Plug Power and FedEx are strong companies for this demonstration.
- It appears that the fuel cell system has performed well.
- The overall strength is the project management by an actual user and planned use in actual driving routes.

Project weaknesses:

- Maintenance issues with the non-fuel cell systems have had great impacts on the project and its future. It is uncertain whether this could have been avoided by better planning and failure mode and effects analysis (FMEA) activities.
- A project weakness is the high employee turnover rate.

Recommendations for additions/deletions to project scope:

- The project is well organized, and there is no obvious need for additions or deletions.
- Regardless of whether the project continues building the remaining 19 vehicles, it would be beneficial for the project team to thoroughly consider and evaluate the learnings from their activities. A report or other documentation from this project could be of great value for other projects in the future. For example, it may be beneficial for an FMEA to be performed, thus enabling a project team to be better positioned to deal with the failure of less reliable or long-lead-time parts.
- The positives and negatives should be identified. It would be helpful if FedEx could clearly mark the presentation figures in future presentations.

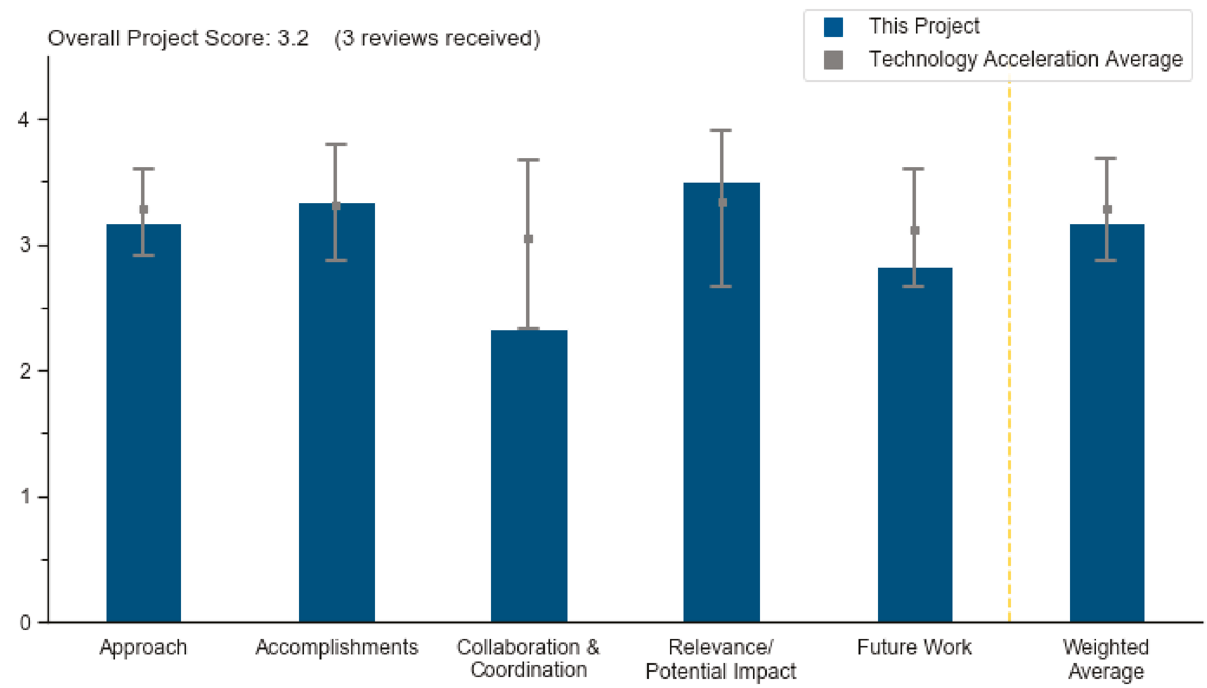
Project #TA-012: Northeast Demonstration and Deployment of FCRx200

Abas Goodarzi, US Hybrid

Brief Summary of Project

The project's objectives are to (1) design, develop, test, and demonstrate one fuel cell range-extended plug-in hybrid utility vehicle (FCRx200) at a commercial operator's site; (2) given the success of the initial prototype, receive approval to proceed with fleet development to deploy and operate a minimum of 20 FCRx200s for at least 5,000 hours or 30 months per vehicle, whichever occurs first, at the commercial operator's site; and (3) conduct an economic assessment, a payback analysis, a life-cycle cost analysis, an incremental capital cost per unit analysis, a fuel savings analysis, and a payback time analysis (concerning the use of hydrogen-fueled fuel cell range extenders in commercial fleets), as well as analysis of comments from the operator detailing the experience during operation. The economic assessment will be facilitated using data collected and submitted to the National Renewable Energy Laboratory on a quarterly basis. Upon project completion, the team will be able to make recommendations on the marketability of the FCRx200 vehicle.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The objectives and critical barriers appear to have been considered.
- The approach to work is good, except the project lacks a definition of the role of National Grid and does not make clear who would benefit from the extended range of battery vehicles.
- The principal investigator listed four factors for Approach/Scope that give specifications for components. There was no discussion on interfacing the fuel cell with the battery system, beyond a statement it will be done.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The accomplishments appear consistent with project objectives and DOE goals.
- The project shows good progress toward goals, except that Phase II is in doubt because of the lack of a Phase I vehicle.
- There was not much discussion about accomplishments in the presentation or the handout. The team completed a safety plan. There are problems with Nissan changing the vehicle and the fact that Nissan does not plan to deploy the FCRx200 vehicle in North America. The Summary slide states that the integration of the fuel cell range extender and the storage and fueling interface were completed.

Question 3: Collaboration and coordination

This project was rated **2.3** for its engagement with and coordination of project partners and interaction with other entities.

- A good project team has been utilized.
- It is late to find out the vehicle will not be offered in the United States.
- Unfortunately, the collaboration with Nissan appears not to be going well: “No plan for [original equipment manufacturer] (OEM) to deploy vehicle in North America.” US Hybrid reports Phase II of the project has a high risk, primarily because of the OEM’s lack of support. Fueling infrastructure in the Northeast has been limited, and while this is not the responsibility of this project, the project depends on it. Limited fueling infrastructure could be the reason Nissan is no longer supportive.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project makes good innovative use of fuel cells, such as use as a vehicle heater.
- If the project team is able to complete Phase II, it could have a good impact on validating the technology for broader use.
- Demonstrations of fuel cell vehicles are critical to the technology’s moving forward.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The team did an excellent job of identifying future work needs, but how the future work will be executed is a problem.
- The proposed future work in the presentation identifies only work in 2019. Additional information should be provided on specific activities planned for the remainder of the project term (i.e., through 2022).
- There is no workaround for the lack of a Nissan vehicle.

Project strengths:

- The excellent use of fuel cell as range extender and heater is a project strength.
- US Hybrid is a strength; the company has a commercially available fuel cell system that has been demonstrated in the Nissan vehicle and versions of the fuel cell system operational in buses.
- This is a good project team, and learnings in early project activities are being applied.

Project weaknesses:

- The presenter stated that the safety plan will be provided to the Hydrogen Safety Panel (HSP) after the go/no-go decision (as stated, this was necessary to ensure that all players, including operators, are included). While it is good to have all project partners involved in safety planning, providing the plan to the HSP for review at such a late date (and considering there has been no other interaction with the HSP) could result in safety issues being identified too late to be easily or cost-effectively addressed.
- Nissan or another OEM is needed to complete this project. If a new OEM joins, that action will extend the project for at least one year.
- There are no plans for Phase II.

Recommendations for additions/deletions to project scope:

- The project needs an active OEM to move forward. DOE should assist US Hybrid in identifying an OEM to complete the effort.
- The project team should think about utilizing “used” Nissan vans for Phase II.

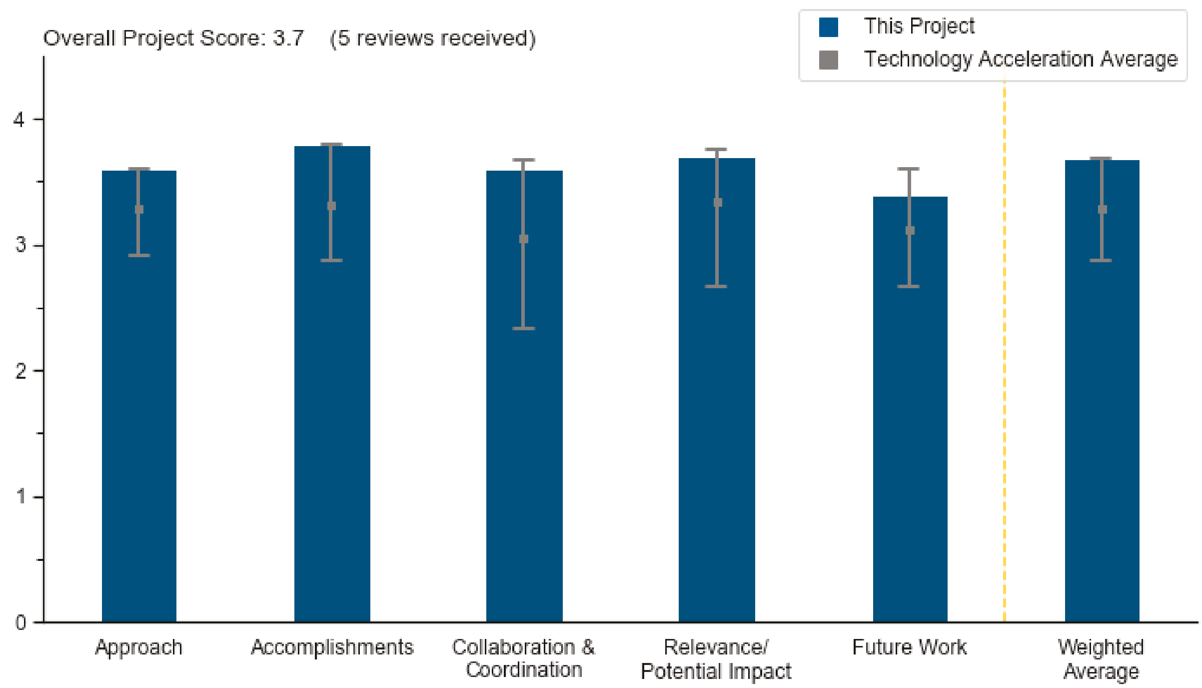
Project #TA-013: Fuel Cell Bus Evaluations

Leslie Eudy, National Renewable Energy Laboratory

Brief Summary of Project

The objectives of this project are to validate fuel cell electric bus (FCEB) performance and cost compared to U.S. Department of Energy/U.S. Department of Transportation targets and conventional technologies and to document progress and lessons learned on implementing fuel cell systems in transit operations. Annual FCEB status reports compare results reported from transit partners and assess progress and needs for successful implementation of FCEBs, addressing barriers to market acceptance.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The principal investigator (PI) has assembled an excellent cross-section of technologies and is sensitive to removing technology that is not relevant (e.g., prototype and/or demonstration units). The data are defensible and presented well and will help the industry identify the parts of the drive train that most need improvement (such as isolating the fuel cell power plant from the rest of the drive train). Others in the community (notably the California Hydrogen Business Council Heavy Duty Strategic Action Group) have proposed to perform such a study for the heavy-duty (HD) market, comparing fuel cell electric vehicle (FCEV) zero-emission vehicles (ZEVs) to standard technologies. In this way, this study’s value and relevance to the community is already being demonstrated. Many in the community seek comparative studies to use as educational material introducing hydrogen fuel cell technologies. This study provides that defensible, unbiased, well-thought-out, comprehensive data and analysis that are being sought. The approach for this work is very good, making the results defensible, credible, and important to the community. Overall, this is a nice project.

- The approach of gathering, processing, and reporting data from multiple demonstrations provides tremendous value. In this case, particularly in the areas of fuel cell power plant (FCPP) durability, maintenance hours and costs, and fuel cost, the project is turning out excellent value; and the long timeline allows for a significant body of data that gives good confidence for the progress needed to reach milestones.
- The approach is sound. The focus on refreshing the data is great, given that the technology is changing rapidly during the course of the study.
- The overall approach of the work is presented well. It is recommended that the wording on slide 4 be simplified to be clearer and more concise.
- The approach seems appropriate.

Question 2: Accomplishments and progress

This project was rated **3.8** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- This project continues to provide valuable timely analysis tracking the performance of FCEVs and comparing them to each other and conventional technologies. The accomplishments and progress are in line with the growth and deployment of the FCEV technologies. Equally important is that this PI keeps the suite of technologies in the sample consistent with what is realistically expected to be deployed. This is nicely done.
- It is quite difficult for a project that has access to a wealth of data and has been going on for many years to continue to share useful results and prioritize key takeaways; this team continues to be successful at overcoming this challenge. The results of this work are routinely referenced in the field and help drive innovation for other non-light-duty fuel cell mobility applications. There are a few suggestions to further enhance the results. (1) The project should combine key data categories to generate insight into the total cost of ownership (TCO). Bringing together the upfront costs, fuel costs, and maintenance costs would be very useful when compared to other technologies. 2) If possible, the team should share additional insight regarding bus fueling (fueling and charging times, how to achieve lower-cost hydrogen, fueling infrastructure costs, etc.).
- The accomplishment of having durability exceed the ultimate target of 25,000 hours is impressive. In addition, the project has been able to adapt as the fleets have evolved to continue to provide data relevant to the current state of the technology. The project has also been able to move from demonstration mode to providing data relevant for early commercialization.
- Understanding real-world applications and barriers is essential to DOE objectives, as it allows for the right focus for several other investment directions.
- The accomplishments are very good and useful; however, to make the data more useful, the team should consider the following. (1) The overall FCEB cost per mile does not seem to be an accurate enough comparison to the baseline bus cost per mile, as indicated in the note found in the presentation that states, “Not all are equal comparisons.” If possible, the team needs to improve this accuracy. (2) For the Stark Area Regional Transit Authority buses, the baseline is “[compressed natural gas]/diesel hybrid.” Since those are really two different baselines, the baseline comparison should be split into two. (3) On the “Hydrogen Cost Data Summary, $/mi” slide, including the number of buses in the FCEB fleet and the baseline fleet would allow the reader to make a judgment on accuracy based on sample size.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- This is a perfect assembling of entities for collaboration and coordination. This group of collaborators collectively represents operators and original equipment manufacturers, providing a good cross-section of entities encompassing the bus transit sector of the public transportation sector.
- The project effectively manages collaboration among four stakeholder groups representing public transit agencies and companies involved in building and integrating FCPPs, battery suppliers, bus service providers, and hydrogen fueling station operators.
- The quantity of data received demonstrates the project's good coordination with relevant stakeholders. The team is also encouraged to engage with key infrastructure stakeholders to better understand their perspective for fueling bus fleets (either at a dedicated depot or at retail stations). This may fall outside of the current scope, but fueling operations and costs are major aspects of bus fleet operations that could be better understood with more input from infrastructure companies.
- The following are suggestions for future collaboration and coordination: (1) The current participation is in California and Ohio, which is not a bad representation of two different climates; however, eventually it would be good to get more severe climates (e.g., cold and hot and humid). (2) It would be good to get feedback from the drivers that utilize the buses and the technicians that service them so that they can share the positives and negatives from their perspectives, versus those of the baseline buses.
- Collaboration with the studied fleets is critical to the project. It is not clear that other research organizations should be involved.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- At the current stage of deployment of FCEVs (e.g., light-duty, material handling, HD, maritime, etc.), studies like this one are critically important for benchmarking the technology and highlighting the maturity and potential compared to conventional technologies. Much education is still needed with the public and with policymakers, among others, to demonstrate the value and potential for FCEV technologies to take their place in the ZEV sector. This study (and other like studies, which are to be encouraged) goes a long way toward providing defensible evidence on the performance of FCEVs, which can be used to educate those sectors of society that need to deploy, use, and make policy about them. This project is perfect for providing defensible arguments to the stakeholders. As such, the impact of this work is huge.
- The project has a high degree of relevance, not only in the areas of operational and cost metrics for the buses themselves but, perhaps more importantly, as an early source of operational and cost data for emerging medium-duty (MD) and HD applications that have central fueling.
- Understanding real-world applications and barriers is essential to DOE objectives, as it allows for the right focus for several other investment directions.
- This is a highly impactful project with minimal investment required. The project is well done.
- From the presentation, it was clear that some of the FCEB targets are already being met, which is fantastic news; however, it was not clear from the presentation what the baseline buses' comparative targets were for lifetime, availability, etc. Perhaps they are the same as those in the "ultimate target" column, but this was not clear.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work is a perfect natural growth of the existing work. This project was not scored a 4.0 because this exact approach and effort should be extended to other HD applications, such as Class 8 HD trucks (e.g., long-haul and drayage Class 8 vehicles, as well as smaller Class 6–7 vehicles), material handling, airport handling, and portside applications. This is an extremely important activity and needs to extend beyond buses.

- The opportunity to add additional fleets will keep the data being reported by the project fresh and allow for trends to be seen as the technology and operation of FCEBs mature. It would be beneficial to see more emphasis and analysis on true "all-in" fuel costs and per-mile cost comparisons.
- Obviously, continuing the data collection is key, and the desire to expand the scope to include fuel cell truck projects is also appreciated. This will be of great interest in a rapidly growing market. It is also suggested that the team more deeply consider the fueling infrastructure component of the value chain, given the huge impact that it has on the TCO for commercial operations.
- Understanding the infrastructure costs, various scenarios, and how they scale is critical to identifying the barriers to adoption.
- The proposed future work looks good and appropriate. The focus, of course, needs to be on attaining a larger sample size and more data on baseline buses for comparison.

Project strengths:

- The project's strengths are (1) that it has already quantified the comparison between FCEBs and the baseline buses and (2) that it has shown that the fuel cell stack seems robust and that it is the balance of plant (BOP) and other propulsion-system reliability issues that need focus. On that note, perhaps there should be some funding programs to drive improvements in those areas.
- The project has a systematic approach to gathering data and a very thoughtful analysis of the data. The alignment of the cumulative costs of maintenance to the introduction date was very well done and very pertinent to the study's objective.
- This is a highly impactful and referenceable project that demonstrates the successes and remaining challenges for FCEBs. The value of this project is considerably higher than the limited allocation of DOE funds that is required.
- The project's strengths include its significant sample size and solid, long-term relationships with the project partners.
- This is a very important activity, well-conceived and well executed, with demonstrated value to the community.

Project weaknesses:

- It can be challenging to bring new ideas to reoccurring data collection projects and maintain focus on presenting the key results. This project is effective at sharing major updates, but there is still more that could be done to address key questions for industry and potential future operators. A stronger focus on overall TCO will have a greater impact beyond studying each element of cost separately.
- The activity needs to be extended to other emerging applications being pursued in the community, including those in Class 8 HD drayage, long-haul trucks, HD material handling, maritime (on- and off-ship), and airport ground support.
- The project's weakness include the following: (1) The comments saying that the fuel cost comparisons are not all equal makes it difficult to compare. (2) Furthermore, the comparison of the FCEB fuel costs to baseline buses should be improved. This should perhaps even be done in an appendix to the presentation for those who want to see the detail behind the comparison so that it is a thorough, apples-to-apples comparison. (3) For propulsion system issues, it would be good to itemize the ones that are required for the fuel cell system versus the ones that are due to the electric propulsion system to differentiate these two challenging areas. For example, it is not clear whether cooling system leaks are due to the cooling system for the fuel cell system or the electric drivetrain. If the leaks are tied to the fuel cell system, even though the fuel cell stack seems reliable, this means that its BOP is not reliable and needs to be improved. On the other hand, if the leaks are tied to the electric drivetrain that is commonly seen in a battery electric bus or hybrid bus, then it is a common reliability issue between these clean transportation propulsion technologies and is worth quantifying further. In the end, it still stacks up against the reliability of the FCEBs; however, it will help quantify how much work is required to improve the reliability of the fuel cell system and its BOP versus that of the other systems, such as the electric drivetrain, that are common with other propulsion technologies.

Recommendations for additions/deletions to project scope:

- It would be useful for the project team to do the following: (1) The team should better quantify durability and reliability and separate them into different bins, such as fuel cell and BOP versus the electric propulsion system, which can be considered a separate technology since battery electric and hybrid electric systems also use it. (2) The team should consider the emissions differences when using FCEBs versus the baseline technologies. (3) The team should determine the other technologies and challenges that must be addressed in order for FCEBs to be successful, as well as any advantages an FCEB would have over other technologies. For example, air conditioning on an FCEB or battery electric bus will have a significant electrical demand. It should therefore be determined whether this is an area that needs technical advancements to improve efficiencies or reliability, as well as whether an FCEB would have more range or reliability, since it is consuming hydrogen to create the energy to run the air conditioning system. This technology is versus a battery that must be plugged in to recharge and that uses a considerable amount of the electric bus battery's energy while in use.
- It would be beneficial to see additional detail related to fuel costs, including capital and operations and maintenance costs per kilogram and per mile for the FCEBs. These data will help in understanding the true comparison with competitive propulsion technologies and in understanding the commercial landscape for developing a fueling infrastructure for future MD and HD fleets.
- The project team should focus on showing total TCO from the data already collected today and expand data collection as needed to accomplish this. The team should also engage closely with infrastructure providers to capture their perspective and insights into the station side of the business.
- Understanding the infrastructure costs, various scenarios, and how they scale is critical to identifying the barriers to adoption.
- The project team should expand the scope to other emerging applications. This project should be kept funded.

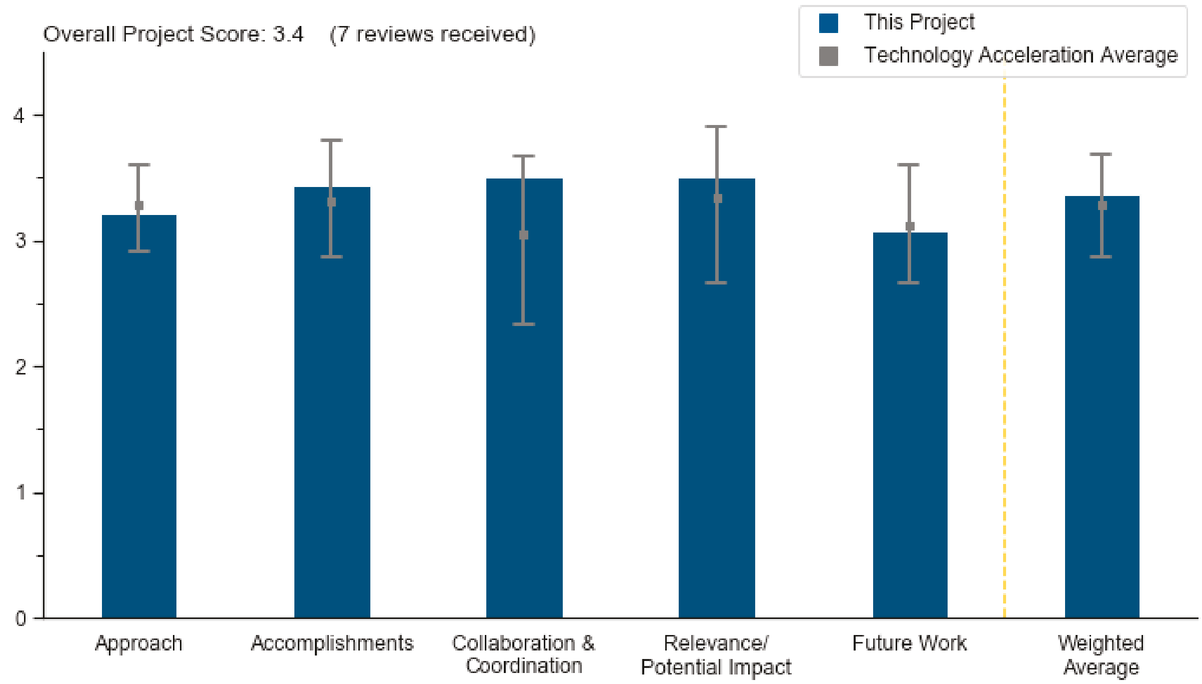
Project #TA-014: Hydrogen Station Data Collection and Analysis

Sam Sprik, National Renewable Energy Laboratory

Brief Summary of Project

This project evaluates hydrogen infrastructure performance, cost, utilization, maintenance, and safety. Data analysis supports validation of hydrogen infrastructure, identifies status and technological improvements, provides feedback to hydrogen research, and provides results of analyses for stakeholder use.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The overall approach is good, and it is good to see the project leverage the existing California Energy Commission (CEC) agreements to access data. In addition, the project tends to look continuously for new ways to analyze and synthesize the data it receives, which is a strong point. Finally, the new work on queuing is unique and directly addresses a data gap that has been an issue for governments supporting station development and needing to be well versed in operations. Since this aspect of the project has looked at only a couple of stations so far, it should be expanded so that those running the project can develop insights through more significant levels of supporting data. However, the tie to the CEC is too strong and is thus a weak point because the project has not identified a way to continue to receive data independently of CEC contracts. The project may need to find a way to garner support and participation from station operators on its own.
- Using actual California station data to evaluate performance is a very good approach to understanding and categorizing station reliability. This data is most likely the best set of aggregated data for doing this analysis. It is encouraging that the team focuses on the most utilized stations to identify reliability issues.

- The investigators have done a good job of accessing data from California stations and earlier infrastructure projects. The investigators have produced a wide variety of data products.
- The data collection methodology follows a comprehensive approach while data analysis explores a set of key performance indicators (KPIs) crucial for assessing the performance of the hydrogen refueling station (HRS). Queuing data and analysis is a novel element added to the analysis last year. It should be expanded to more stations based always on the availability of monitoring equipment. No information is provided on the template questionnaire used for collecting information as well as the frequency of updates.
- While the objectives are clearly identified, the project could be improved by better understanding who is using the data and how it is being used. If the lack of data is the high-level barrier, then the team should have some insight into why that data is needed.
- Drivers are notably absent from the evaluation. The approach should be extended to include their experience of stations. It might be difficult to organize such a study, but it could prove extremely valuable. In the end, the success of hydrogen fuel cell cars is dependent not just on consumer buy-in but on consumers' buying cars.
- The project is an ongoing effort, but the number of KPIs could be reduced.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project collects a series of KPIs aligning with and serving DOE's main goals. The amount of hydrogen dispensed, availability, maintenance, and a number of other important parameters are covered. Further analysis is also provided to investigate the roots of downtimes and various interlinking indicators. As the source of origin for hydrogen is gaining importance, the identification of green hydrogen sources could be considered as part of the questionnaire. This and other similar analyses contribute to the technology and also program monitoring while comparing results with the Hydrogen and Fuel Cells Program targets. However, no information is provided on whether HRSs have fulfilled their targets and commitments.
- The project team's collecting data from station operators is excellent. The data presented and its analysis are extremely relevant. For example, it is nice to see, with the reduction in dollars-per-kilogram maintenance costs, that station design and operation are reaching a certain level of maturity. It was surprising to see the percentage of incidents related to the dispenser versus the compressor; it would be good for the project team to spend time analyzing this in more detail.
- The analyses that have been developed beyond the standard summary composite data products are outstanding. The queuing investigation detailed availability analysis and fueling behavior trend analysis are particularly insightful and useful right now.
- The accomplishments during this period were good and start to provide a good picture of the status of fueling technology in an early-stage market. This work should set the stage for further development needs, either through new project funding or leveraging existing work (i.e., hoses, nozzles, and technologies to help manage queuing).
- The data compiled is the best available set of real-world data describing infrastructure operations.
- While the project has shown a rapid growth of stations overcoming many commercial barriers, the fact that the contract for data collection has run out with one data provider renders the data set less representative of commercial use of hydrogen.
- The purpose of this effort is to use data for future innovations and research, but most of the data is based on existing operational equipment, which is several generations behind on current technology (and status of technology development). It is increasingly unclear how this data is valuable to facilitating future innovation and directing research efforts.
  - Regarding the queuing model, no benchmark has been identified for the project, so unless one was established (perhaps gasoline), this should be abandoned because it is a waste of taxpayer money.
  - The "missed fuel opportunity" is not needed. Station operators are aware of the impact of this on their revenues (even in a pre-commercial market).
  - The team should consider removing the Air Products $9.99/kg initiative that tried to see whether the market would respond to lower fuel costs. When this did not make a significant difference, Air

Products raised prices back up to previous levels. Removing this anomaly from the data provides a better reflection of fuel pricing (or digs into what actual margins or cost components are).

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The project brings in a relevant suite of stakeholders. In addition, it is good that the project looks beyond just the station developers and the government funders. Including other public–private or similar organizations should help the project maintain relevance with the information needs of the broader industry and ensure that the developing U.S. hydrogen fueling market is one of the most well-informed global markets, with actual in-service data.
- The CEC made National Renewable Energy Laboratory (NREL) data collection a requirement for those HRS operators receiving California state funding and is paying NREL to collect data. Collaboration and coordination appear to be sufficiently broad.
- Collaborating with California and station providers is an excellent method.
- The project collaborates with a large and highly relevant group of California stakeholders: the representatives and leaders of the hydrogen/gas industry. The project did not explain why several station collaborators are no longer reporting data and whether they will be approached to continue for the next year.
- The investigators have worked well with the California infrastructure project. The investigators may need to be more proactive in working to ensure continuing data access where mandatory reporting has ceased.
- The project collaborates with the California Fuel Cell Partnership effectively, as well as with the individual refueling station operators to collect data. Nevertheless, international collaboration would be advisable through a comparative analysis for benchmarking and considering a number of publicly available KPIs. In addition, in cases where there is lack of data, more effort should be put on accessing or retrieving missing information for the sake of a robust analysis. Although already partially conducted (gasoline stations), the project team could attempt collaborating with conventional fuel refueling stations to compare similar KPIs.
- As stations in the Northeast are rolled out, it would be interesting to reach out to the operators of these new/future stations to perform the same type of data collection and compare with experiences in California.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Data collection and analysis is an essential element for providing key statistics and conveying messages about the performance of key applications. In this respect, this project, while focusing on HRS KPIs, reveals key results from the operation of the refueling stations. This, alongside a more inclusive overview and analysis on other applications, such as vehicles and stationary fuel cell systems, could provide the basis for a comparative assessment of the hydrogen and fuel cell applications against other technologies. Furthermore, an historical analysis of the available data will provide insights on the evolution of the technology and identify major achievements and weaknesses that necessitate further research.
- This project is highly relevant in measuring the key enabler to fuel cell vehicles: the hydrogen infrastructure. The results can be used by policy and industry decision makers to target commercial barriers and understand when they have been overcome. The team's ability to add new data sets during the course of the project has increased the potential impact of the data sets. The future addition of medium- and heavy-duty vehicle information will further strengthen the project.
- This is one of the most immediately relevant projects in the Fuel Cell Technologies Office's Technology Acceleration portfolio. The data capture is absolutely essential to supporting the ongoing work of publicly available analysis and transparency on the effectiveness of state investments.
- Real-world data is critical to both calibrate existing infrastructure performance models and to develop new models. The data is vital to inform potential investors in hydrogen fueling.
- The data presented is extremely valuable to designers and operators of stations.

- This work starts to shed light on the reliability issues station operators face and the key components affecting reliability and performance. Resolving the queuing issue would most likely involve a second dispenser and additional capital expenditures. This becomes problematic at an underloaded station that has high demand only at certain times of the day. The team should come up with recommendations as to potential solutions, other than a second dispenser.
- The purpose of this effort is to use data for future innovations and research, but most of the data is based on existing operational equipment (including HRSs integrated with technology five years old and older), which is several generations behind current technology. It is increasingly unclear how this data is valuable in facilitating future innovation and directing research efforts. For vehicle fueling data, this data may be most valuable for scenario modelers, as actual hydrogen infrastructure providers can request this information from fuel cell electric vehicle original equipment manufacturers.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project has a clear path forward to gather data from new California stations. The investigators should work with older stations so that the stations will continue to report data even though compulsory reporting is no longer in force.
- Getting ahead of identifying the needs for future stations is an intelligent next step for the project. While there was not much detail available regarding the potential new analyses in the coming year, past experience through the project does indicate that new and valuable insights will arise.
- The proposed future work includes plans to update data collection, which will also require securing/ extending contracts with data providers. Identifying needs for future stations increases the relevance of this work.
- The proposed future work should look at how the various hydrogen supply chains affect the following: station power consumption, losses from hydrogen source to nozzle, and compressor maintenance costs. The future work should also address how the various compressor and chiller designs affect costs and reliability.
- The project work could consider station design (layout, etc.) to try to understand whether it affects incidents like queuing behavior and overall consumer experience.
- The project provides a number of key bullet points in terms of future work. Although they are valid, no reference to lessons learned is mentioned, while linking them with concrete examples of future work. In addition, challenges encountered in the past, as well as ways to tackle them, should be considered as part of the future steps. A more detailed analysis would be useful and welcomed; nevertheless, more information is necessary to fully comprehend the next steps of this projects. Lastly, more ways to evaluate existing data should have been mentioned as part of future work.
- NREL should not engage in identifying needs for future stations.

Project strengths:

- The project's strengths are that it is addressing needs in the developing hydrogen fueling market that exist now and for which there are large knowledge gaps for industry and government stakeholders. This project is an essential part of "proving the concept" that hydrogen stations can be successful, can be operated reliably, and will be used if developed. In addition, while this project has an aspect of continuous data capture, project scientists also continue to seek new ways of capturing and analyzing the data, which is helpful for a growing industry that does not always anticipate its own information needs.
- The project exemplifies in the international context a detailed analysis on KPIs. All major parameters have been collected, analyzed, and visualized comprehensively. Detailed information is presented with monthly/ daily/hourly granularity, which is rarely available. The team undertaking the work is dedicated and committed, with extensive experience in the field.
- This project is developing highly relevant data sets on hydrogen dispensing, data that can guide work and investments by many California agencies, as well as developers. The addition of queuing and station availability has increased the project relevance. Analyzing both traditional and renewable hydrogen infrastructure can also be useful in guiding DOE programs and investments.

- The project summarizes issues and status of the fueling station network in California, highlighting early market status and challenges. The project also begins to set the stage for justifying new developments and focus areas and for ensuring hydrogen price points are eventually achieved.
- The project has assembled a comprehensive data set. The project has produced a broad and useful array of data products. The project will continue to add new data as new stations come on line in California.
- The project team is providing valuable data collected on a relatively large number of stations. It provides interesting information for industry and the public and deserves continued funding.
- The historical data track record of HRS development evolution is a project strength.

Project weaknesses:

- The project's biggest weakness is the tie to contracts that are outside the control of the project scientists or DOE. While leveraging CEC contracts has helped get a high level of early participation from station operators, it is becoming clear that the project will need to develop some alternative structure for ensuring that it continues to receive data beyond the life of the contracts. Moreover, if station deployment is truly successful and becomes more industry-led in the coming years, then there may not be state government contracts to leverage, even though there may still be a need for data and analysis. The project likely needs to develop a supplementary method for ensuring participation and data capture more long-term.
- Older California stations will no longer have to report data, but clear strategies to encourage stations to continue data reporting were not evident.
- The project needs to maintain the availability to collect data from all stations and continue to work with the most robust data sets possible.
- The project seems to cover many areas but does not drill down into any key areas. In addition, it would be good to see progress over time by picking the key issues affecting reliability or costs as the station network matures.
- The desire to collect more data without direction on what is most valuable to industry is a project weakness. Adding data collection points based on "collecting data for data collection's sake" is also a weakness.
- The absence of perspective from drivers is the main weakness, but it is not too late to collect such information through a survey and analyze the data.

Recommendations for additions/deletions to project scope:

- The project should support expanding the queuing analysis further for future work. The team should collaborate with state partners for two purposes: (1) to identify additional cost detail that could be useful in state efforts to understand the developing business case for hydrogen stations and (2) to develop a metric for effectiveness of state funding based on the methods used to choose stations to fund and the observed performance. The project should also incorporate analyses similar to the missed fueling opportunity analysis to identify insights not just for the observed data and the known locations, but for what the data could be saying about locations that have thus far been overlooked. This will likely require a tie-in to some geographic information system (GIS) analysis.
    - The project should also evaluate whether it currently collects or could easily collect data from fueling events that do not reach full state-of-charge. The evaluation of the data should focus on whether common causes of incomplete fills can be identified. This could help lead to insight on whether the fueling protocols need to be re-evaluated and/or re-tuned, as short fills may be caused by out-of-bounds operation that may not truly need to stop the filling process. In addition, it would be helpful to perform an analysis of drivers' reactions to short fills. It would be helpful to know (1) whether they attempt multiple fills and, if so, the number of fills; (2) whether it depends on the operating status of some particular pieces of equipment; (3) how often consecutive short fills occur; and (4) whether the reaction changes with the number of these happening.
- The measurement of green hydrogen as a fraction of the refueled hydrogen should be added in the questionnaire. Improvements in terms of monitoring performance data in real time are considered useful while enhancing the accuracy of the results and providing users with information on HRS availability. In addition, queueing data, if expanded to a considerable number of HRSs, could be used for further planning of new HRSs. Future work should include a plan for continuing data collection and ensuring the quality and

quantity once the number of HRSs increases to a few hundred. A comparison with bus and medium-/heavy-duty vehicle HRSs could perhaps enrich the existing analysis.

- The project scope should include identifying who is using the data sets and how final data sets will be used. This information will help ensure that future work is aligned and is most valuable to achieving industry improvements in hydrogen delivery and availability.
- The team should delete inclusion of the queuing model, “missed fuel opportunity” efforts, and the tracking of station types.
- The investigators should work to encourage and motivate stations no longer compelled to report data.
- The team should look at queueing as a separate topic.

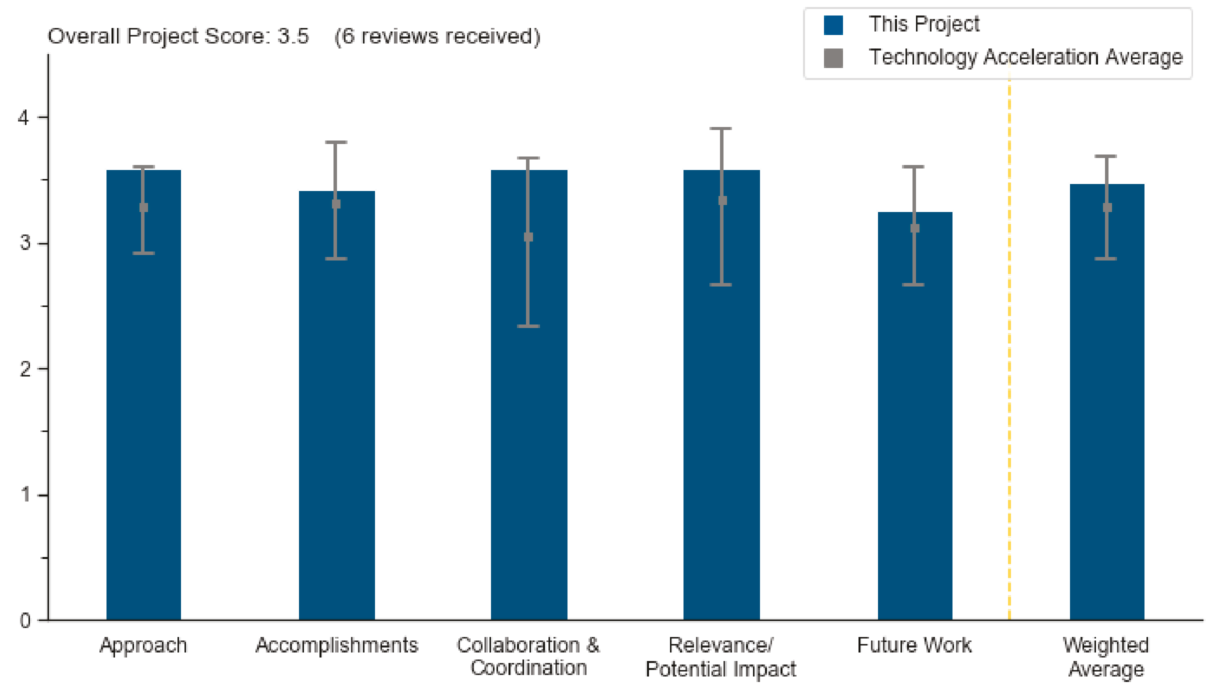
Project #TA-015: Dynamic Modeling and Validation of Electrolyzers in Real-Time Grid Simulation

Rob Hovsapian, Idaho National Laboratory

Brief Summary of Project

This project is demonstrating the fast-reacting performance of electrolyzers and characterizing the potential and highest economic value of their installation to enable participation in energy markets and demand response programs. A novel approach of distributed real-time simulation is used with electrolyzer hardware at the National Renewable Energy Laboratory (NREL), in conjunction with power system simulations at Idaho National Laboratory (INL).

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The team demonstrates a good approach to the problem of integrating electrolyzers into the grid. There is an appropriate level of effort to ensure satisfactory results, and the models estimate well the impact of renewables and electrolyzers supporting the grid. There is a good mix of hardware in the loop, modeling, and industry feedback.
- This work is timely, as it is necessary to address the integration of hydrogen systems and to design the electricity market to supply energy services to both hydrogen users and the grid. The migration to the Institute of Electrical and Electronics Engineers (IEEE) protocols for energy storage is another step in the process to get hydrogen accepted into the tool chest of distributed resources needed for electricity grids with high renewable energy penetration, an inevitable requirement given decarbonization and renewable energy costs.

- This project provides unique data and insights based on its approach. It will be good to see the work expand its runs and outputs to longer-term studies. While it is logical to look at single incidents initially, which seem to be the current project focus, it will also be interesting to see how the electrolyzer reacts to multiple consecutive demands or needs on the network. It would also be interesting to see how the front end controller and system might respond to events that would cause multiple possible demands on the electrolyzer and its output.
- The milestones and go/no-go gates for this multiyear project are well defined and align well with the project objectives and identified barriers.
- The combination of testing and modeling will provide a good basis for evaluating a wide range of implementation types.
- Controllers for mating the electrolysis systems with the grid and other renewable sources of power must be developed and sophisticated enough to handle the vagaries of the performance characteristics of the electrochemical process. Regarding the electrochemical system, the performance of such a device can vary widely based on environmental condition effects as well as operational variability, efficiency, and stability of the stack. It is a chemical plant. It is necessary to understand the impact of the variability, not just of the stack but of the entire electrolysis system, but it was not clear that the number of hours dedicated to such understanding would be sufficient to develop a robust controller system.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The work modeling the impact of electrolysis on penetration of photovoltaics (PV) in microgrids is promising in terms of the electrolyzer matching solar–PV dynamics. The questions now move to the other side of the supply/demand equation, such as how much hydrogen can be used at this level of system integration. The following questions are unclear: what impact this has on hydrogen balances, distribution, and storage; how hydrogen can be used within the sub grids; what the degree of consistency with hydrogen demand models is; and most importantly, how much the hydrogen costs.
- There is good progress across milestones and go/no-go decision points. Two of the five milestones are expected to be complete by May, including the go/no-go pass decision. The project is proof that electrolyzers can make grids more robust and capable of increased renewable energy or more efficient operation of thermal power plants.
- The project is on track to meet milestones. It has demonstrated electrolyzer functionality to provide distribution grid support in a simulated, real-world environment of several utility grid configurations with varying levels of renewable penetration. To provide full value, the work needs to quantify the financial benefit of the services provided and net them against impacts on fuel production.
- Results to date show good performance and input into modeling tools.
- The accomplishments to date are good, though it was a bit difficult to discern what was completed in the last year compared to prior years of work.
- It is not obvious what electrolyzer was used, nor was the history of such an electrolyzer made clear. Different electrolyzers perform differently. The controller logic should be general enough that it can be modified to be useful with other electrolyzers currently available for testing. Ten hours of electrolysis testing and characterization is not enough to provide guidance for controller development. Furthermore, it would be important to include electrolyzer "hiccups" when evaluating performance characteristics, and then assess the effect on controller logic.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- There is outstanding collaboration across multiple utilities for key market data input; good integration across NREL and INL, showing benefits and strengths of two laboratories working together; and deep integration of IEEE industry standards for interfacing with the grid. The university partners are an important part of the project and will enable a broader distribution of the efforts. The geographic range of Humboldt State University (in Northern California) to Florida provides a good range across the United States.

- This project has leveraged a wide range of expertise, with relevant academics, national laboratories, and energy and utility companies included in the work. In addition, it appears obvious that the project has responded to prior reviewer comments to bring in more of these types of collaborators.
- The project appears to be leveraging a well-coordinated team featuring national laboratories, utilities, universities, and regulators. This team is stronger than those of most peer projects.
- This is a good line-up of collaborators. Electric Power Research Institute (EPRI) was looking at storage and integration of hydrogen systems a couple of years ago (Matthew Pellow). Perhaps EPRI could contribute to collaboration. It would be good to know if there is an opportunity to get hydrogen on the agenda of California Independent System Operator resource planning.
- Having partnerships with grid power producers is a big step in getting buy-in and validation of the potential value of electrolyzers on the grid.
- Every group involved is well suited to contribute.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project relevance is clearly shown by the number of industry partners and results that show how electrolyzers can provide flexibility for both renewable energy and better operation of thermal power plants. This project will provide three clear benefits: (1) additional renewable energy, (2) lower-cost hydrogen production, and (3) better quality grid electricity to customers. The integration with universities is important for work force development and knowledge sharing.
- This project is highly relevant. This platform is a fundamental building block to developing a high-penetration clean energy hydrogen system. Having a physical system that demonstrates the concept and generates physical data is very helpful.
- Understanding how to manage and control the integration of an electrolysis system with renewables and the grid is a necessity. A successful outcome would provide numerous options for the utilities and the ability to meet the goals of the Hydrogen and Fuel Cells Program.
- Demonstrating and validating that there is significant value to the grid by using electrolyzers in load balancing is valuable, as grid management remains one of the biggest limitations in the growth of this industry. This project aims right at the center of this issue.
- The project begins to set the foundation for quantification of grid benefits of electrolyzers. The project will make an important contribution to understanding the viability of electrolyzers as grid resources connected at the distribution level.
- The project is looking to answer questions that are central to the H2@Scale effort and are currently relevant in areas attempting to expand their hydrogen-based programs.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- Future work with hardware in the loop and the clear example of the impact of 225 kW stacks on frequency and voltage regulation clearly demonstrate to grid operators that electrolyzers have value in providing better-quality electricity to customers. Saving fuel and reducing emissions from thermal power plants are important electrolyzer benefits, which may not be understood by those outside of a narrow set of people who have explored this or implemented the approach.
- These are good next steps. After a full scope of system integration is determined, it would be good to determine how results can be turned around to identify performance requirements as a list of specifications for electrolysis process, ramp rates, need for black start capabilities, operating range, capacity, etc. The next step will be to determine where in the electrical system (at what level) to connect to optimize the grid, hydrogen production, and hydrogen cost.

- The proposed future work provides a logical extension of the current project. Valuation of grid services is critical in understanding the ultimate potential impact of the work. The team could possibly extend analysis to transmission-level systems.
- Extension of the ongoing work as proposed is valuable.
- The proposed future work is good, though it is not entirely clear how the optimization module discussed will actually be a different study from another current H2@Scale cooperative research and development agreement project, which is also a collaboration between Pacific Gas & Electric (PG&E) and NREL.
- The industry needs to better understand electrolyzer performance characteristics. Decay rates and performance variability must be realistic and should be incorporated into the controller logic. It is recommended that these aspects be considered, if they are not already.

Project strengths:

- There is a good integration of partners. The project brings a clear quantitative benefit of electrolyzers that can be understood by multiple stakeholders. The renewable forecasting at higher penetrations shows how the grid can be built out and reach beyond early projections of 20% variable renewable penetrations to 30%, 50%, or higher. Deep quantitative analysis of grid nodes and the optimum placement of electrolyzers are strong aspects of this project. The optimization of electrolyzer set points to reduce the cost of hydrogen while meeting minimum utilization of the electrolyzers is a key question in the business case for electrolyzer-based hydrogen production.
- The project has created a platform for testing integration strategies to determine process requirements, design controllers, etc. to meet growing interest in hydrogen integration with renewable generators, fundamental building blocks for future clean energy systems.
- Project strengths include high-fidelity, hardware-in-the-loop simulation with supporting analytics, adaptation to early issues with controller design to develop a superior approach in collaboration with stakeholders, and establishment of quantitative impact on grid operations in actual utility system environments.
- Collaboration with grid generators is a project strength. This is a highly impactful topic needing data and modeling to demonstrate the potential and value to the grid.
- The project's strong point is the uniqueness of the approach, which is also going to provide high-value data to the industry and decision makers in stakeholder organizations.
- Team qualifications, collaborators, and grid knowledge are project strengths.

Project weaknesses:

- Being able to distribute this deep technical knowledge to utilities on the East Coast and outside those listed in the project would be an important aspect of leveraging the most value from this multimillion-dollar effort. A better demonstration of the value of grid services would be helpful.
- The team needs to work with additional innovative partners on grid integration. Perhaps the team could work more closely with independent power producers who hold expiring power purchase agreements or distressed system operators facing politically unpalatable curtailments.
- Electrolyzer operational characteristics are a project weakness. Nothing was presented regarding the evaluations and studies of the interaction of the grid and other renewable power generators with electrolyzers.
- Broader implications of the work are not possible to determine without understanding the value of the grid services studied.

Recommendations for additions/deletions to project scope:

- As an outcome, it would be good to see the opportunity for three groups to discuss next steps: (1) the project team, (2) the grid producers, and (3) the industry members who are likely to implement the electrolyzers. This project provides an opportunity for groups 2 and 3 to better plan deployment and capture the value of grid management. It is sometimes not obvious to members of group 3 how working with the grid producers is possible.
- The team should consider more detailed electrolysis performance characteristics, if this is not already being performed. Electrolyzer sizing (megawatts) should be determined to optimize efficiency and grid–electrolyzer dynamics. The controller must also take into account safety aspects of the "system." A failure mode and effects analysis and/or a generalized hazard and operability analysis review should be performed, and the results should be used to guide further development and refinement of the controller.
- The team should increase the scope to allow results to be implemented at a pilot or demonstration level with a utility. The team should determine the best venue for sharing this knowledge with policy makers, utilities that are moving from 20% to 30% penetration of renewables, and those regions with more than 50% renewable energy penetrations.
- The project should look at system response to strings of consecutive events—these could be strings of similar events under varying conditions—to see how the controller decides to react under similar signals in varying situations. In addition, the reaction of the controller to potentially conflicting signals should be evaluated to determine whether there is a risk of non-reaction or non-desirable and non-optimal reaction.
- It is unclear what electrolyzer requirements look like or what the implications are to storage and hydrogen uses in terms of hydrogen produced. Grid constraints are also unclear, particularly given the advent of battery electric vehicles.

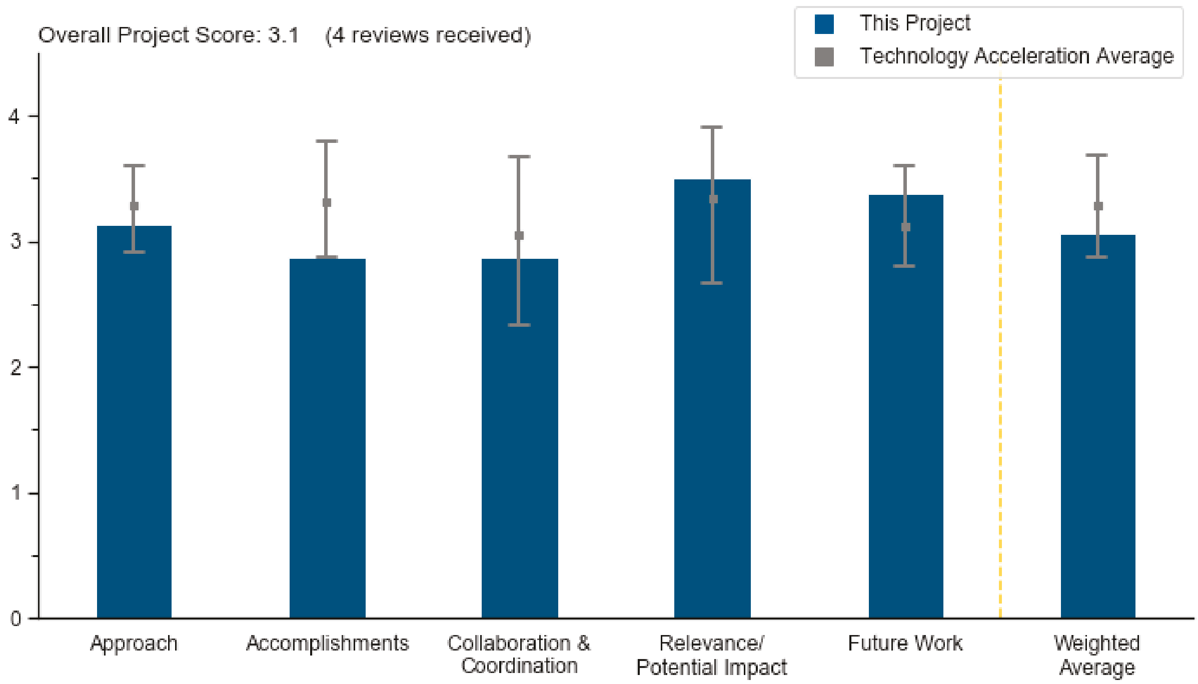
Project #TA-016: Fuel Cell Hybrid Electric Delivery Van

Jason Hanlin, Center for Transportation and the Environment

Brief Summary of Project

This project aims to increase substantially the zero-emissions driving range and commercial viability of electric-drive medium-duty (MD) trucks by integrating a hydrogen fuel cell into the powertrain. Investigators will develop and validate a demonstration vehicle to prove its viability and then build and deploy up to 16 vehicles, which will perform at least 5,000 hours of in-service operation. The project will also develop an economic and market opportunity assessment of MD fuel cell hybrid electric trucks.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Building real-world hardware and getting real-world data, while at the same time educating operators and customers, is a very valuable approach at this time. In particular, the approach has brought forward specific design, test, and operation challenges (for example, DC-to-DC issues and fueling readiness) and prioritized work on getting those solved.
- The project demonstrates a sound approach to accomplishing tasks. The data collection and analysis of the performance of fuel cell trucks in this application should help the industry develop a fully commercial product. The timeline for the pilot demonstration is optimistic. The team should encourage maximum usage during the demonstration to help identify and correct issues before the Phase II trucks are built.
- The project scope is well aligned with DOE barriers. Phase II will be critical to understand “real life” behavior, gain experience and miles, and identify barriers.

- This project was initiated in 2014 and has encountered significant delays. The project could benefit from an experienced original equipment manufacturer (OEM) or integration company to better plan and work through the issues.

Question 2: Accomplishments and progress

This project was rated **2.9** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- It is great to see the pilot truck finally completed and delivered for the demonstration period. The team has done an excellent job of mitigating early issues that caused delays. The team was also successful in acquiring funding to cover the whole project as planned. New funding includes moving to a refueling pressure of 700 bar to maximize truck range. This will help the truck design meet the needs of a broad range of users.
- The project shows good progress to date. Although the project is aimed at understanding the system, component issues could cloud the results.
- The DC–DC converter is a critical component in any fuel cell system. While this project should not be designing custom electronic equipment, it should have spent more time selecting the appropriate component. Progress has been slow and is at risk of becoming irrelevant compared to similar MD truck conversion projects. It is hard to determine whether goals have been met until real-world data have been collected.
- While it looks like Phase I deliverables have largely been met, it is not clear whether some of the delays due to problems (e.g., DC-to-DC) have resulted in delays from the original schedule and whether those delays might have changed the go/no-go date, thus affecting the issue of whether one year of demonstration can be completed before the funding opportunity sunsets.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- The group of collaborators includes state, local, and federal governments, technology providers, integrators, and end users, in addition to the fuel supplier, so the full team encompasses real-world experience end-to-end through the supply chain. Real-world experience is a benefit despite some of the scheduling challenges, which may have arisen related to the coordination between the number of entities involved.
- The project has great collaboration with partners. One concern is with the OEM partners' ability and commitment to commercialize the truck. This will be important to ensure the project leads to an actual market product.
- The collaboration with the team entities seems to be good.
- There seem to be some major problems with the team in terms of successfully integrating a fuel cell system into the truck.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project continues to be well-aligned with DOE objectives. MD trucks are a large segment of the market, with the potential for high-volume production that would lead to lower costs for many components shared with other platforms. The growth of fuel cell trucks in the market could also help increase hydrogen station utilization and justify the need for more station coverage.
- With the increasing focus on MD and heavy-duty (HD) applications, this project looks very timely and relevant with its look at the "last mile" delivery fleet model. It would be good to see more emphasis on the fueling infrastructure/process since that is really a key driver/enabler of commercial viability for commercial fleet applications.

- Relevance with DOE objectives is in alignment, highlighting issues with fuel cell conversion of existing delivery vans.
- Lack of vehicle systems experience in real-world applications is an important barrier that this project addresses head-on.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work (Phase II of the project) is on target for achieving project objectives.
- The proposed work is reasonable. The short timeframe for the demonstration and go/no-go decision could be the biggest challenge for the team.
- There is a need for all problems to have root cause solutions and appropriate validation before the project proceeds to the go/no-go point. While this may cause some headaches managing the project, especially with calendar constraints on funding, it is critical in bringing the demonstration from a one-vehicle demonstration up to the planned fifteen-vehicle "pilot" fleet, which is a critical next step to commercialization.
- It is unclear whether the conversion to 700 bar tanks is a good idea, given all the other problems encountered.

Project strengths:

- One strength for the project is that the team included user input in designing the truck. This helps ensure the truck meets user needs. In addition, the economic assessment is important to help other potential users to understand the technology and costs for better planning. The larger fleet of trucks in Phase II will be important to prove out the design for this application.
- The project structure (demonstration, validation, go/no-go, then pilot fleet) is a strength. The principal investigator has had to deal with a lot of evolution of the project to keep it on track, so the flexible project management is also a strength.
- This project is well aligned with DOE objectives. There is a sound approach for the prototype in Phase I and deployment in service and data collection in Phase II.
- This is directly aligned with DOE goals to get fuel cell systems on the highway.

Project weaknesses:

- The tight timeframe for the go/no-go decision point does not leave much wiggle room for mitigating issues. The technology partners need to take an active role during the demonstration to identify design flaws and engineer corrections before building the Phase II trucks.
- The relative lack of product experience and business stability of the partner companies has been a challenge, which has resulted in both schedule and technical issues for the project.
- This is a small team, and several immature components threaten to cloud the system performance and its evaluation.
- It has taken too long to integrate the fuel cell system, and at the go/no go decision point, the team should consider whether it is worthwhile to continue deployment of this particular system.

Recommendations for additions/deletions to project scope:

- For Phase II, very precise data related to refueling/infrastructure should be maintained and communicated. Since this project is demonstrating the type of MD/HD commercial fleet that is getting a lot of attention now as a fuel cell market, there is going to be much scrutiny of fueling costs, any issues/concerns that arise, and operational convenience. It would especially interesting to see a "total cost of fueling" analysis, with the price per kilogram and, more importantly, the cost per mile including capital and operations and maintenance components, so that the team can provide some real data on total cost of ownership for this type of fleet. Shell has good station cost information based on information the company has shown publicly, so the project team should encourage Shell to participate fully in this part of the analysis and reporting.

- The project is developing a significant knowledge base of lessons learned that are valuable to the community at large and can push the state of the art in terms of fuel cell electric vehicle integration. The project is encouraged to disseminate these lessons learned beyond their publication in the final report.
- The project could benefit from an independent analysis regarding the fuel cell technology proposed compared to the state of the art.
- The project should ensure active participation of technology partners during the pilot demonstration phase.

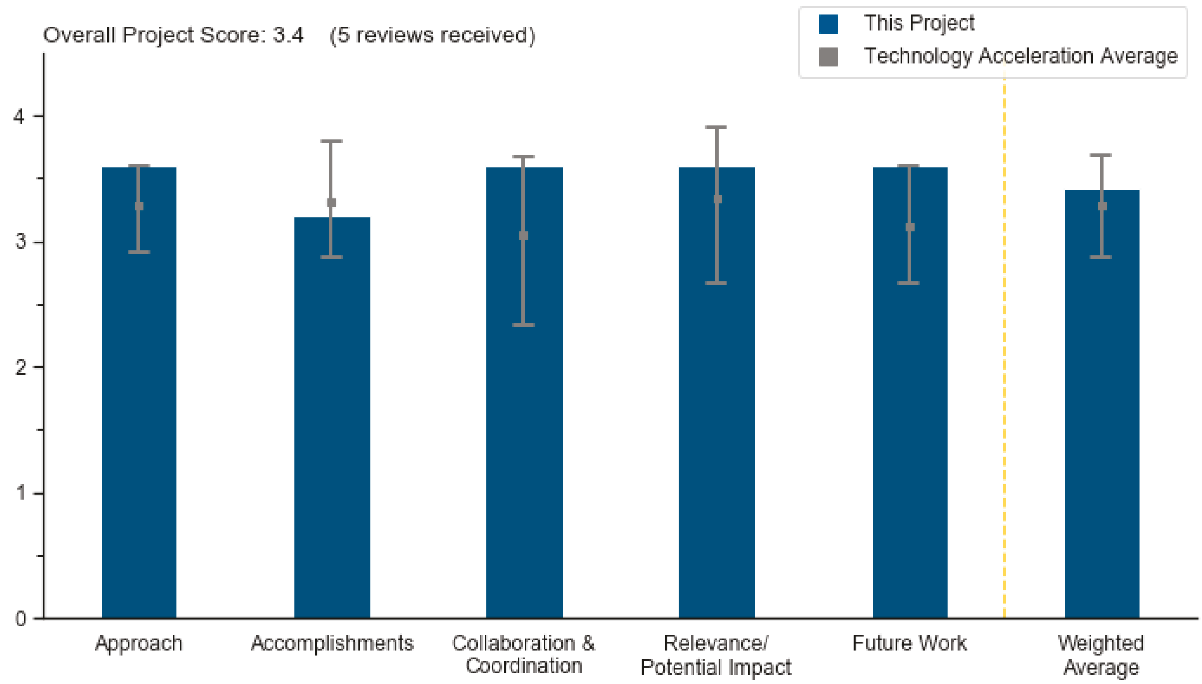
Project #TA-017: Innovative Advanced Hydrogen Mobile Fueler

Sara Odom, Electricore

Brief Summary of Project

The objective of this project is to design and build an advanced hydrogen mobile fueler (AHMF). The developed mobile fueler will be deployed to support a network of hydrogen stations and vehicles, and fueling data will be gathered for analysis by the National Renewable Energy Laboratory (NREL) Technology Validation Team. To reduce risk, the mobile fueler is based on an existing conventional station design, and project efforts are coordinated with station providers and automotive manufacturers.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project appears to directly address three key Fuel Cell Technologies Office (FCTO) barriers. Once deployed, the mobile fueler will be able to provide real-world operational data to NREL. A special DOT permit allowing transport at 95 MPa has been issued for the system, which reduces the cost and improves logistics of transportable hydrogen storage. The demonstration phase will help local authorities familiarize themselves with codes, standards, advantages, and concerns around hydrogen fueling infrastructure. This was clearly laid out in the presentation.
- This project has an excellent approach to addressing the lack of hydrogen infrastructure. Self-contained design makes it easier to site with a smaller footprint. U.S. Department of Transportation (DOT) approval for transporting high-pressure tanks is important for industry.
- The team has designed and is currently building a mobile hydrogen fueler. The approach is strong, and the mobile fueler will deliver hydrogen in a fully code-compliant manner—the same as a stationary fueling

station. Having the unit fully self-contained is valuable, but it would have been preferable to have a fuel cell or other green power source rather than a diesel generator.

- The project approach appears to result in technology progress for mobile and stationary hydrogen fueling stations (HFSs) (and in this instance, a liquid nitrogen [LN_2]-based cooling system, compact Welcon-like heat exchanger/chiller, and 95 MPa DOT-permitted storage tanks).
- This project is aggressive in that 3–5 fills in the first hour, and 20–40 per day, is a challenge for stationary systems, let alone a mobile one. However, the team assembled to take on this challenge is extremely capable. While the project has experienced some difficulties, the overall approach and the team's handling of the setbacks has been appropriate, if not good. Several of the novel approaches are particularly impressive, e.g., using LN_2 to increase efficiency and decrease the real estate and weight requirements. It is also clear that this project is on track in construction of the fueler, even with difficulty in hardware delivery and other supplier issues.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The design phase appears to be complete, and construction has begun. The schedule was delayed for DOT certification, which is reasonable because those types of approvals always take longer than expected. Completion of the DOT certification process is a major accomplishment and a really valuable step in improving hydrogen transport options. Construction has begun, and the team reports that 50% of the components have been procured. It is a concern that the system might not be ready for field testing by mid-2019 since the testing portion is supposed to last 18 months. It is good that the team plans to deploy at a facility already permitted for use as a hydrogen station, as that should reduce the permitting time for the new system(s). It is a little concerning that site selection is not complete yet. There will likely be unexpected hurdles in getting the system landed at a location for testing (e.g., local permitting issues, especially for the diesel generator, challenges in getting shore power identified and supplied to the system, etc.).
- The team has made good progress with the project. It is great to see DOT approval for high-pressure tanks on the road. The fact that other clients were waiting for this approval shows this was beneficial for the industry.
- Currently analyzing frame and fire protection design for 95 MPa storage tanks is an accomplishment, and lessons learned could transfer to truck-mounted systems (or from truck-mounted systems to this system). It may be good to attempt to use the definition for station capacity used in California (either from previous California HFS grant funding opportunities [GFO] or to be assessed with a new NREL/California formula).
- It seems this project has overcome the scheduling and cost overrun difficulties of the past and is back on track for a successful completion.
- The project has already seen cost overruns and schedule delays. The new project controls now in place will, one hopes, get the project back on track. Acquiring the special DOT permit is an excellent accomplishment that can have an impact on the community, in addition to benefiting this project specifically. The sooner the fueler can be deployed, the sooner it can collect data and support the expansion of (and the current) hydrogen fueling networks. The reporting should include performance data of the LN_2 precooling system. With the target of three sites in 18 months, the fueler needs to be completed, sites need to be selected, and it needs to be deployed as soon as possible.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- The collaborators and coordination for this project are very appropriate for achieving the desired outcome. The team includes a very well-established industrial partner capable of executing and continues the deployment of this system. Partnering with NREL in data analysis is appropriate, and working closely with those states needing this for deployment (California and Northeast states) is spot-on.

- The partnership coordination seemed really good, especially given the input from Air Liquide during the Annual Merit Review (AMR) presentation. The research team has clearly benefited from Air Liquide's technical expertise. It is concerning that the site selection process is not yet complete, but presumably Air Liquide is working diligently to identify the sites and will support the effort to get the system deployed quickly and into testing.
- This is a well-balanced team of contributors to accomplish project goals. The addition of a site partner will be important for demonstrating the system and assessing customer acceptance.
- The team is strong, with the right background to build and deploy the mobile fueler.
- This is a strong team, and coordination appears to be good.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project is very relevant and timely. California is predicting that, with the projected growth of HFSs compared to that of vehicle demand (just light-duty fuel cell electric vehicles [FCEVs]), demand will outpace growth in the next couple of years. Equally important is that places like California and the Northeast have worked hard to ensure that coverage is appropriate; HFS reliability remains an issue. In early stages of build-out, a solution to reliability is redundancy; this mobile refueler addresses this very critical issue. This project is very relevant, and its impact in early deployment is huge.
- This project aligns well with DOE goals and addresses barriers of hydrogen supply. This project could help build out fueling infrastructure, which can facilitate early adoption of hydrogen vehicles. This also allows easier introduction of hydrogen fueling to areas that are not yet familiar with FCEVs.
- The mobile fueler enables the establishment of new markets and support of current markets for hydrogen vehicles. If the LN_2 cooling system is effective, it could be deployed at other stations or provide technological pieces for liquid hydrogen cooling systems for liquid hydrogen stations.
- DOE should consider funding 10 additional units to bring manufacturing experience for this type of system from technology readiness level (TRL) 1–3 to TRL 5–8.
- The project appears to clearly address at least three key FCTO barriers and will provide some valuable information to advance hydrogen fueling knowledge. It is not totally clear what direct benefit this fueling system will have on the industry. It is unclear whether this system is designed to provide temporary fueling capabilities while a permanent station is being built, or to test out demand in certain locations before investing in a permanent station, or to provide redundancy for permanent stations. It is also unclear whether any of these scenarios are key issues within the HFS space right now. It would be valuable to get a sense for how this fueler will be deployed in the real world and at scale.

Question 5: Proposed future work

This project was rated **3.6** for effective and logical planning.

- This is a well-laid-out plan to complete the project. Economic analysis will yield important data for the industry. The team plans to use the system past the scheduled demonstration period, which is a bonus. It would be useful to see the data submitted for this longer period to add to the analysis for the industry.
- The proposed future work is in line with what one would expect for the construction and completion of a prototype piece of hardware. The project has overcome some difficulties and is on track to complete the unit as proposed in this project.
- Preventing any more schedule slips is crucial to achieving all project goals. There are bound to be issues that need to be worked out after the initial (and potentially subsequent) deployments. The team needs to keep sufficient time in the schedule to work out these bugs. The proposed schedule and work plan will enable meeting the key objectives outlined in the project.
- The project should build, build, build (and test/verify that things work as designed).
- The schedule on slide 15 of the AMR presentation shows site selection completed by the end of the second quarter of 2019, which is only two months away. It is a concern that even when site selection is completed,

it could take several months to deploy and commission the system. That is going to squeeze the schedule if the contract calls for 18 months of testing. Beyond the project, it would be helpful to get a better sense for how Air Liquide will use the system. It is unclear whether the system is for research and development testing of various components or whether it will be field-deployed to support construction of permanent fueling stations. It is also unclear whether this system has a practical real-world application for industry.

Project strengths:

- The fully code-compliant H70 mobile fueler is demonstrating new technology (a LN_2 cooling system) and the path to DOT approval of new technology (transport of 95 MPa H_2). This innovative mobile fueler can provide support of the current fueling network and expansion into new markets. The flexibility of running fully contained, with hydrogen storage and power onboard, or with external hydrogen storage and "shore" power enables operation in a wide range of environments.
- DOT approval for transportation of high-pressure hydrogen is a significant strength. Compact design should facilitate installation and address customer concerns over the footprint.
- The project team appears very capable of completing the design, construction, and operation of the system. The project was well scoped, with achievable goals and a clear deliverable: an operational mobile fueling station.
- This strong, capable team has already demonstrated the will and ability to rally collective resources to ensure a successful completion.
- Project strengths include a 70 MPa mobile fueling solution meeting SAE J2601 T40 with same capacity as early stationary retail HFSs, DOT permit/approval for 95 MPa, inclusion of a compact heat exchanger/chiller, and testing of the system in the field.

Project weaknesses:

- Earlier concerns from previous AMRs have been addressed with the progress presented this year.
- This appears to be a one-off mobile fueling solution. Running a generator on regular low-sulfur diesel using renewable diesel (not biodiesel) where possible instead would improve the selling point in emission-sensitive areas where 480 V 3-phase is not available.
- The schedule delays associated with the DOT certification are going to put stress on the testing phase, and a good deal of value is to come from that phase.
- Gathering performance and efficiency data, education, and expansion of the fueling network are key objectives, making the schedule delays problematic.

Recommendations for additions/deletions to project scope:

- If possible, the project duration should be extended to accommodate a full 18 months of testing (if delays have reduced that testing phase). It would be helpful to include a case study or scenario that clearly lays out the value of this system once the project is completed. For example, if this is backup for a permanent fueling station, the team should show the cost of deploying the mobile fueler and how that generated benefit for the permanent fueling station if there was an unplanned outage for a certain period of time. The team should make it clear to the fueling industry that this system can provide real value.
- Publishing as much information as possible about the high-pressure DOT permitting process will enable others to follow a similar path for other tanks. Reporting performance metrics (and design information) on the LN_2 cooling system could lead to technological breakthroughs for hydrogen cooling.
- The team should emphasize that AHMF has 480 V 3-phase plug-in capability in all presentations. The team should define station capacity using either the new draft California Air Resources Board/California Energy Commission (CEC) definition or a previously used CEC definition (pick any previous round of requests for proposals/GFO funding, as long as it is clear which definition was used).
- DOE should keep this project funded to its completion. Succession funding to evaluate and test in the field with hydrogen station equipment or device performance should be considered.
- It would be helpful to see the system updated to address medium-duty vehicles. The team should continue to supply data for long-term analysis.

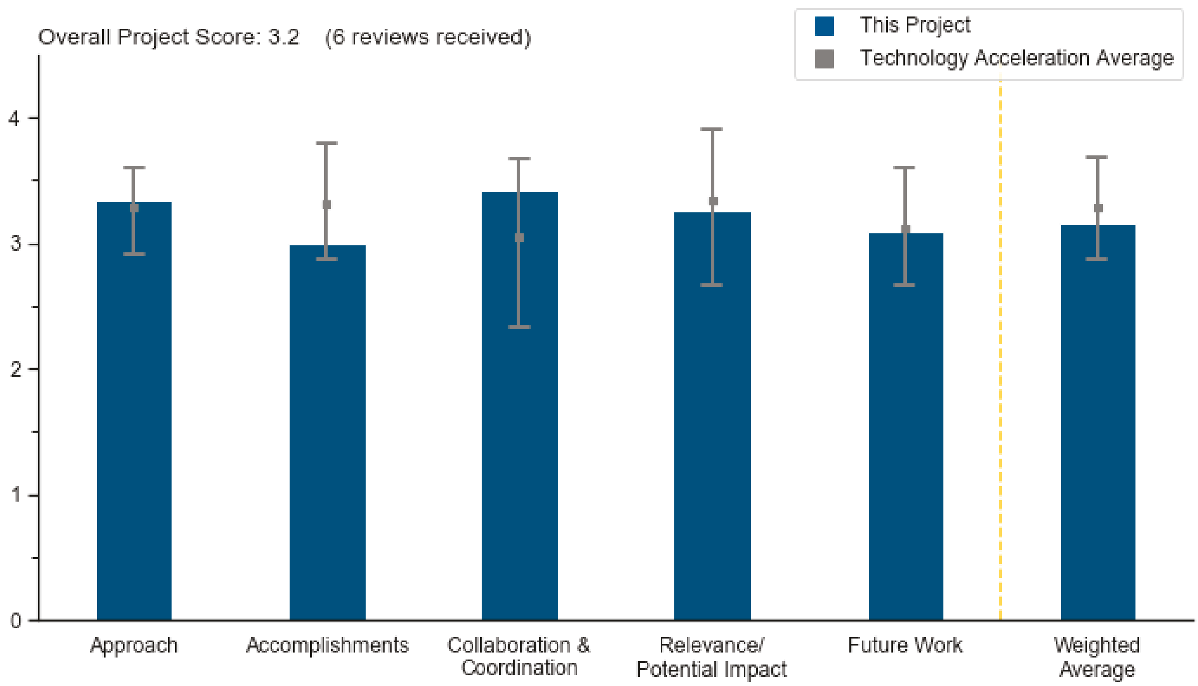
Project #TA-018: High-Temperature Electrolysis Test Stand

James O'Brien, Idaho National Laboratory

Brief Summary of Project

The project objective is to advance the state of the art of high-temperature electrolysis (HTE) technology by discovering, developing, improving, and testing thermal–electrical–control interfaces for highly responsive operations. The project will (1) develop an infrastructure to integrate support systems for 25–250 kW HTE testing units, (2) support HTE research and system integration studies, (3) measure cell stacks, performance, and materials health under transient and reversible operation, (4) characterize dynamic system behavior to validate transient process control models, (5) demonstrate integrated operation with co-located dynamic thermal energy distribution/storage systems, and (6) operate the system with co-located digital real-time simulators for dynamic performance evaluation and hardware-in-the-loop simulations.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is an excellent approach to providing initial understanding of HTE on a large scale. To have a full portfolio of realistic hydrogen sources, it is very important to have the ability to test realistic operating parameters for HTE with foreseeable high-temperature sources of heat and electricity, and on a reasonable scale.
- The project has a clear rationale and approach to performing both intermediate-scale and large-scale HTE.
- The approach is well formulated. However, the objectives discuss goals for integrating the HTE system with both renewable and nuclear energy resources. Presumably, these will each provide different challenges of electrical and thermal energy flows for the HTE system to address or to which the system will be exposed. The approach does plan to report on HTE performance in response to such changes, but the

project has not yet clearly defined how these will be tied back to separate scenarios of integration with renewable energy sources, nuclear energy sources, or both. It would be very helpful to see the work presented in context of these conditions, rather than reporting on the HTE as if it were responding in a standalone state.

- The approach is good with regard to the test station design and build. The development of an over-instrumented test stand is necessary to generate the information from the electrolysis unit and its interactions with subsystems and the heat source. It is not clear that the station was built with an element of flexibility so as to modify its engineering and subsystems, as test results may require in the future. It is not clear why the OxEon Energy, LLC (OxEon) stack was chosen over a larger, more established industrial and industry-engineered supplier's stack. This is not a stack design initiative. The OxEon stack was built for NASA and is typically not a general purpose industrial gas production design. The project should rely on generic stack degradation data, not just data from a single stack design or supplier. The testing plan should be based on data. No such data were seen in the Annual Merit Review presentation (not even data from the 2000-hour, 5 kW tests that were referenced). Dealing with a proprietary stack design is informative but limiting.
- The project seems to be working well to establish HTE testing capabilities. The relevance of working on oxygen-producing units (i.e., solid oxide electrolysis [SOE] and the Mars Oxygen ISRU Experiment [MOXIE]) is not clear. There should be clearer tie-ins to hydrogen production and plans for redesigning or repurposing these units to optimize hydrogen production rather than oxygen.
- The project objectives were not clear from the presentation. The overall scope of the project is understood, but there is a need for clear metrics (e.g., cost targets, efficiency targets, output pressure targets, etc.) and clarity in terms of superlatives for how this system is differentiated (for example, perhaps it is the highest-temperature electrolysis system or the most efficient high-temperature system). The concept of an HTE system has tremendous value, but it is unclear how this project is differentiated. The team needs to clarify what the value proposition is. This is crucial for a successful project.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Much good development work on the test system has been completed, and it is encouraging that the team seemed to find a good solution for procuring the HTE stack. However, it is unclear how the project is to meet milestone 2 (listed as on track), given that this seems to include final production and delivery of the 25 kW electrolysis stack, integration with the test system, validation of the installation, and several test cycles.
- Completion of the 25 kW facility will allow for critical integrated testing of realistic HTE configurations. The team should consider the value of heat exchanger designs and materials to realistically match the anticipated heat exchangers for high-temperature reactors, such as high-pressure helium to steam heat exchanger. Since the facility exists, extending the realism to the heat exchanger connection anticipated in a reactor may be of value. The accomplishments in developing the solid oxide electrolyzer cell (SOEC) stack at the 5 kW level are very promising.
- The investigators have set up the equipment on schedule. The accomplishments are more activity-based than results-based. There should be targets for device performance as well as just for getting the device to work.
- The significant accomplishments and progress of this project are related to the construction and installation of the test cells.
- The project is relatively new. There appears to be satisfactory or good progress to date versus the project scope.
- The results of the test station build seem appropriate; however, the performance of the station was not addressed. If it is not running well, the team needs to determine whether the problem is the station or the stack. Also, it was not reported if a failure mode and effects analysis (FMEA) and/or hazard and operability (HAZOP) review(s) were carried out to assess the station's engineering design logic, safety, and functionality. This process is standard in industrial engineering programs and leads to a better understanding of the entire process. No instrumentation was seen in the piping and instrumentation diagram

(P&ID), nor were what variables and responses will be monitored and varied in future operational tests with the stack. Stack performance will be difficult to understand if the OxEon stack is considered proprietary. Therefore, the cause of any degradation rate will not assessable. The 5 kW stack should be tested 24–7 so its operating characteristics can be assessed.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The project is employing an excellent mix of partners, including the industrial collaborators. This is also an excellent collaboration between the DOE Office of Energy Efficiency and Renewable Energy and the DOE Office of Nuclear Energy. Idaho National Laboratory has a rich history in high-temperature ceramic electrolysis and fuel cells. The principals at OxEon also bring a rich history in developing solid oxide fuel cell (SOFC) and SOEC systems. FuelCell Energy, Inc., has a good deal of high-temperature commercial fuel cell system design experience. Pacific Northwest National Laboratory (PNNL) and Sandia National Laboratories (SNL) are excellent national laboratory partners for this type of project.
- The presenter showed good interactions with partners and is taking a helpful and supportive role in spurring enterprise outside of the laboratory as part of the overall project effort (several small businesses were mentioned).
- The project has appropriate collaboration with NREL, PNNL, SNL, and industry (OxEon, formerly Ceramatec, Inc.).
- The project has assembled a group of collaborators in national laboratories and in the HTE industry.
- The collaborations with industry seem appropriate. However, it does seem like this project is quite separated from other energy system experts across other national laboratories, such as NREL. It would seem appropriate to implement more collaboration with these laboratories, especially to bring context to the testing results.
- The collaboration level is appropriate. It is not clear how much collaboration is taking place with SNL on the work reported in TA-015. This may be a redundancy.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- HTE has long been anticipated as a potential key element in large-scale market-based hydrogen supply. From high-temperature nuclear reactors, the expected production of hydrogen may be closer using HTE than from thermochemical conversion. Early-stage testing anticipated by the HTE will provide the key initial datasets for integrating HTE systems in realistic configurations.
- HTE is an important technology that should be part of the overall technology portfolio. The thermodynamics of electrolysis improve dramatically with temperature. There are many sources of waste heat (beyond nuclear power plants), so there is a great opportunity for this project to have impact beyond its current scope (for example, in steel mills that also can use hydrogen on site). Nuclear plants can also utilize other sources of revenue for their excess generated power.
- The relevance is important, as is the potential impact. Studies and related efforts such as these are necessary for ascertaining knowledge and learning if this concept is ever to be used.
- The scope of HTE has changed significantly in the past decade, changing from very large-scale hydrogen production to the current smaller-scale, intermittent production that is the topic of this work.
- The project goals overall seem to be aligned well with DOE Fuel Cell Technologies Office goals; however, it does seem to be too early to fully and accurately assess the potential impact. In addition, with current popular and political opinions surrounding nuclear energy, this project's results may not have a chance at full utility in the real world. On the other hand, if the project results find significant benefits and can communicate those benefits well, the project could provide a very useful resource for helping to better inform future decisions around nuclear energy resources.

- The project has activity-based goals and targets rather than clear performance-based goals. For maximum relevance, it needs clear goals tied to hydrogen production targets.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- All of the proposed future work for fiscal year (FY) 2019 and FY 2019–2020 looks very promising and is completely appropriate for the activities at this stage. One thing that might prove to be a critical issue is the need to keep degradation below 0.5%/khr. It could be valuable to evaluate any degradation rate early to identify that as a challenge. It is unclear what is meant by establishing a large-scale test capability in FY 2019–2020.
- Most of the elements and initiatives in the proposed future work are consistent with the objectives. It is not clear how the 25 kW stack will be tested and proven out, and the long-term degradation data collection obtained, in a single test rig. It seems like most of the effort is about the stack rather than determination of the interactions and resultant effects of key operational variables of the HTE on performance. The future work should also include subsystem effects.
- The proposed work is well in line with what must be completed for the overall project goals. The only concern is that it may be a highly challenging and ambitious schedule to complete all the 25 kW testing and procure, integrate, and validate a 250 kW installation.
- The project should implement performance-based goals. The relevance of MOXIE and SOE technologies for hydrogen production should be clearly established and described.
- The overall project scope is fine. No go/no-go decision points were seen, which is worrying.
- Establishing key metrics is important to track project progress. It is not clear where the value of ~0.5% degradation over 1,000 hours originated. Metrics for other electrolysis projects have 1% over 1,000 hours. The thermal energy delivery system (TEDS) heat transfer system should be evaluated at scale. The "old" goal of the nuclear hydrogen initiative was the idea of using He-cooled steam from a very-high-temperature reactor at elevated temperature with trace contaminants (potentially tritium). The team needs to clarify what the current heat transfer materials and mechanisms are, as well as whether they will also operate on an intermittent basis and how they will perform.

Project strengths:

- The project has a solid team of collaborators and partners. The current state of the SOEC technology and the opportunity to test it on a large scale in this project's facility should be very valuable to the DOE Hydrogen and Fuel Cells Program and nuclear program.
- The overall project strength is its potential to provide new insights on nuclear energy resources that could spur a redirection of current trends for this resource. The project also has a well-structured approach that will provide real operational data, potentially providing highly convincing information for decision makers.
- This is an applied project that aims to demonstrate intermediate-to-large-scale HTE with commercial materials (i.e., SOEC stacks). The work has resulted in impressive facilities and promising results.
- The project's strengths include its significant national laboratory resources (i.e., engineering and equipment). The project is building on knowledge of SOFC technology and related systems design and controls.
- The use of SOXE is an important testing platform, and this work is important.
- The project has established DOE expertise in the implementation and operation of HTE equipment.

Project weaknesses:

- The project represents a significant and unique integration of complex components into a high-temperature thermoelectrochemical system. The potential for unexpected technical challenges may be higher than with other complex systems. There does not seem to be a plan to deal effectively with such unexpected challenges.

- The project weakness is clearly the relatively low availability of HTE units. It seems that if the project partner is delayed or somehow unable to fulfill development for this project, then the overall project's accomplishments could be at risk. It is likely wise to continue searching for a second procurement source, just in case the primary source has any issues.
- Too much emphasis has been put on an unproven stack technology (which was developed for non-industrial, small-scale application). As it is presented, this is a test stand development effort. The test stand does not seem to be flexible with regard to testing and proving out related subsystems. No mention was heard of an FMEA or HAZOP review to guide system development. The team needs to better understand the variability in heat sources using the test stand and then understand the impact on stack performance and efficiency.
- The "intermittent" nature of the proposed electrolysis systems is questionable. This is asking a good deal of existing or known materials systems including seals, electrolytes, electrodes, etc. Perhaps an economic analysis could be pursued using a fraction of the electricity produced in a quasi-steady-state matter coupled with hydrogen storage, instead of multiple on/off cycles.
- Clear metrics, go/no-go decision points, and overall project management seem to be lacking. The team must have clear "objectives" to measure success.
- The project goals are not tied to specific targets.

Recommendations for additions/deletions to project scope:

- It is recommended that the team add context to the analyses so that they demonstrate the potential real-world impacts to policy- and decision-makers. Sample tests of system performance should be tied back to representative events in the typical, occasional, out-of-bounds, and problematic operations of the other energy resources into which the HTE is integrated. Evaluations should then be made not just of the HTE's performance and ability to absorb and meet these demands but also of the effect it would have on the remaining energy resources' operations.
- The researchers should perform an FMEA and a HAZOP analysis as a guide for making a better test station. They should also obtain a stack from a second source and test and compare the results; perform an analysis whereby the hydrogen compressors in the cycle are replaced with an electrochemical hydrogen compressor; perhaps run the economics; operate the stack and system on the test stand so that pressure is generated and assess the test stand's ability to evaluate the effects of pressure; and reference the P&ID, as the gas does not seem to be thoroughly dried to industry standards (-50°C dew points) in this current generation of the test stand. The overall losses in the entire system should be assessed to provide performance and efficiency metrics so as to guide development of HTE systems in the future. The team should also check with the TA-015 team regarding front-end controller development efforts.
- It may be worthwhile to consider evaluating different heat exchanger configurations that employ anticipated renewable or nuclear thermal inputs.
- The project should establish performance-based goals tied to hydrogen production cost targets.
- Overall program management would be important. This should be more than just a proof-of-concept project.

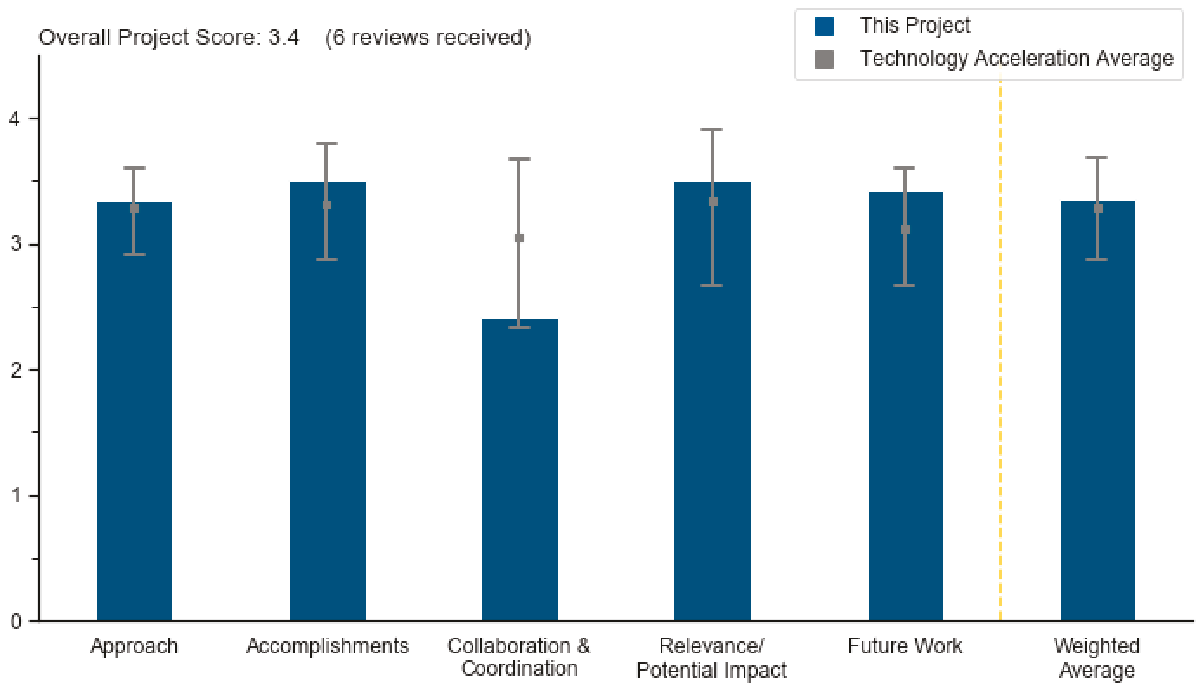
Project #TA-019: Modular Solid Oxide Electrolyzer Cell System for Efficient Hydrogen Production at High Current Density

Hossein Ghezel-Ayagh, FuelCell Energy

Brief Summary of Project

This project seeks to demonstrate the potential of solid oxide electrolysis cell (SOEC) systems to produce hydrogen at a cost less than $2 per kilogram, exclusive of delivery, compression, storage, and dispensing. Project activities aim to (1) improve SOEC performance to achieve greater than 95% stack electrical efficiency based on lower heating value of hydrogen, resulting in a significantly reduced cost of electricity use for electrolysis; (2) enhance SOEC stack endurance by reducing the degradation rate; (3) develop an SOEC system configuration to achieve greater than 75% overall (thermal and electric) efficiency; and (4) improve subsystem robustness for system operation compatible with intermittent renewable energy sources and their load profiles.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project's technical accomplishments are impressive and represent the potential for a step change in hydrogen production and power integration methods for the industry. The scaling-up process and test methodology are consistent with the technology readiness level of the development and size of the project.
- The approaches are excellent and logical.
- The approach is very comprehensive.
- The approach is very well thought out and explained. The only suggestion is that the economic analysis be completed at a large scale, perhaps 50 tonnes per day or more. Solid oxide electrolysis (SOE) is probably not as suitable for distributed production sites (of 1.5 tonnes per day).

- The approach seems reasonable for the steady-state electrolysis operation. It is unclear if this is a practical, real-world scenario; the possible electricity source was not discussed. Renewables are intermittent, so it may be nuclear, or it may be just grid-powered. It would be good to see the technoeconomic analysis (TEA) for this type of operation.
- The project is close to the end and has quite a bit of funding left. The researchers said they plan to buy equipment. Usually, it is best to buy equipment at the beginning of the project and use it throughout the project. Given that the project is scheduled to end September 30, 2019, and that an equipment procurement can often take several months, it is not clear how the equipment purchases will benefit the project.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Year after year, the team continues to show good progress and report results of improvements in stack and cell performance, as well as degradation.
- The project has made excellent progress toward the overall project objectives.
- The project is meeting and exceeding targets and milestones; this is very good.
- The project has good accomplishments and progress, especially in studying degradation over long times. At 50%, the steam utilization seems quite low. The team has a creative modular design.
- The project has demonstrated multiple years of operation at high currents. The cells and stacks seem very sensitive to uncontrolled disruptions in operations. The team needs to build better test stands, perhaps with backup power, to minimize the disruptions. The researchers tried to repeat the work, but the repeat of the cell had a higher degradation rate than the best-performing. The post-test analysis was very interesting. Cr migration and Ni depletion are challenges that have been solved in solid oxide fuel cell (SOFC) operation, so the team may be able to take some strategies from SOFCs and apply them to the project technology.
- The performance metrics were met for the electrolysis stack. However, demonstrating a complete and scaled-up system has not yet been done and will consume most of the project funds.

Question 3: Collaboration and coordination

This project was rated **2.4** for its engagement with and coordination of project partners and interaction with other entities.

- The amount of collaboration for this project is sufficient.
- Collaboration with other organizations and national laboratories is highly recommended.
- Collaboration remains the biggest weakness in this project. Without independent verification of the process or the results from a collaborative team, this project suffers from a credibility gap. Projects are always stronger when there is a diverse team working with the results and verifying outcomes. It would be particularly helpful to have a third-party TEA to validate the economic projections.
- There does not seem to be much collaboration. There does seem to be some coordination within FuelCell Energy, Inc. (FCE) with Versa Power Systems, Inc. (Versa) (which is owned by FCE) and some loose coordination with National Energy Technology Laboratory (NETL).
- There seems little collaboration up until this point. Perhaps NETL will participate in the TEA, but this was not mentioned.
- There is very little collaboration. Only two other collaborators are listed on the project, and one of them, Versa, is a subsidiary of FCE. NETL is referenced but, as stated, contributes only indirectly.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- If this project is successful, it could represent a breakthrough in the approach to energy and fuels, leading to a scalable platform with flexible applications, as is needed in this industry.
- Bringing down the cost of hydrogen at the nozzle is key to the success of the technology, so this has significant relevance and potential impact.
- Hydrogen is a core problem to be solved. This project addresses the efficient production of hydrogen with an SOEC system and provides a benchmark.
- The project aligns well with the DOE Hydrogen and Fuel Cells Program.
- The work directly contributes to DOE's solid oxide targets and goals.
- This project is highly relevant to H2@Scale. It has the potential to produce low-cost hydrogen. The scale-up and demonstration are needed for H2@Scale. Given the limited time left on the project, unless a no-cost extension is granted, the demonstration will be of minimal impact.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- This project seems to be very well managed and focused.
- Completing the demonstration and the performance testing will be the critical deliverables for this project, and the team is on a good pathway for completion. It remains to be seen if the schedule will permit sufficient testing before the project closeout.
- The future work is the demonstration. The demonstration is very important, but it is not clear whether enough time remains on the project for the demonstration to gain useful information.
- The proposed future work is appropriate; however, a more detailed description of the proposed approaches (e.g., pressurized operation) may be needed.
- Building a scaled-up complete system and running a demonstration will be most interesting. The question remains whether the stack can scale beyond current proportions. The proposed megawatt installations with numerous small stacks seem problematic. A larger stack would help simplify the proposed future large-scale installation.
- It is great to do cost analysis, and fine to do it for small production sites, but it seems the trend is to use SOE for large-scale production. As such, a cost analysis should be completed for large-scale hydrogen production as well.

Project strengths:

- This project is a novel technology that has the potential to significantly reduce the dollar-per-kilogram cost of hydrogen and can be offered in a modular format, therefore also being relatively cost-effective from the manufacturing perspective (as pointed out by the presenter).
- The technology development is excellent. This is a comprehensive project and technology development pathway.
- The project has done excellent work in stack development and degradation. FCE has many technical experts and is well suited for completing laboratory testing of their materials.
- The project was well funded. The durability tests were very important. FCE did a good job sharing the failure modes, such as the chrome and nickel migration.
- Demonstrating long-term steady-state SOEC data is very helpful and provides a benchmark performance metric for further research or modeling.
- The project's main strength is in the approaches and technical direction.

Project weaknesses:

- This project has no major weaknesses; however, additional coordination with other organizations and national laboratories is recommended.
- The project did not leave enough time for the demonstration unit. There is quite a bit of funding and not much time left. The demonstration should have started in the middle of the project (in year 2) so there would be sufficient time for the demonstration to occur. There is a good deal of valuable information that can be gained from the demonstration.
- The project should discuss scale-up for very large production volumes and include TEA for large production sites. There was no real collaboration with non-FCE entities.
- The lack of collaboration on the project has the potential to weaken the credibility of the results and projections. At a minimum, a third-party TEA is strongly encouraged.
- It is perhaps an oversight not to include some controlled thermal cycling and, instead, to base it only on steady-state operation.
- The lack of transient response data is a weakness, along with the absence of an economic justification or TEA.

Recommendations for additions/deletions to project scope:

- It is recommended that the team continue to build out the full standalone system; the results are highly anticipated. Possible additions could include stack scale-up and the TEA to make the economic case for the technology.
- Further real-world validation (which can include power outages, thermal excursions, etc.) is recommended to show robustness.
- It is a concern that the testing of the demonstration will be tight in the schedule. The results of this testing are critical, and an extended test period should be considered as a possible project extension.
- The team should apply for a no-cost extension.
- TEA for a large-scale production system is recommended.

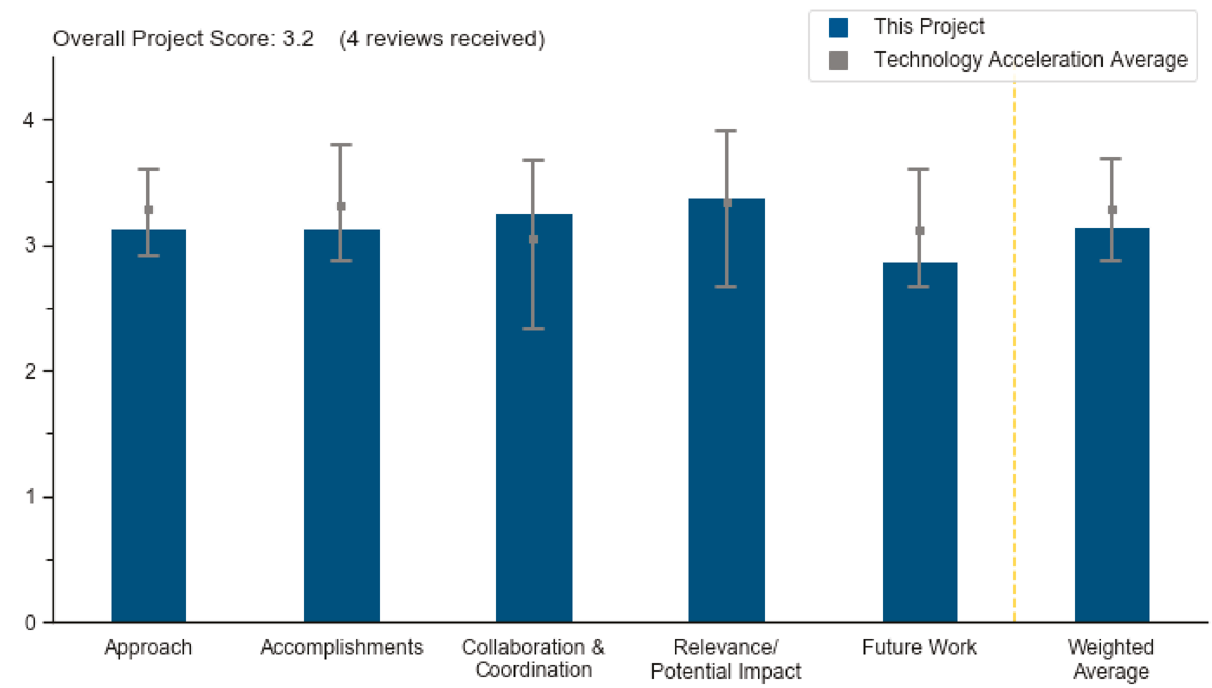
Project #TA-020: Optimal Stationary Fuel Cell Integration and Control (Energy Dispatch Controller)

Genevieve Saur, National Renewable Energy Laboratory

Brief Summary of Project

Current control strategies for building systems tend to be simplistic. The objective of this project is to create an open-source, novel energy dispatch controller to optimize the dispatch of different building components such as combined heat and power, storage, and renewable generation systems. Such a controller, which will incorporate improved forecasting capabilities and model predictive control strategies, would enable these building systems to participate in grid ancillary services markets. A planning tool for sizing building components utilizing simulated dispatch will also be developed.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is a good approach to the challenge of building control and grid integration. The team has a very quantitative explanation and comprehensive set of variables for all the control levers available for optimization, including constraints for the building occupant's comfort.
- The approach to this project is well aligned with U.S. Department of Energy (DOE) targets and the overall goals of the DOE Hydrogen and Fuels Cell Program (the Program).
- The approach appears sound. Focusing on inputs that are readily available and commonly produced by installed equipment ensures the model will be practically applied in real-world scenarios. The researchers mentioned "comfortable temperature bounds" in the presentation, which is an important consideration. This model will only be as effective as it is comfortable for users. Tenants will not care about economic dispatch modeling if they are sweating in their cubicles. It would be good to know whether those comfort bounds

have been defined, either by this group or previously. Progressive development can be seen in this project; the team focused on the model for single-zone building, then expanded to multi-zone. The researchers may have advanced too quickly. Ancillary services are "nice to have," but given that those markets are not well developed in the building space, it might not make sense to make them a core component of the objective. Capacity charges are probably the highest-value component of the electricity bill to pursue. It would also be beneficial to know whether the modeling effort includes rooftop solar. It would be valuable if building owners could try different scenarios with different components and then optimize for capital cost, energy cost, emissions, internal rate of return, etc. There is also some value in "islanding" a building during grid outages. Fuel cells could complement solar storage, especially in areas with low solar incidence for extended periods (days or weeks).

- This project seems to be driven by modeling building energy balances for the Grid Modernization Initiative (GMI). The project needs to generate some results from the model that indicate how it relates to hydrogen technology, fuel cell performance, etc. Developing a base case using natural gas combined heat and power may be useful in validating the model and assessing the "hydrogen advantage," if there is one.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project team has made nice progress, with the inclusion of multizone buildings to ensure comfort across a broad range of layouts and people. This will dramatically extend of the usefulness of the modeling and optimization results. The communication with Volttron and the open-source project is an important demonstration.
- The team has accomplished the expressed purpose of the project: a useable evaluation tool that enables the integration of stationary fuel cells into a building's energy efficiency design. The methods and tools developed by this project will certainly enable building designers and planners to consider stationary fuel cells in ways not previously considered.
- The results presented were concerning. The predicted values versus actual values did not appear to match well. Perhaps there is a metric that can be used to quantify modeling success, like the R^2 value. No results were presented for the single-zone buildings. It may be that the prediction was better for those simpler scenarios. It seems like a good practice to optimize the model on single-zone buildings before taking on a more complex problem. The researchers stated that modeling proved harder than anticipated; however, the key goal for this work has to be developing a good model. Everything else is dependent upon that core objective. It may make sense to abandon some of the later goals (e.g., hardware integration, ancillary services value) in order to focus remaining resources on improving the model. There was no discussion of economics, which has to be the key target for optimization. At the end of the day, building owners want to see the economic benefit to enhancing control of building systems. The value of this type of modeling comes out in the scenarios. From an industry perspective, what is wanted is a model that can reduce energy bills or building emissions by X% using this advanced control logic. The researchers should focus on reaching the point where some key scenarios can be modeled and the economic or environmental benefits can be clearly demonstrated.
- Alas, software tools take hours to develop but only seconds to use. It is hoped that the project will generate results and sensitivity analysis to see what insight these models give.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- Collaborating and sharing information with Washington State University, as well as interfacing with Volttron and the open-source community, are important highlights of the National Renewable Energy Laboratory's efforts toward collaboration, including efforts with Pacific Northwest National Laboratory. A wide range of expertise is needed to incorporate weather forecasting, in addition to building climate optimization. Including the OpenADR Alliance provides additional benefits by opening the door to

ancillary services. Including the University of Colorado Boulder is important for workforce development, as well as for enabling a broader distribution of the project and knowledge that has been gained.
- While the project is primarily an academic exercise, the project team has established enough critical links to private industry to enable a robust feedback loop. This has enabled the project to select reasonable examples and consider real-world applications not previously considered, addressing key gaps from the previous year's reviews.
- This is actually a big problem to solve. It looks like the partnerships are diverse enough to cover the various disciplines required to advance the work, and partners appear to be contributing value to the project.
- Until the project team has results that show something of interest to facility managers and engineers, it will be difficult to find collaborative connections, except among fellow modelers. There may be some intrinsic advantages to hydrogen systems that would capture interest, such as how fuel storage can be located in-structure, etc., which could segue to a compelling reason for hydrogen. This is what was found with backup power systems in Hong Kong: hydrogen storage was easier to site and approve than equivalent diesel fuel systems—in the event of a fire, the hydrogen storage would vent.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This research is absolutely critical to advancing fuel cell deployment in buildings. This kind of modeling is the first step in identifying potential deployments and building the business case for fuel cell integration. This will be a really valuable tool for researchers, project developers, and building owners. This is why it is so important to focus on the quality of the model and its ability to optimize for economics and emissions reduction.
- Buildings are a major energy consumer, and this project will enable future zero-energy buildings through extreme optimization and renewable energy optimization. The open-source nature of the tools will also enable as widespread an update as possible, without the barriers of proprietary high capital cost implementations, which may be more difficult to implement in less affluent areas of the United States or abroad.
- This project will have positive impacts on the design and use of stationary fuel cells as it reduces the barriers to designers and developers when considering fuel cell technology.
- The project does not seem to be directly relevant to goals of the Program. Thinking of building management systems as part of a larger energy system may support both clean energy systems and the core objectives of clean fuels for transportation and decarbonization. There could interesting synergies both on the system design and on the financing, using long-term property mortgage financing. That being said, hydrogen systems do not scale well to smaller sizes, and the source of the hydrogen is unclear.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- Keeping everything open-source is really valuable to advancing this work after the project is complete. Modifying the model for a web-based interface will also help more people use and refine it. It might be valuable for the presentation to cite other examples of open-source software that have been adapted for commercial use. It may have been that Linux was adapted to commercial software used for industrial control software, under the open-source model. Something along those lines would assuage any critics who may be concerned that industry will not want to develop something that is open-source. Hardware testing is not as important at this point. The early value will be for making the business case for optimizing operation. Integrating with actual hardware makes sense only once that business case has been verified. Future work should include using the model to look at scenarios for real building case studies. The team should be showing that the model is effective and then using it to propose optimized dispatch and calculate economic and environmental benefit.
- It is a good to see that the software will be integrated with a web interface to enable more user adoption. The hardware-in-the-loop (HIL) implementation and co-simulation should bring the project more

credibility and give future adopters a better idea of the limitations and opportunities of implementing this energy management solution. Future publications of analysis and lessons learned will be vital for ensuring a lasting value beyond the limited scale of the project.

- A stronger emphasis should be placed on communication. Publication and dissemination should be the main focus. Further research and HIL implementation are less critical to the project's impact than communication.
- The proposed future work is okay, but there is a concern that the project may run out of time before value is derived from the work.

Project strengths:

- The project addresses a key barrier to the use of stationary fuel cells in building energy systems. By creating a robust and accurate tool with relevant examples, the team has generated a work product that has the potential for significantly impacts on the market. This tool provides building designers and developers the information necessary to select stationary fuel cells, information to which they certainly did not have easy access in the past.
- The project's strengths include its open-source nature, the peer review with the sheer number of partners, and the focus on technology transfer that will ensure that the knowledge can be implemented outside the national laboratories with colleges and various other partners. The hotel case study is an excellent choice.
- The team and its partners represent a broad skillset and the experience to cover the many facets required for a modeling effort like this. This work is highly relevant and, if successful, will be very valuable to the fuel cell market.
- Software tools have been developed in the context of the GMI program, addressing identified barriers.

Project weaknesses:

- This project needs to increase the effort to communicate the results, thus ensuring the potential to accelerate private building developers' use of stationary fuel cell technology.
- There is a lack of progress and measurable results. More scenarios and an analysis of how well the model matches to the real world need to be seen. The project is running out of time, and it is concerning that resources are being used for hardware testing and ancillary services when they could be better spent improving the model.
- The project's weaknesses include bridging from research and development to opportunities for actual commercial or open-source implementation.
- At this point in the project's development, it is not clear how relevant hydrogen systems are. The team is running out of time, and it is not certain that the results will get to market.

Recommendations for additions/deletions to project scope:

- The project team should brainstorm with architects, building designers, and developers of other applications that could benefit from power from fuel cells and see what the models have to show. There may be input that could inspire the use of hydrogen fuel cells. For example, there may be applications such as data centers that could benefit from using low-voltage, direct current (DC) power, where energy could be delivered through a gas network, or applications in which fuel cells could convert hydrogen to DC power at point of use, with some heat recovery. New solid-state light sources could benefit from low-voltage DC power that could be produced by fuel cells at the point of use, etc. It will be interesting to see how Japan will use hydrogen to power the 6,000-unit Olympic Village for the 2020 Tokyo games.
- The project team should increase efforts to distribute the knowledge (e.g., through publications, analysis, and case studies) and ensure that open-source software with documentation is available in a single project portal page that does not disappear at the end of funding. The team should try to quantify the savings from implementing the software for different building types in order to encourage adoption.
- The project should remove HIL testing and the work on ancillary services. The project team should also show at least one case study (a real-world building or a DOE prototype building) in which the model showed the value of integrating a fuel cell.

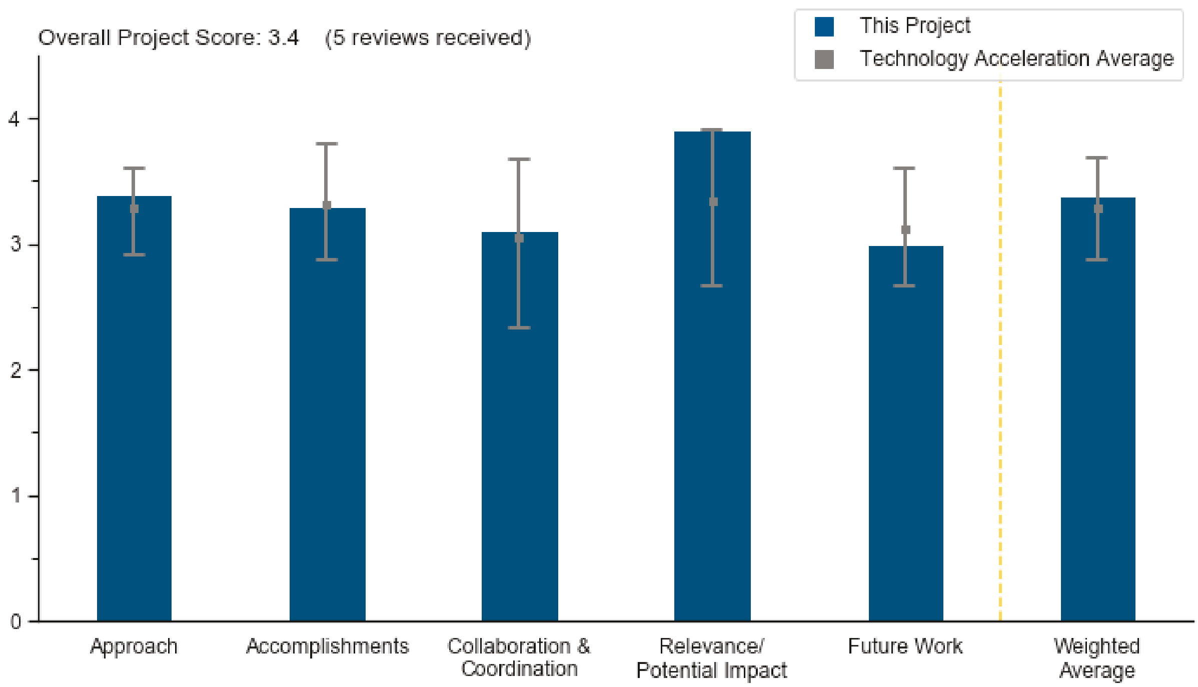
Project #TA-021: Integrated Systems Modeling of the Interactions between Stationary Hydrogen, Vehicle, and Grid Resources

Samveg Saxena, Lawrence Berkeley National Laboratory

Brief Summary of Project

Hydrogen technologies offer the unique ability to simultaneously support the electricity and transportation sectors, but the value proposition for such systems remains unclear. This project is developing an integrated modeling capability to establish the available capacity, value, and impacts of interconnecting hydrogen infrastructure and fuel cell electric vehicles (FCEVs) to the electric grid. The potential to support the grid and the potential to balance resources from flexible hydrogen systems, such as dispatchable production of hydrogen by electrolysis, are quantified. The project is also developing methods to optimize the system configuration and operating strategy for grid-integrated hydrogen systems.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project provides a good economic evaluation with a focus on California, where the biggest challenges will be experienced with excess renewable energy. The model includes historical prices for a realistic framework for evaluating the benefits of hydrogen production from electrolyzers. Optimization is occurring between the grid and hydrogen, with detailed inputs from the Scenario Evaluation, Regionalization, and Analysis (SERA) model on the use of FCEVs and the demand for hydrogen. By using PLEXOS simulation software, the project team will have a full picture of existing electricity demand. This is a comprehensive approach that should provide a realistic set of results.
- The project approach is well aligned with both the project objectives and the Hydrogen and Fuel Cells Program objectives. The project is also well described and effectively communicated. It is clear that the

researchers understand the detailed subject and have worked hard to resolve the most relevant information to make it easily understandable for a larger audience. It is this final, critical step of "distillation" and communication that separates satisfactory projects from excellent projects.

- As illustrated on slide 3, the conceptual overview is straightforward and readily understandable. The barriers addressed by the project, as shown on slide 2, are not specifically included among the barriers listed in the Technology Validation (now Technology Acceleration [TA]) or Systems Analysis (SA) sections of the Fuel Cells Technologies Office (FCTO) Multi-Year Research, Development, and Demonstration Plan. The project approach is to develop a hydrogen–vehicle-to-grid integration model that utilizes and integrates work done on multiple models; this approach is logical and efficient as a means of achieving the challenging objectives of this project. As described in slides 6–10, the approach is comprehensive and thorough, and it incorporates real-world data. The approach has outstanding potential to achieve the project objectives cited on slide 3. However, the primary focus of project activity seems to have been on developing a more extensive modeling capability. Evaluated as a TA project, the approach is "good." Evaluated as an SA project, the grade would be at least "excellent."
- This work is very good. However, there are some components that should be considered to make it more robust in future work, such as the daily volatility of gas prices and the availability of electricity rates in the regulatory framework.
- It is good that the work is building on other modeling work that already exists and is integrating those models to explore this area. There are some scenarios that will, one hopes, be produced in the wrapping-up portion of this project going forward; their summarized results and output are highly anticipated.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The cost comparisons for multiple hydrogen infrastructure scenarios, as reported on slide 13, are impressive. The accomplishments cited on slides 13–15 are a testimonial to the potential benefits associated with an improved, more extensive, integrated modeling capability. The potential will be realized, however, only to the extent that the integrated model will be used to inform decisions by stakeholders, including vehicle manufacturers, hydrogen producers, electric utilities, and regulatory agencies. The project team has responded well to prior comments from reviewers and input from stakeholders (as seen on slide 16).
- This project makes a solid contribution to both the Hydrogen Production R&D subprogram work, in terms of understanding the economics of production and distribution, and to the H2@Scale framework by developing specific scenarios for the availability of hydrogen and electric power.
- This work supports the rollout of FCEVs and supports understanding of the infrastructure and value that could be derived from that infrastructure.
- The accomplishments of this project are significant in that the analysis has a significant impact on the stakeholders. It is well explained but could be more concise. The results beg the question of practicality. Onsite electrolysis has been implemented at hydrogen refueling stations in California, elsewhere in the United States (at DOE facilities), and globally. It may be that the researchers were not granted access to the data from those installations, or they may have simply not asked industry partners for data. Many might consider onsite electrolysis in California as bringing about some significant practical barriers, with respect to negotiating rates and relevant scale for the grid operator. While the results show a great advantage to onsite electrolysis, perhaps there is something in the implementation that is worth investigating.
- Good progress has been made on four of the five stated questions, and progress has been made toward the project's goals by studying the following: (1) the benefits of central versus distributed hydrogen production; (2) the potential level of renewable energy integration with hydrogen production; (3) the economic impact of hydrogen on the grid through PLEXOS; and (4) the impact of the accelerated hydrogen demand from medium-duty (MD) and heavy-duty (HD) hydrogen trucks. The last portion of the project through September 2019 will likely cover higher penetrations of wind and solar. The team has made a credible effort toward integrating multiple complex modeling systems, including SERA, PLEXOS, and renewable profiles. Unfortunately, there are a few items that could be improved. It is unrealistic to expect shipping delivery organizations to use hydrogen if MD and HD vehicles are not evaluated. This would be especially relevant if hydrogen cost targets are met, i.e., lower-cost hydrogen could be used for transport.

As liquid is stated as the preferred delivery method for most stations being built now, it seems the model is missing a key distribution option.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- It is very good for the project to build on models from the National Renewable Energy Laboratory (NREL) and others and to collaborate with data coming out of California.
- There is good integration with multiple laboratories and some input from an industry think tank. It would be helpful to collaborate with some industrial gas companies or station providers to give more realistic input on future station developments.
- Within the project, the collaboration among team members from Lawrence Berkeley National Laboratory, NREL, Idaho National Laboratory, and Emerging Futures, LLC, seems appropriate and effective. There are concerns regarding insufficient coordination with teams working on other hydrogen-related modeling activities, e.g., H2@Scale. During the question-and-answer portion of the presentation, a question was asked about the intersection of this project and H2@Scale activities. The response indicated there is awareness and some communication but that coordination across projects is limited by time availability and is not a high priority. The issue of whether there is overlap and duplication among modeling projects being funded by FCTO should be addressed.
- The project's collaboration was primarily referred to in terms of utilizing the models from NREL and others (SERA, V2G-SIM, PLEXOS, etc.). Otherwise, there was not much reference to specific discussion or coordination with the partners. The presenter acknowledged this in terms of time limitations for getting the work done. It seems like there are some additional opportunities here for more peer interaction and likely related refinement or improvement of the results.
- This project appears to suffer from a lack of non-academic stakeholders. The conclusions reached regarding onsite electrolysis generation ignore significant barriers to the practical implementation of such a solution. Industry stakeholders are needed to validate the conclusions and provide critical feedback to conclusions reached through economic theory. A workshop, or similar discussion of the project among stakeholders, would greatly benefit this project.

Question 4: Relevance/potential impact

This project was rated **3.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The output of this project is very highly relevant to H2@Scale; one of the greatest benefits of using hydrogen as an energy carrier is making renewable energy available at times other than when it is being produced. Therefore, this work is going to inform the economics of which applications make economic sense, as well as where and at what scale.
- This work will be very valuable for utilities and others evaluating the infrastructure needs.
- The effort gives high-level input for the direction of hydrogen and the potential for renewable integration. The work can be considered as a general pointer for integration and for how hydrogen can be used to benefit the grid. The project may be taking on too much, but there is good progress to date.
- The potential benefits to stakeholders are summarized on slide 5. This summary underscores the project's relevance. In response to a question asked after the session, Dr. Greenblatt stated that an independent transmission system operator engaged the project team to provide information for its analysis and decision-making. Stakeholders' use of results provides a tangible indication of relevance.
- This project has significant potential impact, particularly in California, where the largest commercial hydrogen energy market exists. Unfortunately, the analysis is incomplete and belies a false conclusion for policymakers, which industry partners will now need to dedicate time and effort toward correcting. This type of work is counterproductive to the overall goal of sound policy and progress toward cleaner air and lower carbon intensity. Industrial partners are needed in this project to provide sufficient insight into the practical aspects of the developed theory. With this critical insight, the clear barriers to market evolution

can be determined and demonstrated. Through such collaboration, strong, dynamic, and market-based solutions can form virtuous cycles that encourage positive behavior. For example, the researchers should consider the Low Carbon Fuel Standard hydrogen capacity credit program recently instituted at the request of industry. Similar policies could further incentivize the acceleration of grid-scale electrolysis, with all the benefits cited in this work.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The last part of the work will be the most valuable. Finding the tipping point for increased renewables should only make hydrogen more attractive. The energy markets are enormously complex, and considering the stock of hydrogen, the spark spread between natural gas and electricity, and the impact of out-of-state liquid, there is still much to be done.
- The work that is to be done during the remainder of the current project (through September 2019) is described well on slide 19. The analyses will appropriately utilize the modeling results accomplished by the project. Including the results synthesis and dissemination in the remaining work this fiscal year (FY) is a plus. There was only a single line describing work that could be done with funding beyond FY 2019; this is not sufficient to make a case for additional resources. The grade for this element would be higher if there were more specificity about follow-on work beyond FY 2019, how that work would address barriers and benefit stakeholders, and how the work would complement other FCTO-funded activities.
- At this point, it appears that the future work consists primarily of summarizing and reporting the results. It will be valuable for the principal investigator to do some sensitivity scenarios related to the price of renewable power, as it is possible that the increased demand for stranded renewable power will result in the price's rising. It was also proposed that it would be helpful to have an understanding of the model's sensitivity to the interplay of electricity prices and natural gas prices.
- The proposed technical direction for the project is well aligned with the project objectives. The proposed future work should include the feedback from other stakeholders.

Project strengths:

- The project team has extensive experience with the development and application of the multiple models that have been integrated. The modeling and analytical capabilities within the national laboratories are superb. With sufficient stakeholder collaboration, analyses resulting from the integrated models have the potential to be valuable inputs for organizations with an interest in fuel cell and hydrogen technologies.
- The project does a good job of integrating and building on other models that describe the "building blocks" of the overall ecosystem. The project also does a very good job of addressing a very important element of implementing H2@Scale and renewably producing hydrogen for fuel.
- The project has good modeling if the narrow scope and artificial framework is acknowledged. More aspects and market dynamics will need to be covered to get the most use out of this project. There is nice integration of SERA and PLEXOS, which are very complex but allow for good linking of diverse markets.
- This is very good work.

Project weaknesses:

- At least so far (and this may resolve with the final work on the project), there has been no reference to the economics of hydrogen production. It needs to be shown if there are modeled scenarios that will produce hydrogen at or near the DOE target cost for hydrogen fuel. This is the key value of this project; there is a need to identify the many scenarios where work can be stopped, as well as the few scenarios that need focus, based on economics.
- This project has strong technical strength yet lacks critical feedback from industry and policy stakeholders that would guide the practical application of the results of the analysis.
- The project needs to (1) receive more industry input from those building hydrogen stations, (2) improve the integration of other energy streams, from renewable natural gas to liquid delivery, and (3) consider hydrogen as transportation fuel for tube trailers (or liquid, if included in a future effort).

- There seems to be insufficient collaboration or joint planning with other hydrogen-related modeling and analytical activity, much of which is being conducted by the same national laboratories associated with this project. Work such as what has been accomplished by this project should be well coordinated with other systems analysis activities funded and supported by the FCTO, including H2@Scale. There is no clearly articulated link between this project and the barriers cited in FCTO plans. Nevertheless, the project does support the FCTO's goals and objectives. There could be more outreach about the project and its results to stakeholders with financial and regulatory interests in hydrogen and fuel cells.

Recommendations for additions/deletions to project scope:

- It would be very helpful for the project team to include some sensitivity studies of the impact of varying electricity prices and the capital expense of varying electrolyzer usage to narrow down the scenarios that should be pursued.
- If follow-on work to this project is funded by the FCTO, it should be planned in conjunction with and folded into activities under the H2@Scale umbrella.
- The project team should perhaps include liquid hydrogen and the impact of out-of-state biogas in future efforts.

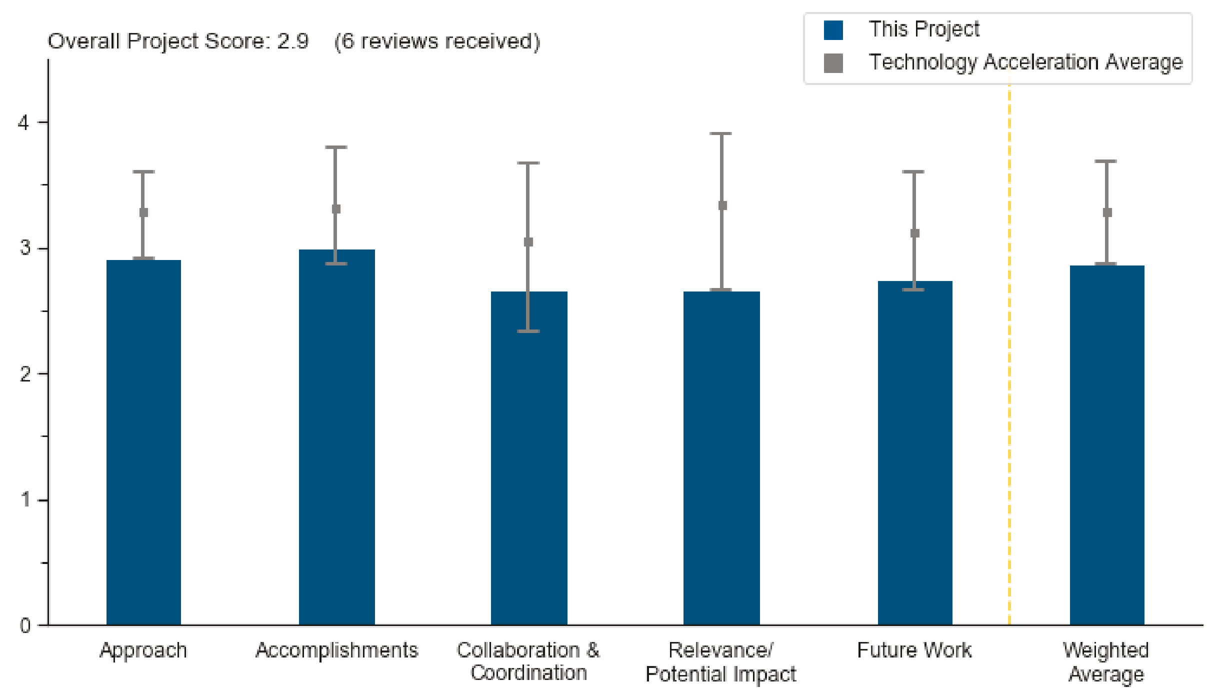
Project #TA-022: H2@Scale: Experimental Characterization of Durability of Advanced Electrolyzer Concepts in Dynamic Loading

Shaun Alia, National Renewable Energy Laboratory

Brief Summary of Project

This project aims to evaluate electrolyzer durability with dynamic loading and assesses the ability of electrolysis-based hydrogen production to be cost-competitive while maintaining performance with extended operation. Los Alamos National Laboratory (LANL) will support the National Renewable Energy Laboratory (NREL) in (1) establishing baseline performance as a guide to catalyst and electrode development and (2) evaluating the influence of low loading, intermittency, and system controls on durability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **2.9** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is essentially determining the conditions under which electrolyzer operation will affect system durability, lifetime, and performance. From a materials perspective, this is an appropriate position, but it would be good to see the project better bridge to the electrolyzer design. The team should consider whether there is an acceptability criterion or a design criterion that could be developed to determine acceptable performance under these conditions. The team should determine how much degradation is acceptable and how a system can be designed or operated to minimize this.
- The research is following a logical path in an area highly relevant to the integration of hydrogen renewable power systems.
- This project should be able to contribute to cost reduction over the service life of electrolysis from numerous intermittent energy sources by extending the service lives. The project does provide useful input to future electrolyzer designs for challenging operating environments. It is very relevant to the success of

such applications. However, while the repetitive trial-and-effect method does a good job improving understanding the results of various catalysts, cell materials, morphologies, etc. in the presence of specifically varying inputs and loads, it does not address the underlying physical chemistry. Getting to the fundamental mechanisms of change within the cell and its materials would serve a wider purpose for future electrolyzer designs needed in intermittent and variable renewable power sources. The cycling tests show that degradation increases with the total number of cycles and cycle frequency, which is not unexpected, but the wave shape effects (flat, square, and triangle) show differences that lead to the need to understand the fundamental kinetic mechanisms for the degradation. The team should determine whether there are time-resolved effects (dE/dT, dI/dT, etc.) that need to be understood. If more fundamental studies were possible, they could more effectively lead to loss mitigation strategies for more universal electrolyzer design criteria. Such efforts do not fit within a $650,000 budget, however.

- The project uses catalysts with much lower loadings than real catalysts and subjects these model catalysts to severe operating conditions to obtain deactivation in a short time. Accelerated catalyst aging is useful to obtain deactivation data in a reasonable time, but accelerated aging sometimes involves deactivation mechanisms that have little or no relation to mechanisms present in the aging of catalysts under real conditions. To understand whether the deactivation mechanisms are the same, the investigators should make greater use of advanced characterization techniques on real and model catalysts deactivated under standard and accelerated conditions.
- It was not until slide 13 that it became apparent that this presentation was on polymer electrolyte membranes (PEMs). The approach is basic: fabrication, testing, and post-mortem. The cycle is missing "revised design." The approach appears to be to test PEM cells with iridium- or rutile-doped electrolyte (several grades of deionized water) for various load profiles and then to evaluate the structure of the catalyst layer.
- The approach to this work seems a bit rudimentary, given the maturity of the industry. It is not clear why there are not more industry partners or why the approach does not include a validation with field experience. The barriers are industry barriers based on feedback from field experience and industrial issues. This experimental approach seems to miss this critical connection.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has effectively built upon previous years' work with much-needed data and analysis on the materials performance. This will provide a good basis for the next steps.
- The accomplishments and progress to date lead toward a number of design inputs for electrolysis in highly variable environments. The testing to relate various electrochemical element component choices to sensitivity to operating environments should be very useful.
- The project has established some useful test methodologies that can be used to evaluate potential mechanisms for performance loss, as demonstrated by the interesting findings regarding the fabrication of membrane electrode assemblies (MEAs).
- The experiments have been carried out carefully, and the mechanisms of deactivation have been identified. Given the fact that the deactivation mechanisms have been identified, the project needs more focus on techniques for extending catalyst lifetime.
- Half-cell and single-cell testing with iridium- and rutile-doped electrolytes promotes catalyst degradation. The increases in Nafion™ content appear to accelerate the degradation.
- The work presented seems to be a repeat of junior-level chemical engineering coursework from the early 2000s. The low loading and effects of square wave on Nafion membrane single cells are well known. Additionally, the effect of fabrication techniques seems specific to the work conducted at NREL, with no correlation as to how production of a single cell with low catalyst loading has any relationship to the cells of a multi-megawatt stack produced commercially. It is hard to understand how the researchers were unable to use the $650,000 provided to develop a project with greater impact. Perhaps this is unfair criticism, but the information provided does not demonstrate any substantial contribution to DOE goals. If this criticism is inaccurate, perhaps the investigator should better explain how the accomplishments will be used by

industry for commercialization, or if this is a standard approach for other researchers in evaluating single cells. This is a guess, as it is not explicitly stated by the presentation.

Question 3: Collaboration and coordination

This project was rated **2.7** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration between NREL and LANL was effective in accomplishing the different efforts of the project.
- Given the performance of commercial catalysts, the project should seek industry collaboration in continuing the work under a new mandate. In the meantime, the project should continue its strategy of publishing and presenting findings.
- It is probably time to bring in more electrolyzer design teams from industry to evaluate how these data and this performance information can better inform their operations and system designs.
- It would have been nice to include a PEM electrolyzer manufacturer, such as Proton OnSite.
- Although the investigators have worked with one other national laboratory, there is no indication that they have collaborated with or sought input from manufacturers of commercial solid oxide fuel cells (SOFCs). These interactions are vital if the project is to yield results that are useful in the real world.
- This project involves two national laboratories operating in a silo, independent of the industry; this has resulted in research for the sake of research. It is unclear whether anyone besides the project participants will see this information other than at the Annual Merit Review.

Question 4: Relevance/potential impact

This project was rated **2.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The topical area of electrolyzers' service-life sensitivity to dynamic operating environments is critical to the long-term success of electrolysis from intermittent sources, such as renewables. This project addresses some of the underlying service-life issues.
- Electrolyzer reliability and durability remain key issues in the long-term reduction of hydrogen production costs.
- Performance degradation is an important issue and highly relevant to the industry's achieving targeted cell-stack lifetimes and life-cycle costs.
- If hydrogen is to be used as an energy storage buffer (e.g., fuel cells or flow batteries), power-load following of the grid is required. Electrolyzers do not like load following. Simple loads were tried (e.g., square wave and triangular wave), and they accelerated the decay. Higher potentials were also an issue, as would be expected from catalysts operating above reversible hydrogen electrode (RHE). The team should try limiting the local oxygen potential to less than 1.0 V above RHE. This could be done with a dummy load.
- Although the project focuses on catalyst deactivation, the investigators have no evidence for what role catalyst deactivation plays in the cost of SOFCs. Without a quantification of the impact of catalyst deactivation on the capital and operating costs of SOFCs, it is impossible to gauge the importance of this work. The project seeks to identify the causes of catalyst deactivation, but it has not produced strategies for maximizing catalyst life.
- This project has significant potential but fails to leverage necessary partners and develop a project with relevance. Lowering the cost of electrolysis through technology improvement is a key factor in the transition to lower-carbon hydrogen production technologies. Electrolysis performance, particularly the better use and durability of catalysts, is a critical area of research. The researchers unfortunately squandered that opportunity with research that is devoid of industry interaction. This is despite seemingly well-positioned capabilities for the production of single cells and a project idea for low loading and high potential, which is seemingly meant to accelerate end-of-life failures or design vulnerabilities (though this is not clear, as it is not explicitly stated). The researchers manage to provide only a research-for-research's-

sake result that has benefit for neither industry stakeholders nor research peers. NREL has done DOE a disservice in the execution of this project.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The work will continue to use testing methods to identify sources of performance degradation, which is good. The team should publish results and get feedback. Continuation of this work should be supported by industry.
- The proposed current-based testing could be helpful in identifying more fundamental mechanisms of performance degradation in a dynamic environment.
- The project investigators should work with commercial fuel cell producers to quantify the potential benefits of the project. The team should work to verify the assumption that the deactivation of low-loading catalysts under accelerated aging conditions is the same as the deactivation of real catalysts under normal operating conditions.
- It is suggested that, prior to full-sized cells, the team should first master local voltage control of a single cell. The team should avoid conditions of mixed potentials on the anode, a condition that may result in excessive local cathode potentials.
- The proposed future work does not address the key issues with this project and does not allow the results to achieve some useful purpose. During the review, the presenter was asked simply, "What is success?" The project team should return to this question, as neither the presenter nor the presentation clearly answered this basic question. It is not the DOE Hydrogen and Fuel Cells Program's (the Program's) management goals or a lack of clear DOE targets, it is not a lack of interest from the industry, it is not a lack of technical understanding by the reviewers, it is not a lack of funds, nor is it a lack of skill or resources. It is the research team and the DOE Program manager who are complicit in not achieving a better result. There is time yet to achieve a positive result, and the team should move quickly to change direction to find a means to define and achieve success.

Project strengths:

- The project makes good use of electrochemical characterization to model the deactivation of model catalysts under accelerated aging conditions.
- Tools have been developed that should be helpful in improving the performance of electrocatalysts in electrolyzers.
- The project partners made significant progress in their planned research, given a somewhat limited budget.
- There is detailed materials analysis of degradation modes.
- The topic of electrolyzer performance is the best part of this project.
- The project's strengths include the team's diligence and energy.

Project weaknesses:

- There is no technoeconomic analysis to validate the assumption that extending catalyst life will have a significant impact on the cost of hydrogen. The project also has a weakness in its assumption that the deactivation of low-loading model catalysts under accelerated aging conditions is related to the deactivation of real catalysts under normal operating conditions. There is little or no activity in the project for improving catalyst lifetime.
- The lack of depth of study into more fundamental details of the electrolyzer degradation process in a dynamic loading environment may make it difficult to understand degradation and failure modes of electrolyzers in a way that could lead to successful design changes.
- The results need to be tied in and made relevant to electrolyzer design and operations from a systems-level perspective.
- The project needs to engage industry in order to continue the work; the researchers should get feedback on the relevance of the test methods, etc.

- This project has many previously outlined weaknesses.
- The project's weaknesses include communication skills.

Recommendations for additions/deletions to project scope:

- The scope of the project is accurate; the project should apply itself to achieving its potential through communication and relevance rather than through further efforts in new technical results.
- With industry support, this project should seek continuation.
- The project should add technoeconomic analysis to quantify the impact of catalyst deactivation and set targets for improvement in catalyst lifetime. The team should also carry out work to compare the deactivation of model catalysts under accelerated aging to the deactivation of real catalysts. The team should also work with commercial SOFC manufacturers to make sure that the work is relevant.
- The team needs to collaborate with industry suppliers to understand any problems in electrolyzer performance that may be caused by variable operating environments. The team should extend the project into more fundamental analysis of basic physical, materials science, and chemical processes in electrolyzers related to intermittent and variable supplies and loads. If at all possible, the project should consider alkaline systems as well.
- The team should look at the effect of local voltage control.

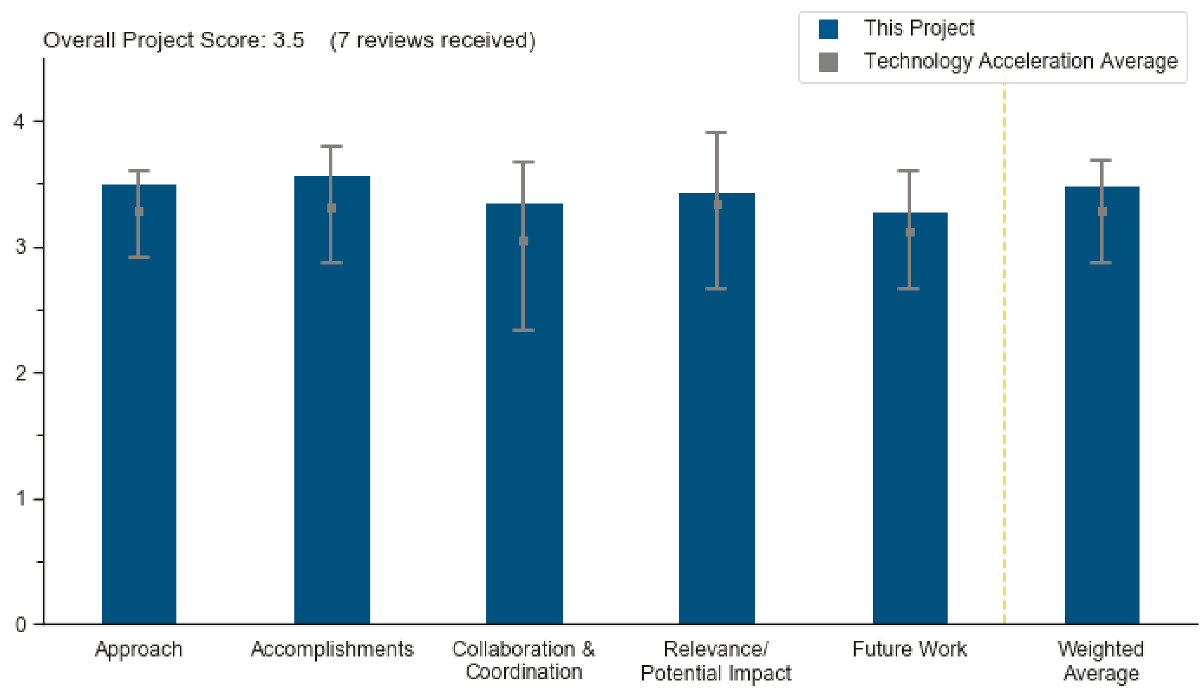
Project #TA-023: Hydrogen Stations for Urban Sites

Brian Ehrhart, National Renewable Energy Laboratory/Sandia National Laboratories

Brief Summary of Project

The primary objective for this project is to create compact risk-informed and performance-based liquid hydrogen reference station designs that are appropriate for urban locations and permit hazard reductions, as well as improve near-term technology. Hydrogen Fueling Infrastructure Research and Station Technology (H2FIRST), a Sandia National Laboratories (SNL)–National Renewable Energy Laboratory (NREL) collaborative project, will partner with industry stakeholders to identify methods of reducing physical station footprints and address the possibilities for station layouts within urban sites.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has clearly identified three Fuel Cell Technologies Office (FCTO) barriers to address and is positioned to address all three appropriately. The FCTO has targeted a 40% reduction in station size by 2022, relative to 2016. It sounds like this was initially a technical target, i.e., whether fueling station equipment can be reduced in size to reduce the overall footprint. A key takeaway from this update appears to be that this is not a technical question but primarily a regulatory question. That is, the work has identified the main drivers of station footprint, and they appear to be fire codes. This analysis, however, is scientifically rigorous and fact-based, which will make it valuable in addressing the regulatory hurdles to reducing station footprint.
- The approach is very clearly defined; the project identifies three critical barriers that guide the focus of the station design. The project also considers the objectives and input of the FCTO, as well as those of the

commercial and policy stakeholders involved in the H2USA initiative. Codes and standards are also integral to the scope of the work.
- The approach for this project is very well aligned with its objectives and the Hydrogen and Fuel Cells Program's (the Program's) goals.
- The project has a well-organized approach to reducing station footprint. The station delivery size appears small for commercial application. Presumably this would be a prototype station.
- The approach uses reasonable assumptions and established industry specifications for the delivery methods and technologies used in the layouts.
- The project appears to cover most of the aspects of hydrogen refueling stations (HRSs), from a modeling perspective.
- The approach is excellent and appropriate for the project work.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project's accomplishments appropriately represent the key questions industry faces when siting stations in compliance with existing fire codes. The work highlights some of the key aspects beyond simply the equipment and takes into account the various challenges faced in real scenarios. The work accomplishes a scientific method for evaluating sites and options in order to highlight the interaction of equipment technology and site layout with the efficacy of hydrogen in the gasoline forecourt.
- The project demonstrates that a comprehensive set of key accomplishments has been achieved. The base case and critical components for station footprint have been established for gas and liquid delivery as well as on-site electrolysis. Codes and permitting issues have been identified for each of these as well. Economic analyses are included. The comparison with a real-world station further strengthens the project.
- The project's accomplishments include its well-organized analysis of station types with explanations of the strengths and weaknesses of gaseous, liquid, and electrolysis cases. The team has clearly identified that the size of the delivery trucks for gaseous and liquid hydrogen is important. The team has also evaluated alternative designs for reducing footprint, identified a co-location case with a convenience store as a real case, and analyzed gas stations to get a comparison base. However, it is not clear if the daily delivery of gasoline fuel is the same as the daily delivery case for hydrogen that was studied here.
- The project appears to provide useful information for station development and future development direction with regard to footprint planning and development.
- The team shows good progress toward evaluating a range of station types.
- This project has made excellent progress to achieve its objectives.
- The researchers have made good progress on developing their base cases and examining some key alternatives to potentially reduce station footprint. The summary table of lot sizes for all cases is an effective way of sharing the data and showing the key results from the study. The summary table of setback distance that could be reduced was also an efficient way of communicating that information. It is recommended that the team provide some additional description of how setback distance can be reduced, i.e., through special measures, but also perhaps some justification for challenging the setback distances with data. The base case is for a 600 kg/day station. California typically looks for stations with a size of 1,000 kg/day, especially if public money is provided. The authors should consider commenting on how much impact station capacity has on the overall footprint and, specifically, how increasing capacity to 1,000 kg/day would affect the study results, at least qualitatively. It would also be interesting to know if there is another way to quantify lot size that takes into account the area and features of the length of the sides. It may be that most station lots are relatively square, so area is sufficient. But if there are oddly shaped lots (like a really long, skinny lot), additional parameters would be required to really understand how the station layout could be optimized for minimum footprint.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The project has sufficiently discussed and vetted information with various stakeholders to ensure that the information is science-based, generically applied, and useful.
- Fifteen stakeholders are identified in this collaborative project with Sandia National Laboratories (SNL) and the National Renewable Energy Laboratory (NREL). There is a strong effort to get the hydrogen community involved.
- Effective and excellent coordination has been demonstrated.
- The collaboration and coordination are good.
- While there is only one other formal project partner, several collaborators are named as informing the project. The project should further illustrate the type of information that is shared between the broader set of collaborators and what additional information could strengthen the project.
- A better approach to this project might be to partner with a site owner or a city planner to look at specific sites for implementation and optimization. In the field, there are huge variables from site to site that are well beyond the simplified layouts used in this study.
- There are a number of collaboration partners listed, but the presentation did not give the sense that many of them had contributed more than equipment data. Fueling station developers and operators should be more involved, especially in considering an atypical station layout, such as underground or rooftop. Questions remain, such as whether those designs are exclusively economic decisions. It is unclear whether developers and operators provided any input on concerns about operations and maintenance, permitting, or aesthetics; whether they have much experience in reducing setback distances; or how they feel about the shorter delivery truck concept. California Air Resources Board's California Hydrogen Infrastructure Tool could be useful for identifying existing gasoline stations that would represent high potential for hydrogen fueling. Those stations could be selected for further analysis of co-locating hydrogen fueling and of what setback reductions or other advanced concepts would be required to successfully integrate hydrogen fueling.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The reduction of station footprint is a critical barrier to commercial fuel cell vehicle deployment, and this project is very relevant. The potential impact of the project is made stronger both by including theoretical designs and by integrating real-world barriers and issues into the analysis. The project's focus on California and the Northeast is also very much aligned with the original equipment manufacturers' plans for vehicles.
- There is significant potential impact for this work, especially as it concerns focusing future research and development efforts. If appropriate, the authors should explicitly state that the key to station footprint reduction is not primarily a fuel cell technology problem but a regulatory problem (e.g., setbacks) or logistics problem (e.g., delivery truck size). Additionally, creating a framework to screen existing gas stations would be very beneficial in developing new hydrogen fueling options and focusing state money (at least in California) on the most cost-effective locations for station development.
- This is an important project that anticipates the design of a hydrogen station in a commercial environment. The project has the potential to place the safety, codes and standards (SCS) and permitting for the future deployment of hydrogen stations on a firm basis.
- This information has a strong impact, not necessarily on the industry participants, who likely already know the challenges, but rather on the overall community. This work helps establish a consistent and defensible dialogue around site challenges and equipment options to allow policymakers and industry participants to engage in productive dialogue. This is a key aspect of the Program's goals.
- The project aligns well with the Program.
- The project has clear potential impact; however, the focus is not on the co-location of hydrogen with other fuels (such as gasoline), while that is what industry is currently pursuing because of zoning and aligning with providing a gasoline fueling experience. Something that should also be kept in mind with all DOE and

H2FIRST reports is that when final reports are finally published, the observations are far behind the status of technology, and this is typically not clarified in reports.
- This project is difficult to strongly support. Most of the work on this project is already being done in the field by the station installation teams and project teams, and the site-to-site variability of elements such as layout, facility hookups, look and feel, and site owner acceptance is a huge issue that cannot be addressed in this study. This type of project may be best left up to the industry players.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The project has accomplished a good deal, and the team is on a good trajectory to complete the key goals for the study. The proposal to incorporate alternative means into SCS is a logical follow-on to this work, given that reducing setback distance appears to be the key pathway to footprint reduction. Exploring underground storage safety codes seems less valuable, given that so few stations will likely find it economical to deploy underground storage.
- Because the project is near completion, the proposed work focuses on finalizing the studies and designs and preparing the final report. The future work proposed under new contracts appropriately concentrates on SCS to further address that barrier.
- It is excellent to see direct liquid burial included in the work proposed for the last few months of this project.
- The proposed future work is appropriate.
- The proposed future work is to complete the project and issue a report; this would be outstanding, like the rest of the project. Unfortunately, real fueling stations supply 200 to 300 vehicles per day, and this approach would address only 30 to 60 vehicles per day. The future work should consider stations with commercial delivery capability.
- The project will end, but the proposed future work could use more evaluation and better detail to ensure that it will be relevant. Validation of alternative means and methods is a very difficult approach and might be stepping over the line between academic work and industry advocacy. Additionally, underground storage may be interesting, but perhaps there are some other areas, with respect to safety consequence and frequency reduction, that might elicit more beneficial results.

Project strengths:

- The team is following a logical and rigorous process for working through this problem. They have developed good results that clearly identify the best levers to pull to reduce station footprint. The real-world case studies are a great way of communicating the impacts to the audience.
- The project is very focused on key barriers and objectives and very much aligns with industry needs for further vehicle commercialization. The end results will inform technical work as well as policy and codes and standards.
- The project's strengths include its effort to assess what factors play a role in reducing footprint based on codes and standards, as well as alternative methods to meet the same intent.
- The project fits a need within the industry's best practices, helping to identify barriers and placing those barriers in easily understood terms.
- The strong team made up of SNL and NREL has made this project successful.
- The project has good conceptual topics and a good use of industry standards for systems and layouts.
- The project's main strength is in the approaches that have been used to conduct the work.

Project weaknesses:

- It would be good to use the station capacity definition that is used in California for state-funded HRS projects. The team also needs to further analyze earthquake-proof overpass-grade-located station equipment. Additionally, by the time the final report is available, it may confuse new industry stakeholders, as it contains good lessons that have been learned but not what the current status is for HRS development.
- The team could benefit from coordinating more closely with HRS developers, and even gasoline station developers or owners, to understand the other barriers to deploying new stations, as well as any tips or tricks for reducing setbacks or the footprint required for delivery trucks. A question from the audience involved using the street or adjacent empty property for the delivery trucks, thereby reducing the required footprint. The project team should find out if this is a common practice in the petroleum fueling space. It would be interesting to get some input from those already in urban refueling.
- Formally including additional partners, or at least clearly defining how collaborators are being engaged and providing information, would further strengthen the project.
- The project team might be considering some opportunities too mundane to address, instead hoping for more challenging evaluations (e.g., underground storage), while the mundane solutions, and particularly some depth of rigorous scientific support, could have a greater impact.
- The project weaknesses include its relevance to real-site challenges. A given site almost always has many more constraints with regard to layout, site owner acceptance, etc. than are discussed in this project. A general study of “typical” sites is not particularly useful for these highly constrained sites.
- The project does not address the delivery quantities of a commercial fueling station.

Recommendations for additions/deletions to project scope:

- The project scope is well considered and needs no additions or deletions.
- It is recommended that the project add a sensitivity analysis to consider the impact of increasing the station capacity from 600 kg/day to 1,000 kg/day. The team should identify the reducible setback distances and explicitly state the method by which each could be reduced (e.g., special exemption, adding firewalls, etc.). The team should also identify a case study that clearly shows how to reduce setbacks and the impact it has on a real-world station location.
- It is worth investigating how significantly the project outcomes would change if the project included larger-capacity stations (such as the limits indicated in National Fire Protection Agency). This relates to the comment about calculations seen on slide 9. For the final report, the team should acknowledge the capacity points at which things would change significantly.
- The project should continue to highlight synergies with other FCTO projects (and state projects, where applicable) on station development and codes and standards.
- It is suggested that the project team work with a station installation team to do evaluate an actual site to see the kinds of challenges and constraints that can be faced.
- This project does not address commercial-size fueling stations. A follow-up project should be initiated that addresses commercial fueling station requirements, and this project should include an existing fuel delivery company such as, for example, Exxon.
- There are no recommendation for additions/deletions to project scope.

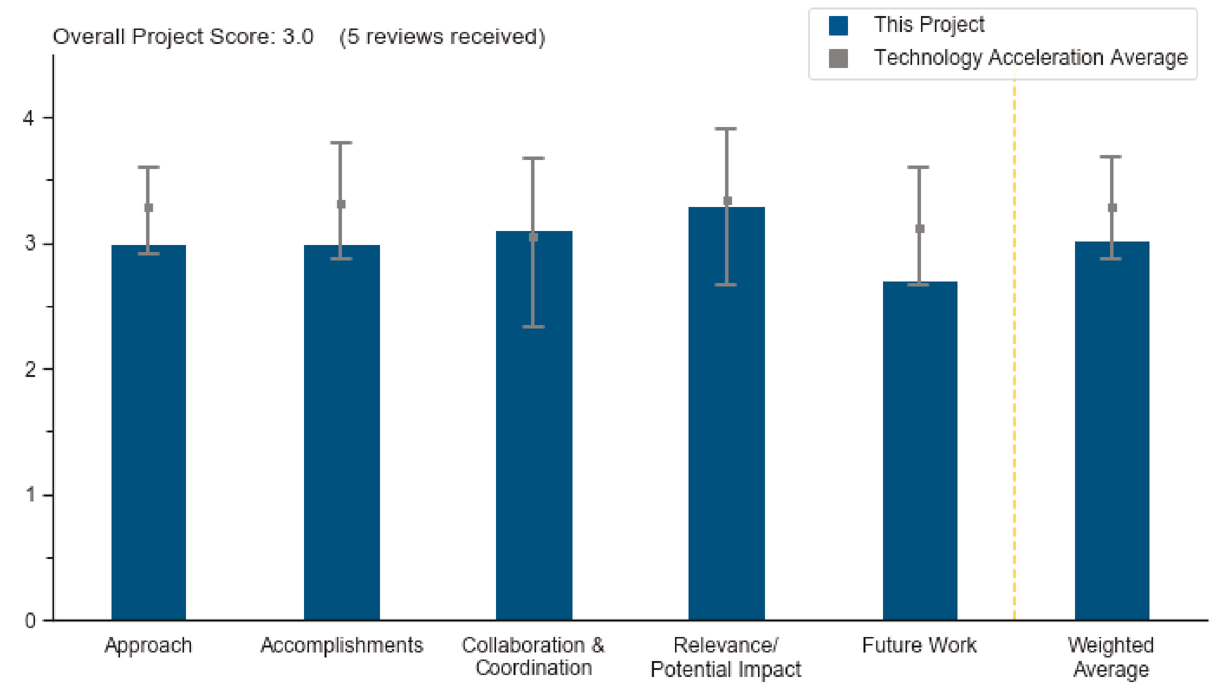
Project #TA-024: Analysis of Fuel Cells for Trucks

Ram Vijayagopal, Argonne National Laboratory

Brief Summary of Project

The primary objective of this project is to reduce the ownership cost of a fuel-cell-powered truck by finding optimal component sizes for the onboard hydrogen tank and battery pack energy storage system. The Argonne National Laboratory (ANL) Fuel Cell Team will support the U.S. Department of Energy (DOE) by creating a design solution that will meet or exceed the baseline performance and cargo capacity of a conventional vehicle.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Technology Acceleration projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project has a sound approach; using a common platform helps identify differences in requirements for the platforms supporting each technology. Investigating the cooling problem is highly relevant to the deployment of fuel cells in Class 8 trucks.
- The approach is well thought out and comprehensive; this is a good use of a workshop to obtain industry input.
- There seems to be a disconnect between the barriers cited on slide 2 and the project objectives stated on slides 3 and 9. The barriers, as described in the Technology Validation section of the Fuel Cell Technologies Office (FCTO) Multi-Year Research, Development, and Demonstration Plan, refer to the need for vehicle operational data that can be related to established targets. Thus, there is an implication that the project focus is on comparing "real-world" performance between fuel cell electric trucks (FCETs) and conventional diesel-powered trucks. However, the first objective (as seen on slide 3) is the development of models that enable comparison of potential FCET energy and cost performance with those of current and future diesel trucks. The second objective is to quantify FCET cooling requirements (as seen on slide 9);

here, the approach is to develop models that enable improved understanding of the thermal behavior associated with the options for FCET cooling systems. While the project's objectives and approach do not directly address the stated barriers, they are consistent with a project that can provide useful information on the potential for FCETs to compete with conventional trucks. The approach utilizes and builds on the significant vehicle modeling capability established at ANL. The team understands the importance of linking the work on this project with related activities and capabilities; other projects intersecting with and contributing to this one are noted on slide 4. This is a plus.

- The approach is set up well, and a deeper understanding of the current draft of targets for FCETs is very valuable. However, there may be more effective ways to accomplish this goal. There are a few key points to be made: (1) The intent behind including a detailed study of cooling requirements is not well understood. This may be a useful exercise, but it was not apparent how this relates to setting targets. (2) The definition for "best in class" seems to be based more on how a truck is operated rather than the technology itself (simulated as lower cargo and lower speed). For added clarity, it is suggested that going forward, the project team should benchmark to one standard diesel truck that follows DOE targets. This will capture lightweighting and other efficiency improvements while reducing the complexity of the study (i.e., showing just baseline diesel as opposed to two different diesel baselines). (3) Finally, the project team should show the current draft targets being used as a baseline.
- The approach of using Autonomie as a simulation engine is sound. However, there are a number of competing parameters that define a "good" or "best" FCET, e.g., battery size versus fuel cell size, motor power versus torque. These require detailed trade-offs, which then require intimate domain knowledge. A formal optimization wrapper would significantly improve the approach, with expert inputs on how to limit the optimization parameters for meaningful results.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The work clearly identifies the challenges facing fuel cell technology in Class 8 applications.
- The accomplishments seem reasonable; there is nothing unexpected or unusual.
- Progress has certainly been made to vet the draft truck targets, and it is highly anticipated that the continued work will set accurate and useful targets to drive innovation. Based on the data presented, there are a number of recommendations that could improve the presentation of future work. (1) It is recommended that the project remove "best in class"; the value of this metric is somewhat unknown, and it is not modeled in an apples-to-apples comparison with the other simulations. It would also help greatly reduce the complexity of the results and focus on key points. (2) The team should use graphs that show analysis and comparison; the current graphs appear to plot the targets of each in a separate graph. To improve clarity, it is suggested that the fuel cell and diesel graphs be combined for the relevant metrics (both technical and cost-related). (3) The project needs sensitivity analysis of key targets. The key intent of this work is to inform the draft targets and help set them appropriately. It is suggested that the project team run a few scenarios of the key targets to better understand whether the current draft targets are appropriate or need to be adjusted. (4) More insight needs to be provided; considerable analysis and data have been presented, but it was difficult to assess the accuracy and impact of the targets. The team should share some insight on these key takeaways. (5) More discussion on how the cooling analysis affects targets should also be provided.
- For the first objective (which is to support medium-duty [MD] and heavy-duty [HD] target-setting), the preliminary results summarized in the technical accomplishments (as seen on slides 7 and 8) seem encouraging for FCETs. It is concerning, however, that the results are determined by the assumptions documented in slide 6, specifically that the targets are expected to be achieved in 2030 and 2050. It would be helpful to provide the results of sensitivity analyses for ranges of technology performance and cost. However, the project's limited funding constrains the team's ability to analyze the multiple cases reflected by this comment. Regarding the second objective (which is to quantify FCET cooling system requirements), the accomplishments are impressive for a project with relatively limited funding and short duration. It seems that exercising ANL's Autonomie model for this work takes advantage of the results provided by other FCTO-funded projects that address fuel cell systems for HD trucks. The results from this

project should be beneficial in determining where to apply available resources for future FCET research and development (R&D).

- It seems that the FCET model has been optimized heuristically. A formal optimization wrapper would likely change the configuration and would likely provide more significant benefits that can change the ranking versus other power plants. Without that certainty in the FCET configuration, the basis for the value predictions is weak.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- Coordination and collaboration with industry is always a good thing; the sharing of papers with SAE International is also great. Assuming that there is good communication between project members, leveraging the assumptions and work from existing projects is excellent collaboration.
- The project's collaborations to conduct analysis and receive feedback from industry are very good. Additional outreach is encouraged if more input is needed when the team is amending targets.
- Collaboration and coordination are difficult to evaluate when specifically limited to and in the context of this project. The graphic on slide 15 indicates that this project is being done solely by an ANL team. Based on the presentation and Dr. Vijayagopal's response to a question, the organizations cited on the right side of the slide provided input in forums related to multiple ANL modeling activities. For example, work on this project has drawn from the results of a workshop that is mentioned; the same workshop has provided information used by multiple other projects. The same "collaboration and coordination" slide was used in ANL's presentation on project SA-044. It is fine to use the views of the organizations shown on the slide as input for the planning and implementation of multiple ANL projects; however, it would be helpful to clarify that coordination with all these stakeholders did not occur in the context of this project alone. SA-169, managed by the National Renewable Energy Laboratory (NREL), is another project that seems to intersect with TA-024. Its approach, which uses FASTSim as a primary modeling tool, also calculates cost of ownership for MD and HD vehicles.
- Hopefully, the investigators will have the opportunity to get data from ongoing demonstrations in the California Ports project. The team could coordinate with Ballard Power Systems, Inc., or involve the Toyota Motor Company and Kenworth Truck Company team. The team should also consider the buses at the SunLine Transit Agency that operate in the summer months.
- There is significant effort in the same area at NREL and Oak Ridge National Laboratory. These are partnership opportunities that would significantly increase the quality and impact of the work. At a minimum, such a collaboration would allow for the cross-validation of the results but hopefully would allow for a significant increase in quality of the results. Collaboration is a missed opportunity in this project.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This is a highly relevant application for hydrogen and fuel cells, given the ability for trucks to scale up in terms of infrastructure, the significant impact they have on emissions, the prospect of future restrictions on the use of diesel, etc., and the value of the energy service provided by trucking. This project should be supported.
- The impact and relevance for setting and analyzing FCET targets is of great importance to stakeholders. The project team is encouraged to obtain any final feedback before swiftly moving to publish the targets in order to drive the industry forward.
- MD and HD trucks are potentially important applications for fuel cell power. This potential is a legitimate topic for FCTO interest and activity. A project with this one's limited scope and duration, however, has limited ability to help achieve the FCTO's technology and cost targets. Regarding objective 1 (as seen on slide 3), it would be preferable for the team to apply the available funding to the development and testing of

fuel cell technologies for trucks rather than analyses of 2030 and 2050 results premised on the achievement of FCTO targets. Regarding objective 2 (as seen on slide 9), R&D on options for achieving cooling system requirements for FCETs seems reasonable. It would be helpful for the presentation to include the underlying rationale that led to the selection of the cooling system as a focus for this project.

- The project has excellent alignment. However, some of the approach's flaws can inject misleading conclusions that are questionable at a minimum. It is counterintuitive to put forward the view that FCETs are better suited for urban or MD applications, rather than long-haul (even if the long-haul diesel power plant is close to optimal).
- There are many areas in HD FCETs that need development and work. The cooling loads will certainly be an important consideration for the operation of an FCET, but it does not seem to be a high priority at this time, as there are so many other technical topics that need to be solved.

Question 5: Proposed future work

This project was rated **2.7** for effective and logical planning.

- There is not much time left in this project, but the work on developing a cooling system to fit the technology will be highly useful. If there is a follow-on project, it would also be good to consider liquid hydrogen. Liquid hydrogen would have a number of benefits, including extending range, dealing with cooling issues, and reducing fuel dwell times. Liquid hydrogen is also compatible with distributing hydrogen in a hydrogen infrastructure at large scale, as well as with public and large-fleet refueling.
- The key is the long-term goal of "making thermal characteristics an integral part of the vehicle-sizing algorithm for all powertrains."
- More support is needed in developing the targets. The proposed details of this work are somewhat vague, but the work scope is important. It will be interesting to hear more about how the scope of cooling requirements is directly related to target-setting.
- Slide 16 provides a general indication about continuing similar modeling work upon completion of the current project. Evidently, no proposal for related work has been submitted to the FCTO. Continuation of the modeling work associated with the "target development process" should have lower priority for FCTO funding than R&D on truck-related fuel cell technologies. The R&D of cooling system technologies for FCETs is appropriate. However, exercising the Autonomie model as part of that activity at this time is questionable and is an issue that the FCTO should address.
- The proposed future work needs deeper consideration. It is strongly recommended that the project team with NREL and consider an optimization wrapper.

Project strengths:

- The topic of FCETs is growing rapidly, and the development of accurate targets will help guide the academic community, the setting of policy, and industry. The team is encouraged to continue the great work in support of this topic.
- This is a highly relevant topic for scaling up hydrogen infrastructure and decarbonizing the delivery services of goods. FCETs may leapfrog fuel cell electric vehicles in terms of fuel demand and overall proposed value.
- This project has the right focus. Running an industry workshop provided a great start, and the approach is generally sound. The analysis of cooling capacity versus battery size is convincing and pertinent to the objectives.
- The project's strengths include its industry input and collaboration; the team should make sure these continue, as well as the project's long-term goal.
- The project team at ANL has significant vehicle modeling expertise, which has been developed and refined over many years. Its models and related analyses are highly regarded and widely used.

Project weaknesses:

- This project is evidently linked with other related analytical activity. However, as a stand-alone effort with limited scope and funding, its presentation does not convey confidence that it is an important element of an integrated plan for the advancement of FCET technology, or an element that provides critical analysis related to that technology. It is not clear that organizations cited on the collaboration and coordination slide have made comments or recommendations specifically related to this project. There is a conclusion that the performance and cost of FCETs will be competitive with conventional diesel-powered trucks; this conclusion seems to have resulted from the assumption that FCTO targets will be achieved. While that has some benefit, it would be much more valuable for modeling and analysis to identify areas with a high potential for adversely affecting the ability to achieve long-term targets and that could provide a rationale for the application of future R&D resources. There is a disconnect between the barriers cited on slide 2 and the project objectives stated on slides 3 and 9.

- An optimization wrapper is needed, coupled with expert supervision of the optimization process, in order to avoid unrealistic corner cases. There is a gap that needs to be filled in the project's collaboration outside of ANL, especially with NREL and other DOE/Vehicle Technologies Office projects.
- The project's weaknesses include the lack of data from Class 8 trucks for testing models. The project scope is unduly restricted, and the team needs to look at the feasibility of liquid hydrogen as onboard fuel for long-haul applications.
- The project's approach for analyzing the draft truck targets could be improved to be more impactful and efficient. It is expected that the targets could be published rather quickly if a few improvements were made.
- This work could possibly be done at a later date, after more critical technical challenges have been overcome.

Recommendations for additions/deletions to project scope:

- The team should add liquid hydrogen and liquefied natural gas to the list of comparables. The team needs to be cognizant of the impact of diesel emission restrictions in the long term. It looks like diesel will be banned in some jurisdictions.
- If modeling and analytical work, such as that accomplished by this project, is continued, it should not be as a separate, "standalone," independent activity with limited funding. The work should be incorporated into a comprehensive and well-integrated modeling and analytical project, designed to support FCET R&D.
- This project should perhaps be made a subset of a larger, more comprehensive HD modeling and testing project.
- The cooling system simulation is interesting, but the justification for how it fits within the target-setting scope needs to be made clearer. Perhaps these resources could be better used to focus more on the targets themselves. It is recommended that more effective analysis be done within the current scope.
- An optimization wrapper is needed, coupled with expert supervision of the optimization process to avoid unrealistic corner cases. There is a gap that needs to be filled in the project's collaboration outside of ANL, especially with the NREL and other DOE/VTO projects.

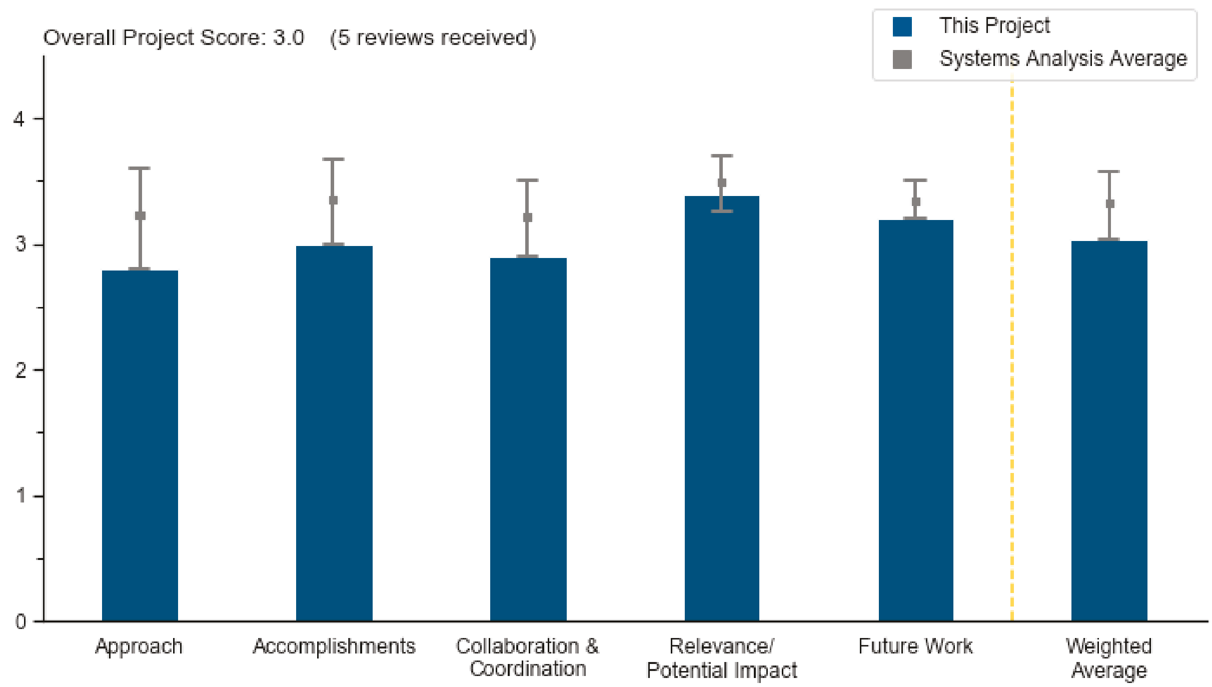
Project #SA-044: Cost–Benefit Analysis of Technology Improvement in Medium- and Heavy-Duty Fuel Cell Vehicles

Aymeric Rousseau, Argonne National Laboratory

Brief Summary of Project

This project aims to quantify the impact of fuel cell system improvements on energy consumption and economic viability of fuel cell electric vehicles (FCEVs). The project will (1) analyze fuel cell stack, hydrogen storage, and fuel cell system improvements in terms of their impacts on the cost of driving FCEVs and (2) evaluate whether current fuel cell and storage technology targets are sufficient to make FCEVs viable.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Systems Analysis projects.

Question 1: Approach to performing the work

This project was rated **2.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has a solid, transparent approach to evaluate the DOE targets and is coordinated with a number of other projects across Argonne National Laboratory (ANL). The project leverages the Autonomie model, which has been used for similar evaluations in previous studies. The business-as-usual improvements are not clearly defined in the slides, but the concept very informatively demonstrates the impact of achieving the DOE targets. The project approach is described with ample clarity and focus. There are a few suggestions to improve the value of the results: (1) The project should include more insight for earlier years (e.g., 2020) rather than just focusing on 2030 and 2050. It is good to understand the near-term challenges and development pathway. (2) The comparison to diesel as the main baseline certainly makes sense, but there could be a stronger focus on FCEV comparisons to battery electric vehicles (BEVs) to highlight the applications in which fuel cells have a superior advantage, assuming a zero-emissions vehicle (ZEV) solution is required.

- The project approach is straightforward and well described. The use of existing modeling (Autonomie, systems analysis cost models, etc.) represents good leverage on past work and others' work.
- The model background and development is opaque. It was difficult to understand the value of the analysis. Many of the slides had acronyms spelled out on a single slide, far removed from the core results. The presentation of the results had too small of an axis, making it extremely difficult to differentiate the technologies and value of the effort.
- It is unclear whether the project approach is related to the barriers identified. The approach provides a process of analytical analysis and modeling when the barriers are related to a lack of performance and reliability data and a lack of real-world operational data.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The description of objections in question-and-answer format is succinct and instructive. Consideration of multiple vehicle powertrains and vocations is useful and adds substantially to the project. The project work substantially aids in answering questions stated in the objectives and in furthering DOE goals.
- The results presented are very insightful and clearly demonstrate clear advantages for fuel cell electric trucks (FCETs). The project is encouraged to expand the results to include years prior to 2020 so that the audience can clearly understand the near-term challenges over the next decade. Understanding these challenges will help drive innovation. There are a few additional suggestions to maximize the value of the work:
    - The project should broaden the description of total cost of ownership (TCO) to include targets for fueling and maintenance costs, expanding beyond just the capital expenses of the trucks.
    - The research team could create a deeper dive, similar to slide 12, comparing only the ZEV technology choices (FCETs and BEVs), as diesel may not be the proper baseline in certain future markets that require a ZEV solution.
    - The principal investigator should clarify whether fueling time has been included and valued in some way. If fueling time is included and valued, it should be shown in this analysis separately, or if this analysis has not been conducted (related to overall TCO), it should be included.
- The accomplishments and progress provided establish the value of the DOE targets in areas of performance relative to truck performance.
- For starting in fiscal year 2019, this project has many results and provides meaningful conclusions. The plots could be presented in a more informative way to clarify the cost components that drive the purchase price over time. One could then see which DOE targets make the largest impact on vehicle price and may be the most important to attain.
- While some work was done to compare drivetrains, minimum information or assumptions were shared, which makes it difficult to evaluate progress and accomplishments.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- This project collaborates mainly within ANL. However, the project team seems to have a diverse background in this medium-duty (MD) and heavy-duty (HD) vehicle modeling and is leveraging the Autonomie model and other projects that have a wider collaboration team that extends across DOE and various original equipment manufacturers (OEMs) and technology manufacturers.
- The collaborative nature of this project has been very good to date, considering the limited data available. However, deeper consideration of utilizing automotive fuel cell technology for MD and HD vehicles is encouraged. Based on the comments received to date, the bulk of the feedback received seems to come from Ballard Power Systems (Ballard). This serves as a good baseline, but Ballard will not be able to achieve the cost reductions compared to automotive stack technology due to high-volume production. OEMs such as Hyundai Motor Company, General Motors, and Toyota Motor Corporation are already

announcing and demonstrating the use of automotive stacks in MD and HD vehicles, which could significantly reduce the cost of the powertrain. Obviously, the durability is currently unproven, but the project team is urged to consider this when setting targets and reach out to additional stakeholders for additional feedback.

- There is good use and coordination of output from other models. Vetting of results with collaborators is not stated.
- It is unclear how the collaborators listed provided relevant information to address the barriers or the accomplishments, as the model results presented relate only to the DOE targets and "business as usual." It is inferred rather than explicit that the data contributed by the collaborators were used to establish the "business-as-usual" case. The investigators do not sufficiently establish the validity of the real-world data, if such were used in this "business-as-usual" case.
- Additional partners could have been included regarding conventional trucks and HD parts suppliers. This would provide more confidence in the effort in which some assumptions were missing.

Question 4: Relevance/potential impact

This project was rated **3.4** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- MD and HD fuel cell applications are very relevant with the current market dynamics and recognition that other ZEV technologies may not be capable of meeting the commercial vehicle application needs. This project does a nice job of identifying how reaching DOE targets improve the competitiveness of FCETs in commercial applications.
- The impact and relevance of analyzing the potential of MD and HD FCETs cannot be understated. Vetting and adapting the targets is a worthwhile exercise, and the work to date is encouraging.
- The project has the potential to provide key insights in the further development and refinement of the DOE goals. The accomplishments provided suggest that achievement of the DOE targets will, in some cases, provide only muted benefits, while in other cases such achievement will provide substantial benefits. Such insight allows DOE to further evaluate the key performance indicators selected for project goals. As such, the project potential is substantial to the overall DOE Hydrogen and Fuel Cells Program (the Program).
- Studies of MD and HD fuel cell trucks are lacking. This project is relevant and is beneficial to both DOE and the technical/policy community.
- With the level of modeling and lack of transparency in the assumptions, it is difficult to judge the project impact. Perhaps with a different presentation approach, there would be better external uptake and motivation for technology investments or regulatory adjustment.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The future work contemplates very relevant questions. The impacts of the proposed evaluations could have impacts similar to the accomplishments demonstrated in this work.
- The suggested expansion of TCO is excellent.
- Future work is clearly defined and described.
- The TCO work should be helpful in comparing the existing technology evaluations. More input on markets and impacts of drastically increasing emissions requirements will need to be taken into account. The most value would be in providing a transparent list of assumptions and clearly explaining how the final model iterations across technologies are clearly described, which would give credibility to the presented results.
- It will be very interesting to see which market analysis aspects of this project are highlighted in future work.

Project strengths:

- This project is very relevant. It is important for DOE to understand how to best set the technology performance and cost targets to improve FCEV adoption for commercial applications.
- The relevance of the project is greatly important, and the impressive modeling tools used for this study are robust. The capabilities of these tools continue to grow and expand.
- In-depth modeling is leveraging expertise from multiple programs. A wide range of results were presented comparing business as usual versus meeting DOE technical targets. Many elements, such as sizing and power, are of interest to industry; cost of components is also of interest to industry.
- The project has a clearly defined methodology. Results are succinctly and logically conveyed. The project examines a high number of cases (vehicles and powertrains) and compares them on numerous relevant parameters.
- The work has good potential for significant impact on the DOE Program. The analysis methods have strong precedence and are well substantiated with scientific methodology.

Project weaknesses:

- The analysis itself is sound. Resources could be more optimized with a stronger focus on key takeaways. With a bit more direction and focus, the impact of this project can be increased.
- The presentation of the results lacks a clear demonstration of the conclusions from the analysis. The graphs are difficult to decipher and provide a confusing display of the results. The presentation should explain the results in a more clear and succinct manner. The effect of the results is lost in the overwhelming amount of detail provided by the presenter.
- There is a lack of transparency of assumptions used for input. There is a lack of clarity in data presented and comparisons across technology options. The presentation was limited as to considerations of component sizing, power requirements, and ultimately how the different technologies, truck chassis, and components differ across scenarios.
- The cost projections for the hydrogen storage system in slide 8 seem too high. A listing of additional vehicle/analysis assumptions should be included in the backup slides.
- This project’s main weakness is the use of DOE targets without any evaluation of the specific targets that are most important to achieve for commercial vehicle applications.

Recommendations for additions/deletions to project scope:

- This project is well defined to evaluate FCET targets, and additional scope is already being evaluated by other projects within the DOE portfolio.
- Suggested additions include (1) pre-2030 targets (e.g., 2020, 2025, etc.), (2) a strong focus on total TCO comparison, (3) specific FCEV vs. BEV comparisons (not just a focus on the diesel baseline), and (4) more discussion on the value of fueling time (as part of TCO).
- The project team could better present the assumptions and results. There should be a clear comparison of TCO, including infrastructure assumptions and how that affects business operations for each of the vehicle classes. The most important aspect would be to benchmark assumptions compared to the state of the art, and to understand fully the future of advanced diesel engine development, when major markets are suggesting eliminating diesel in the coming decade or two.
- The project could consider a historical evaluation of the light-duty vehicle market and the data developed for the current deployment of light-duty vehicles.
- A TCO analysis (including fuel cost) should be conducted.

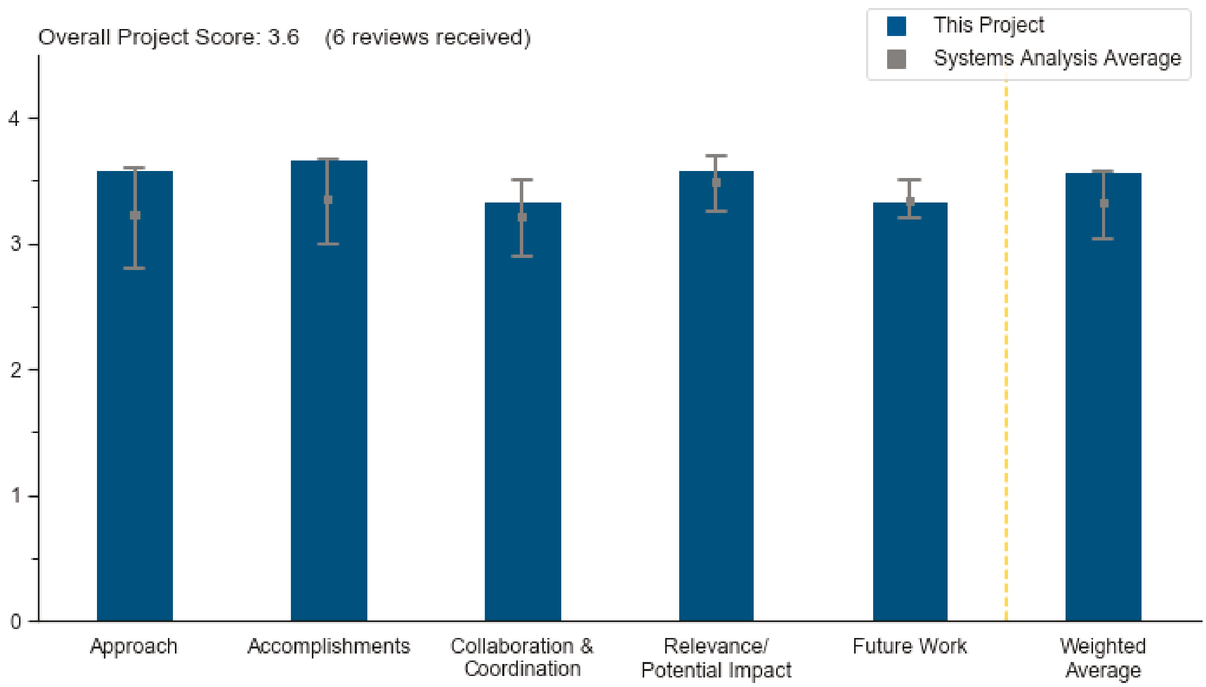
Project #SA-169: Market Segmentation Analysis of Medium- and Heavy-Duty Trucks with a Fuel Cell Emphasis

Chad Hunter, National Renewable Energy Laboratory

Brief Summary of Project

This project provides stakeholders a broad assessment of medium-duty (MD) and heavy-duty (HD) fuel cell vehicle market opportunities and helps guide future U.S. Department of Energy investments in the area. As part of this effort, systems analysis models that assess cost and market barriers to fuel cell vehicle adoption will be enhanced and expanded. The tools and models used in analysis include the Future Automotive Systems Technology Simulator (FASTSim) for vehicle optimization to obtain vehicle cost, fuel economy, and weight; and the Scenario Evaluation, Regionalization, and Analysis (SERA) model for stock modeling and modeling of direct costs, opportunity costs, and other value streams. The SERA model will be used to calculate total cost of ownership (TCO) for each vehicle class and vocation by region.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Systems Analysis projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has an exceptional scope that leverages a vast wealth of tools and knowledge. The key focus on what matters most to stakeholders is apparent and explained very clearly: TCO. The project team is applauded for having a clear objective and minds open to feedback to ensure the greatest impact of this work.
- The use of existing models (SERA, FASTSim) is a strength. This kind of integrated analysis requires numerous assumptions. Therefore, the use of established values and existing analysis tools is a solid approach.

- This is a good approach that mixes modeling and real-world reports, including out-year targets that are peer reviewed by stakeholders and invested industry players.
- The project effectively uses a wide variety of analysis tools to assess fuel cell electric vehicle opportunities in the truck market.
- This project approach is well aligned with the objectives and with the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program targets.
- The approach is logical and addresses the need for information to compare alternative fuel choices in different market segments. As with all these types of comparisons, the results are highly dependent on what input parameters are chosen for the different technologies. The source of the values chosen for the individual technologies is not clear, in particular the 61% number for fuel cell peak efficiency on slide 6. The text suggests that the values are from DOE targets, but the peak fuel cell system efficiency shown for 2020 and the ultimate efficiency match neither DOE Fuel Cell Technologies Office (FCTO) targets for fuel cell system peak efficiency nor results from recent commercial vehicles. Testing on the Toyota Mirai at Argonne National Laboratory has shown a peak fuel cell system efficiency of 63.7% (with a fuel cell stack efficiency of 66%). The target fuel cell system efficiency for 2020 is 65%, with an ultimate of 70% in the 2016 FCTO Multi-Year Research, Development, and Demonstration Plan. At a minimum, the targets should all be set to the value for the Toyota Mirai, and it is suggested that the 2020 and ultimate targets be set at 65% (for the medium estimate).

Question 2: Accomplishments and progress

This project was rated **3.7** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- These results are immediately useful to all interested stakeholders who have been craving an in-depth third-party analysis of TCO across many key powertrain types for a number of MD and HD vocations. The project team's consideration of all key factors is apparent and shows the team's willingness to solicit and act on feedback. The inclusion of cargo and dwell-time considerations is rarely seen in other analysis projects, and it is commendable. The analysis makes the value for fuel cells very clear, and the future results are much anticipated.
- The project's accomplishments are numerous. The team has considered multiple vehicle classes, multiple powertrains, and with low, medium, and high variation of key parameters. There is a nice compendium of scenarios. It is a good idea to benchmark against existing vehicles (e.g., from Nikola Motor Company [Nikola] and Hyundai Motor Company) and different drive-cycle analysis programs (e.g., Autonomie). The breakdown of the manufacturer's suggested retail price for each powertrain is nicely displayed.
- There is excellent quantitative discussion of TCO, including a broad spectrum of costs across other technologies. The uncertainties are critical with this level of first estimates for out-year technologies. The assumptions are clear and realistic. This was a very good presentation. There is a clear path to diesel parity.
- The investigators have established TCOs for a wide variety of vehicle technologies and operational variations. Sensitivity analysis points out the areas where research should focus to enable specific technologies. A preliminary example of an online version of the tool is already available.
- This project showed significant progress from last year, with positive response to feedback and input.
- The project has made good progress to date, providing preliminary analyses for long-haul trucks in 2018 and for Class 4 parcel delivery for 2019. The results have been benchmarked with fuel economy data from the industry and are in good agreement for the short-haul case. In the case of long haul, the FASTSim results for fuel economy are consistent with those from Autonomie but are substantially lower than the reported fuel economy of the Nikola One. The results showing the large payload opportunity costs for electric vehicles for both long-haul and short-haul Class 8 trucks and large dwell costs for Class 4 Parcel delivery are important. It is not clear how dwell-time costs are calculated in the TCO model or what is included in those costs. For example, it is not clear whether it is just the hourly charge for the time of charging and refueling, whether the time considered is strictly the refueling and recharging time, or whether additional time is built in to account for times when the recharging or refueling equipment is occupied by a different vehicle charging or refueling, etc. There is much uncertainty, and the error bars for the preliminary TCO for Class 8 short haul are large enough that the TCO of one fits within the error bars for

all vehicles for all scenarios. It is not clear why the uncertainty is so large in some cases or what can be done to decrease this uncertainty. Maybe the project should narrow the market segments more.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- This is a good mix of stakeholders and interested parties. Robert Bosch LLC and Toyota Motor Corporation are major players in the emerging fuel cell truck space. Cummins knows a lot about the challenges of gaseous fuels, and the Center for Transportation and the Environment has run many projects.
- The project has drawn from numerous sources of data, which suggests a good degree of collaboration (of assumptions, if not verbal communication). A broad set of external peer reviewers was consulted to provide feedback to the team.
- The project team's desire for collaboration and feedback is apparent, and the stakeholder list is relevant and broad. It is recommended that the team do some additional outreach to the infrastructure providers to gain more insight into a large portion of the TCO: the fuel and infrastructure costs. Obtaining this feedback and including an associated infrastructure cost as part of the TCO is a natural expansion of this great work.
- The project appears to be reaching out to the community and collaborating. The list of external reviewers included was appropriate. An expanded list of fleet users in the collaborators and reviewers could be beneficial.
- The project utilizes a sufficient number of partners to ensure the credibility of the results and their relevance to the market.
- The investigators have vetted the model with industrial partners.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is very impressive and will have great positive impact. The project team is strongly, strongly encouraged to publish a version of this model that any stakeholder can use. The value of this tool—to assist all interested stakeholders in better understanding the sensitivities, comparisons, and value of developing, investing, and operating alternative powertrain equipment— cannot be understated. This wealth of knowledge will ultimately lead to more demonstrations of the proper technology for each application (and fuel cell electric trucks are a strong candidate).
- The project will provide transparency to the relatively closed-off industry of fuel cell trucks. This will provide financial investment and some long-term certainty for large-scale hydrogen production, which can further reduce TCO.
- This project does a good job in demonstrating the impact of DOE targets on the overall market. The project provides a fair assessment while identifying the unique attributes of fuel cell trucks that contribute to the TCO.
- This type of analysis is vital to guiding future research efforts and to informing investors. Sensitivity analysis allows stakeholders to identify critical variables.
- Until recently, studies on fuel cell trucks had been lacking. This fills a substantial need.
- The project is relevant and useful for DOE and others to determine what the opportunities are for fuel cells in the HD/MD vehicle market. The large uncertainties and error bars limit the usefulness of the models.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future work toward buses and drayage will be important as California moves to 100% zero-emission buses in 2035, and transit infrastructure plans are due in 2020. The sooner this work is shared, the better. Drayage trucks are an important space in which to leverage existing capital costs, as there are 25,000 fuel cell forklifts already installed.
- This project will end in 2019; however, the potential future work proposed for a new project is interesting. Perhaps the team would consider a region-based assessment and align with H2@Scale analysis efforts to help establish some of the regional aspects.
- The project is almost complete, and the proposed future work is appropriate for completing the project.
- The researchers have laid out a clear plan for completing the project.
- The project did not receive a 4 for this metric simply because of the slight hesitation to publish a full TCO model. If the project team does this, the industry will be forever grateful.
- Making the SERA model available online is appreciated. The remaining classes of powertrains that are to be modeled are not clear.

Project strengths:

- These are all good things to see here: impactful relevance, the leveraging of DOE capabilities, a focus on useful results, and the desire to share a published model for everyone to use. The project team should carry on; the developments going forward are highly anticipated.
- The project provides a very good assessment of the truck market and helps industry participants prepare for the likely market segments. This work also demonstrates the need for more aggressive targets in TCO to make any alternative to diesel competitive (without incentives).
- This project's effort is extremely quantitative and transparent in its various assumptions. The comparison to other fuels and technologies allows for a clear comparison. Many aspects have been considered, and the work is very thoughtful.
- The project's strengths include its good use of excellent modeling tools, its good collaboration with industrial entities, and its clear reporting of ownership costs for technologies and operational variables.
- This is a well-described and clearly executed project. Drawing upon the vehicle and other assumptions from other models and leveraging existing models are great strengths.
- The project's strengths include its ability to compare results across vehicle platforms.

Project weaknesses:

- The project's weaknesses include its slight hesitation to publish the final TCO model. The project team should not think about it any longer and should just do it. The project team is also encouraged to reach out to stakeholders so that they can share their thoughts on the value of this project. It seems likely that all of them will strongly encourage the team to find a path forward to publishing and will be willing to help in any way they can.
- The project would benefit from real-world performance data, but this cannot be helped until more real-world data is available.
- The target fuel cell costs for trucks appear to be based on the cost targets for light-duty vehicles. This is not realistic. Using more realistic targets will increase the cost of fuel cell trucks even further above the cost of diesel trucks. The battery cost of $145/kW seems too low. This may mistakenly be the cell cost, when it should be the battery pack cost.
- The project results are reasonably well presented but are still a bit complicated. There is still room for improvement in communication. The team seems not to have reached its full potential for communicating the results.
- It would be nice if parts of this work could be open-source, or if a user tool could be provided for organizations that are considering expanding or implementing hydrogen infrastructure and equipment for the first time.

- There are large uncertainties for many of the TCO parameters. The project team is not using more realistic models for how trucks are bought, used, and resold in a secondary market.

Recommendations for additions/deletions to project scope:

- A few natural progressions would be (1) to include more of the infrastructure piece of the puzzle (i.e., fuel cost, infrastructure cost, scalability of different fuels, etc.); (2) to continue to include more vehicle types and vocations; and (3) to publish the model and continue improving it based on stakeholder feedback.
- The project team should work closely with Nikola and others to obtain data. The team should also examine economics as a function of volume- and weight-limited operations. The weight-limited case includes 30% volume-limited operation. The full range of operations should be examined, from 0% weight-limited to 100% weight-limited.
- The development of an online tool is a good focus; however, the team should also consider a simple reference with key data and suggestions for future researchers and industry strategists, with references for trustworthy data.
- It would be good if, where possible, some aspects of the model could be released for external use, as well as inputs of individual assumptions or expected cost targets.
- For fleet vehicles, taking a closer look at the cost of infrastructure based on fleet size could be beneficial.

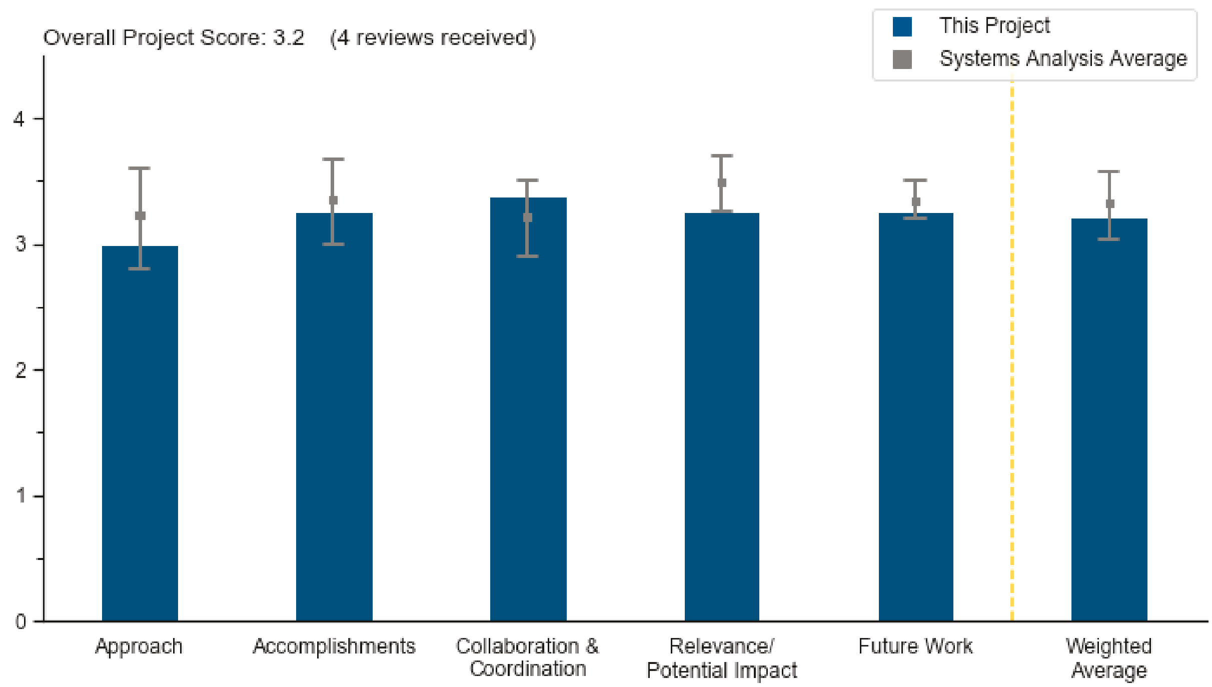
Project #SA-170: Analysis of Cost Impacts of Integrating Advanced Onboard Storage Systems with Hydrogen Delivery

Amgad Elgowainy, Argonne National Laboratory

Brief Summary of Project

This project seeks to evaluate the impact of onboard hydrogen storage systems on delivery and refueling costs. Argonne National Laboratory, in collaboration with the U.S. DRIVE Partnership: Hydrogen Interface Taskforce, Lawrence Livermore National Laboratory, and Energy Technology Analysis, is addressing inconsistent data, assumptions, and guidelines by developing new delivery and refueling pathways in the Hydrogen Delivery Scenario Analysis Model (HDSAM) for onboard systems. By improving understanding regarding refueling pathways for onboard hydrogen storage and providing better models and tools to better evaluate relevant sustainability impacts, the project team aims to accelerate development and deployment of cost-effective refueling pathways.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Systems Analysis projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach is solid and well thought out. The presenter identified limitations to the approach, such as the boundaries of the system, and included some of these in future work (e.g., incorporating upstream supply chain aspects). The only additional item to potentially consider would be the impact on the vehicle cost that the advanced onboard storage systems would incur. The presenter noted that this was important and that there are limited data available, but if a feasibility or scoping-level cost estimate could be completed to ensure the vehicle storage cost would not dramatically increase, that would be helpful in understanding whether the refueling station changes were worth studying. Perhaps that aspect justifies further funding, as it would be very interesting to see whether both the refueling station cost and onboard storage equipment cost could be reduced simultaneously.

- The project approach is very effective in using existing U.S. Department of Energy tools to evaluate the future barrier between future onboard storage technologies and infrastructure.
- This remains focused on one piece of the puzzle related to bringing down the cost of hydrogen fuel and improving station reliability. This is certainly useful analysis, and the project could benefit from a broader consideration of the supply chain to assess the key challenges that need to be addressed. Examples include (1) upstream supply and distribution (local vs. centralized production, cost of liquefaction, hydrogen delivery options and costs, etc.); and (2) onboard vehicle storage implications (new technology development required, cost, storage durability, storage volumetric and gravimetric density, etc.). Not every aspect needs to be studied in depth, but focusing on just one section of the supply chain makes it difficult to understand the value of completely switching to new technologies. This insight would be very useful to the industry. It appears that similar comments have been made in the past but have not yet been reflected in the project scope.
- The approach to analyzing the impact of alternative vehicle onboard storage approaches is properly developed and applied. The lack of analysis of vehicle cost impact limits the value of the analysis. It is not clear how the work addresses the barrier of "stove-piped/siloed analytical capability" noted in the presentation.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- In the past year, the project has made significant progress in determining the contribution to refueling cost for various on onboard storage technologies. The refueling cost results are helpful in understanding the potential opportunities or barriers for certain onboard storage technologies.
- This project has made strong progress since the 2018 Annual Merit Review, as demonstrated by the accomplishments presented and the journal paper developed.
- Good progress has been made, and the key takeaways are clear. However, the results remain focused on one aspect of the overall project scope. For this project to maximize impact, a broader analysis of the supply chain is strongly encouraged. The presenter articulates the key point that delivering liquid hydrogen (LH_2) to the station is beneficial for essentially every station pathway. If this is the case, it seems odd that this is not done for every station today. Analysis of LH_2 may unlock this riddle and help key stakeholders better understand whether LH_2 is indeed worthy of their investment. A key question raised when discussing hydrogen delivery is the most efficient and cost-effective method of delivering the gas based on the distance and the scale required. The project team is encouraged to consider a comparison of different delivery technologies based on both delivery distance and amount of hydrogen delivery required.
- The project has identified avenues to reduce the cost of dispensed hydrogen, which is a key barrier to fuel cell electric vehicle adoption. However, additional work is needed to understand the impact on total cost of ownership. The project has largely met the analytical objectives established for the project.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The team has done a great job coordinating with multiple stakeholders on approach, data, methods, and validation.
- Individual team members and contributions are described in the presentation and appear to represent the primary areas relevant to the work.
- It appears that reasonable feedback from within the national laboratory network and industry has been solicited. However, the results feel somewhat academic in nature, even though the key intended audience is industry (to aid station design decisions in order to reduce cost). The team should reach out to more industry stakeholders from both the infrastructure and original equipment manufacturer perspectives to clearly understand what challenges they face and what value they would like to see from this work.

- The project has a high level of collaboration with various national laboratories and technology teams, although the collaboration could be improved by including infrastructure companies.

Question 4: Relevance/potential impact

This project was rated **3.3** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The project is extremely relevant to the DOE Hydrogen and Fuel Cells Program (the Program) since the future onboard storage technologies must be compatible with the infrastructure. The results of the analysis could assist DOE in shaping portfolios for both onboard storage technologies and infrastructure. Also, the project outcome can help in establishing research targets for both onboard storage technologies and infrastructure.
- The current limited scope is very relevant to the needs of the hydrogen supply chain, and the project's impact could be greatly improved by expanding the scope beyond the study of a few station technologies. Without significant scope changes over the next year, the value of these results may be lost, when instead they could play an integral role in a very useful supply chain analysis.
- This project is relevant, as refueling station costs are quite high today. However, the bulk of the refueling station cost benefits seem to come from economies of scale and technology maturation over time, as demonstrated by the cost estimates going from $6–$8/kg (current) to $1.94/kg for conventional 700 bar gaseous hydrogen refueling. However, it should be noted that, while reducing the dispensing costs by ~$0.5–$0.75/kg may not be substantial on an absolute basis, it does indicate a significant (~30%) improvement. One thing that was not specifically pointed out was the different capital and operating expense splits of the technologies. Lower upfront investment of the metal hydride and sorbent technologies may reduce the risk to station developers and owners, which could lead to faster station development. This could be an interesting aspect to explore further.
- Cost reduction for hydrogen compression, storage, and transport is crucial to reaching cost targets for dispensed hydrogen, so the work aligns strongly with Program goals. However, the lack of the cost impact of the onboard storage systems limits the ability to draw conclusions from this phase of the work.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed future work should be very interesting, particularly the system boundary expansion and the life-cycle emissions analysis.
- The proposed future work seems very good and appears to address reviewers' comments from the 2018 Annual Merit Review.
- The proposed future work is relevant but should also include vehicle cost impact and compare to LH_2 pathways. Also needed are the technology readiness levels of the relevant components, the timing of potential deployment, and the ability to integrate the components into the then-existing supply and delivery chain.
- The future work is good but could be improved by using the analysis for determining the optimal onboard storage operating conditions for infrastructure cost and compatibility. The previous work also assumes dedicated hydrogen stations for each technology rather than evaluating compatibility of multiple onboard storage concepts at the same station. In addition, the assumptions from the previous analysis could be explored based on a sensitivity assessment.

Project strengths:

- The strength of this project is the team involved in performing this analysis. The principal investigator, in particular, has extensive history and technical expertise in the area of onboard storage technologies and infrastructure. The project results are explained effectively, and assumptions are documented.
- This project evaluates early-stage research and development and does a nice job of systematically evaluating each technology. A variety of technologies are evaluated, and the results are presented in easy-to-understand ways.
- The project provides detailed analytics not previously available on technologies that may improve the dispensed cost of hydrogen in the time horizon beyond five years.
- Strengths include thorough analysis capability and a desire to reduce fuel costs while improving station reliability. The project is encouraged to leverage these strengths and goals on future expanded work.

Project weaknesses:

- The project weakness is the lack of infrastructure company involvement to validate the results. Also, there are some inconsistencies that need to be explained; for example, the hydrogen refueling price on slide 3 does not align with the price on slide 12. The cryo-pump cost should be further analyzed, especially for the different hydrogen delivery pressures (700 bar vs. 350 bar cryo-compressed).
- The defined limited scope limits the positive impact of this project, and the response to previous review comments demonstrates that stakeholder feedback has not been fully captured. The proposed future work attempts to address these comments, and hopefully there will be significant improvements going forward.
- The system boundaries could be defined for more appropriate system-level costs. The future work looks to improve upon this, but the impact on the vehicle cost could be important to consider as well.
- Weaknesses include the vehicle cost impact's not being included, as well as a lack of discussion or analysis of deployment timeline and integration in the existing supply, delivery, and dispensing chain.

Recommendations for additions/deletions to project scope:

- The project should consider the following additions: (1) broader analysis of upstream supply chain considerations, (2) broader analysis for the onboard vehicle storage implications, (3) assessment of scale and delivery distance implications, and (4) increased industry engagement and feedback.
- The project should add the analysis for determining the optimal onboard storage operating conditions for infrastructure cost and compatibility. The previous work also assumes dedicated hydrogen stations for each technology rather than evaluating compatibility of multiple onboard storage concepts at the same station. In addition, the assumptions from the previous analysis could be explored based on a sensitivity assessment.
- Additions to scope could be to assess any non-cost-related factors that these technologies could affect. For example, these different storage technologies could affect refueling time, reliability, consumer perception/ acceptance, noise levels, footprint, etc. These factors are clearly out of scope but could accelerate the adoption of hydrogen refueling station technology.

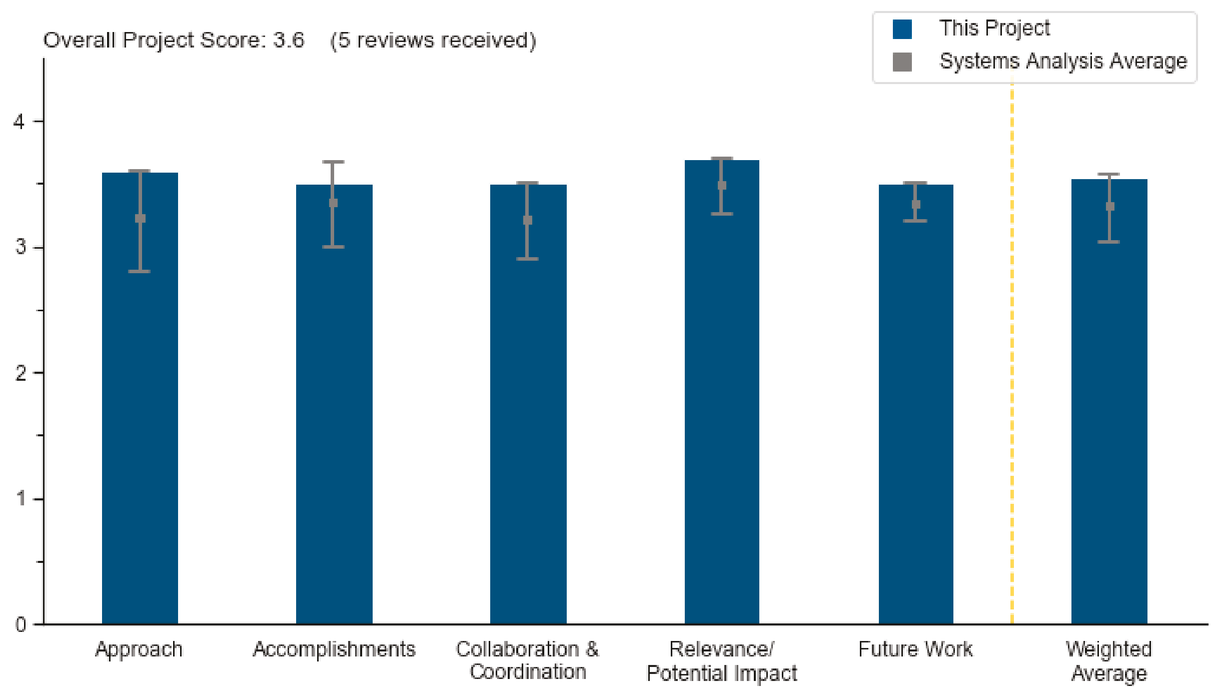
Project #SA-171: H2@Scale Analysis

Mark Ruth, National Renewable Energy Laboratory

Brief Summary of Project

H2@Scale is a concept that explores the potential for wide-scale hydrogen production and utilization in multiple energy sectors in the United States. The objective of this project is to improve the fidelity of the H2@Scale value proposition. The analysis seeks to quantify the potential economic, resource, and emissions impacts from wide-scale hydrogen production and utilization. In addition to conducting nationwide analysis, the project will also identify regional opportunities and challenges. H2@Scale analysis integrates many transportation, industrial, and power sector analyses and tools.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Systems Analysis projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This is a complex project, and incorporation of a large team using a variety of already existing models is a good approach. Definition of terms, the breakdown into technical and market potentials, and examination of each individual market's supply and demand are all good elements of the approach.
- The approach is very well described and leads naturally into the presentation. The approach is comprehensive and simple, indicating that the researchers have a strong mastery of the subject.
- The supply–demand equilibrium framework is a solid approach for the work. Folding quantitative demand elasticity into the analysis, where available, would improve the strength of the analysis.
- Utilizing a suite of existing models to accomplish new analyses is an intelligent structure for this work. However, one of the barriers identified was the development of new tools to fill in gaps in analysis capabilities. It is not clear what new tools or models are really being developed or, to be fair, whether new tools even really need to be. The project may need to re-evaluate the premise that new tools/models are

needed; perhaps it is only that existing tools need to be leveraged in new ways. In addition, while there was mention of a consumer choice model for forecasting the light-duty vehicle market demand, it was unclear whether a similar model or consideration was implemented for the heavy-duty demand. This may have had an impact on results, as the hydrogen demand for heavy-duty applications seemed small, especially compared to light-duty applications and taking into consideration the much larger per-vehicle hydrogen use for heavy-duty. The modeled hydrogen demand for heavy-duty vehicles also seemed much less sensitive to the evaluation scenario, which seems to indicate it was more of an exogenous or rule-of-thumb assumption. Finally, it is unclear how much the consideration of demand from metals markets truly affects the results, since it seems masked by assumptions about renewables in the corresponding scenario descriptions. Also, given that the metals market is assumed to have some price elasticity in some of the cases, it seems like there could be the same assumption investigated for other markets. In fact, this might help define a path for greater adoption, if consumer price elasticity is assumed to be greater at first and then decrease over time.

- The project's approach and vision of hydrogen as an energy carrier and integrator across multiple industry sectors is bold and broad.
    - However, given the current and projected U.S. energy export levels, the national energy security justification for hydrogen is less compelling. The primary driver for investors and consumers is the potential environmental benefit of hydrogen over existing energy systems. As such, the project needs to quantify and incorporate the life-cycle greenhouse gas (GHG) benefit for the various hydrogen sources or industry sectors and use it as an additional constraint parameter in market growth potential.
    - For the most part, the framework approach used to estimate future economic potential is reasonable. However, the project should modify or expand the national scenarios to include more realistic and likely ones. Given that more than 95% of current hydrogen sources come from non-renewable sources, there should be a plausible national scenario in which decarbonization of existing hydrogen sources, such as via carbon capture and storage (CCS), is seriously considered.
    - Another suggestion is to add a national "high natural gas resource" scenario, in light of the current boom of U.S. liquefied natural gas export investments based on long-term, abundant, low-cost natural gas supply.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has shown good progress over this performance year, completing novel national supply and demand estimates for all key demand and supply sources. Several scenarios on key market variables were also completed. These analyses are a necessary foundation for assessing the potential value of H2@Scale to the energy, industrial, and transportation sectors. Some approach to valuation of GHG emission reductions should be added to the analysis without any endorsement of a particular policy framework. Perhaps the low natural gas resource (or a high natural gas price) scenario is a proxy for this in some respects. Carbon regulation should be part of the analysis in states that have adopted such regulation.
- The accomplishments have significant impact on the overall project and DOE goals. Additionally, the project presentation does an excellent job of conveying the information. The information provided is comprehensive, and the presentation enables the reader to easily identify the key conclusion of the accomplishment.
- Developing supply and demand curves for each market is very good. The explanation of the results and formatting of graphical results are very clear.
- The preliminary supply–demand curves and the economic potential results look interesting. Given that the project is only few months old, this is a good start.
- The completion of the economic potential evaluation was a major accomplishment for this past year. A recommended addition to that would be to compare that potential to known benchmarks (such as incumbent conventional fuel market sizes) to help provide context to those who will eventually make decisions based on these results. This analysis should look at both the magnitude of the calculated potential and the rate of growth. If possible, comparison to other advanced or new technologies could also be helpful.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The collaboration effort, including the stakeholder engagement in framing and launching H2@Scale over the last two years, is excellent.
- The project is highly collaborative and is coordinating with researchers and market analysts in each relevant technology and market.
- The project boasts a robust group of collaborators and has clearly benefited from the input of this team.
- Multiple laboratories and industry stakeholders are represented. Noting in the analysis where industry vetting was conducted would strengthen the work.
- The collaboration between national laboratories, with different modeling and analysis capabilities, is exemplary. In addition, the outside collaborators appear to be a fairly balanced mix of fuel providers and policymakers. However, it does seem that there might be room to add more collaboration with representatives of the end-use industries assessed in this study. There also does not seem to be much representation from the renewable energy and electric utility industries, which seemingly would be instrumental to this work.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- Quantification of potential growth in hydrogen demand that might be enabled by the H2@Scale initiative has been lacking and is necessary to build industry and government support for the concept. This work makes an important contribution to addressing that gap and applies an equilibrium demand approach not used previously in this sector.
- Studies that are looking at the full-scale potential of hydrogen, and attempting to complete the analysis with a holistic vision, are currently some of the most necessary information resources for decision makers. The proposed future work on regionalizing the results will also be particularly impactful in this regard. In addition, the team may want to consider hyper-detailed analyses for smaller focus areas, such as individual metro areas of interest—or ideally, a combination of select metro, urban, suburban, and rural areas. Exploration of potential impacts of the broader H2@Scale vision on these more localized communities would be very insightful work right now.
- This project goes to the core of H2@Scale, as it will assess whether the entire concept is economically feasible.
- The project is very relevant to the stated objectives of the H2@Scale project.
- The broader H2@Scale effort is indeed very relevant with respect to promoting hydrogen use in the United States, per Hydrogen and Fuel Cells Program objectives. However, the project does not adequately address a few critical questions on relevance. It would be good to know whether favorable market size and resource availability alone are enough to advance the hydrogen economy—in other words, whether new hydrogen sources will be commercialized without demonstrating meaningful environmental or GHG benefits over existing or fossil fuel sources.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- Each of the three pillars of future work is merited: expanded economic potential estimates, transition analysis, and development of illustrative business cases. The future work all feeds logically into assisting DOE with research and development target setting.
- The proposed future work is consistent with the project objectives and very much aligned with the next logical step of the scientific investigation.
- The proposed future work on estimating hydrogen transport and storage costs is the next logical step.
- The proposed future work is a logical next step for the analysis. Additional empirical validation of demand elasticity would be useful.
- The proposed future tasks on transportation costs and regionalization of results are great additions and will be valuable for supporting ongoing efforts to expand support for hydrogen and fuel cell vehicles. In addition, it would be good to look at the price elasticity question. That is, early consumers may have some price elasticity, whether real or "virtual" due to policies and subsidies, that could increase the near-term market size and have lasting effects in the long term. However, as the technology matures and becomes more mainstream, the broader audience will have less elasticity in its purchase choices and should be modeled accordingly. Useful insight could be provided through an analysis of the potential benefit of a phased or transitioning deployment target path compared to one that holds ultimate economic equilibrium as the metric at all points in time.

Project strengths:

- The project's strengths are its breadth of analysis, its holistic approach, and its ability to incorporate existing capabilities at many national laboratories to develop large-scale and insightful research results in a relatively short time.
- The project research activities are well aligned with industry needs and facilitate a strong basis for industry to consider in the development of a comprehensive national hydrogen infrastructure. The future work in evaluation of regional markets is also a strength.
- The work addresses a critical knowledge gap by quantifying the long-term demand potential for hydrogen in the transportation, energy, and industrial sectors.
- The project's greatest strength is the success in integrating so many elements of past National Renewable Energy Laboratory analysis into a comprehensive assessment of the supply and demand curves.
- The project is ambitious and well thought out, with broad scope and reach.

Project weaknesses:

- Weaknesses are the limited validation of demand elasticities and the absence of timelines for demand growth.
- Communication of the results is a weakness. The researchers do not clearly indicate the one or two key aspects of the results in the accomplishments. This forces the user to spend extra time considering the results. While the researchers wish to refrain from commenting on policy (and this analysis effort is very close to the policy discussion), the communication of the results would still benefit from some summary notes that indicate perhaps already obvious aspects of the results.
- The project's weakest point is that the results seem to rest heavily on low-temperature electrolysis's reaching $100/kW. This is a very challenging price point to achieve.
- The project's weakness is likely that the devil is always in the details. As noted in the presentation, some of the more global assumptions may not be appropriate or correct when the analysis is carried out on a more focused region. Thus, the regionalization (and hopefully even more finely granular) analyses will be an important step toward ensuring the results of this analysis are valid and useful.
- The project lacks some sort of a metric to gauge the environmental or life-cycle GHG benefits of the various sources or applications, a critical driver for a hydrogen economy. Also, the H2@Scale effort does not differentiate between technology readiness levels of the various hydrogen sources or industry sectors

under consideration, e.g., steam methane reforming vs. electrolysis, or established markets (refineries, ammonia, iron, etc.) vs. new ones such as synthetic fuels made from CO_2.

Recommendations for additions/deletions to project scope:

- The project team should consider adding two national scenarios: a blue hydrogen scenario that envisions steam methane reforming with CCS, and a likely national scenario of "high natural gas resource." The team should also consider adding a market constraint based on quantified environmental benefits of the various sources or industries. Developing a technology roadmap to meet the research and development targets would be very helpful to current and future researchers.
- The regionalization effort is very good and should go further to look into smaller areas, such as cities and towns, and possibly to expand the scope of applications that might be considered at this level of detail (distinctions between privately owned light-duty vehicles and corporate, rideshare, and ride-hailing fleets, microgrid potential, localized hydrogen energy storage potential, etc.).
- No additions to or deletions from the project scope are recommended.

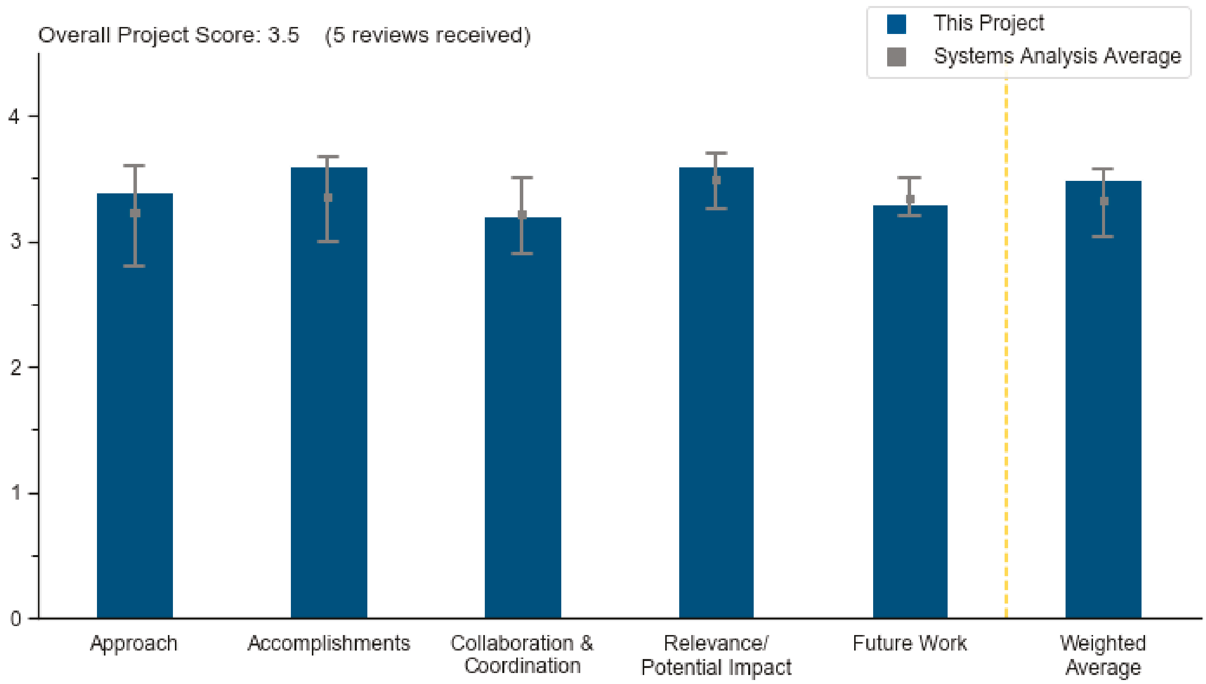
Project #SA-172: Hydrogen Demand Analysis for H2@Scale

Amgad Elgowainy, Argonne National Laboratory

Brief Summary of Project

Hydrogen from clean energy sources can enable renewable energy penetration and serve energy sectors beyond transportation. This project evaluates potential growth in hydrogen demand for existing and emerging applications. Performance and energy market data are collected for both current and potential future markets, including fuel cell electric vehicles, petroleum refining, ammonia production, electrofuels (synfuels or e-fuels), steel refining, biofuels production, and injection into natural gas pipelines. A final report will document all data sources, the modeling approach, and the analysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Systems Analysis projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach of this project accurately addresses the barriers stated and is well integrated into the remaining H2@Scale program.
- The project breaks down demand into key sectors (refineries, ammonia, etc.) and clearly labels the source of data for each. The diagrams of source data are particularly useful and effective.
- The work covers several important sources of current and future demand for hydrogen. The analytical approach for estimating hydrogen demand for refining and ammonia is well developed and makes good use of underlying data to correlate hydrogen demand. The demand analysis for electrofuels (e-fuels) and steel appears to be gross potential, and details for other sources are not contained within the Annual Merit Review presentation. It is assumed that the full report will provide more detail on these areas.
- It seems that a good deal of focus on the hydrogen consumed to support fossil fuel reforming was driven by the U.S. Energy Information Administration's (EIA's) *Energy Outlook*. While this is a respected and

consistent methodology, it would also be insightful to look at cases that differ significantly from this fuel mix. This could be especially insightful for regional analysis, where localized policies and programs may be pushing for energy and fuel demands that would not match EIA projections. In particular, as presented, the work seems almost to assume that fossil fuel demand for transportation would not be undercut by electricity and hydrogen demand as transportation fuels, which may not comport with expectations in all areas of the United States. In addition, for some of the analyses (particularly the e-fuels analysis), it seemed as though estimates for demand were driven primarily by current sources of supply. If true, this seems like it would be misleading, or at least too circular in its logic.
- The approach used to estimate the hydrogen demand from oil refineries, ammonia, and steel plants is laid out reasonably. However, the assumptions in the demand estimation for the e-fuels are unclear. For the three existing markets, the study does not seem to make a distinction as to whether the source of hydrogen is renewable, which is nice to know but not necessary for this analysis. However, for e-fuels, hydrocarbon combustion products CO_2 and water are converted back to hydrocarbon products; if the process is to make sense, there needs to be a clear statement that the input energy (electricity and/or heat) can only be renewable. Otherwise, the conversion process will result in more emissions to the atmosphere. Note that the e-fuels concept is inherently a reverse combustion process. Therefore, the market demand estimates should reflect this reality.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project provides a comprehensive summary of the current hydrogen demands. This demand summary establishes a strong foundation for assessment of overall market growth. The interaction of this project with other H2@Scale analysis efforts is very well established and demonstrates a very positive synergy of the overall H2@Scale initiative.
- The project team has substantially completed the demand analysis for the applications in scope. This rigorous analysis of potential hydrogen demand makes an important addition to the H2@Scale foundations.
- The team did an excellent job in using historical data to estimate future hydrogen demand for the three existing markets. Obviously, there are more uncertainties for those early or non-existent markets, such as e-fuels, which needs to be reflected in the final results.
- The results are logically and clearly explained. The title of slide 11 states that refinery hydrogen demand has increased significantly. While numerically true, this may be due to recovery from the ~2008 recession. Thus, graphing hydrogen demand prior to 2009 may clarify whether demand is just returning to previous values or is indeed exorbitantly rising. The data source for future trends would benefit from further explanation. For instance, the graphs on slides 12 and 15 are suspiciously flat or evenly increasing. This suggests gross assumptions about future demand predictions. While no one can foretell the future, additional commentary on the confidence level of these underpinning assumptions would be useful.
- The major weight of the accomplishments in the past year seems to have centered on fossil fuel reforming. While this was a good and necessary step, it seems a bit unclear why this received so much attention, especially given the plethora of established demand forecasts for gasoline, diesel, and so forth that could easily be translated into hydrogen demand with relatively good accuracy. Some of the other markets seem to be greater unknowns, especially given that the analyses are assuming there would be some fundamental change to these industries' operations if they were to have a closer tie to a renewable hydrogen resource. It seems the effort could have been more focused on larger unknowns rather than the incumbent, and much more well-known, industry.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The team is collaborating with relevant and experienced groups. No holes in the team are perceived. The presentation would be improved by briefly describing each collaborator's contributions.
- This is a very strong cross-laboratory team. Industry partners are noted in general but not identified, and greater clarity on input received from industry would improve the work.
- It looks like the team has collaboration with key national laboratories and unnamed industry partners. It would be good to disclose what role each collaborator has played in the study.
- Internal collaboration is good between national laboratories, but it does seem that there is a dearth of external collaboration. Since the project is looking to assess hydrogen demand across many different real-world and existing industries, it seems like a more natural collaboration environment would be one that is more heavily focused on industry partners. The project should work to include more industry collaboration as it progresses.
- This project will benefit from collaboration with more industry participants. Workshop activities around the initial results could offer opportunities to engage many perspectives and add nuances to the analysis.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project has significant potential impact on the Hydrogen and Fuel Cells Program goals and the strategies of private industry. National-scale strategies require this type of in-depth, comprehensive analysis to develop the vision. This vision is further refined as industry stakeholders identify synergies.
- This is a highly useful and informative analysis that synthesizes multiple unwieldy sets of data. Understanding demand and the corresponding hydrogen prices necessary to fill that demand is a very relevant and useful task.
- Quantification of potential growth in hydrogen demand that the H2@Scale initiative might enable has been lacking. This work makes an important contribution to addressing that gap.
- There is no question that this work is very relevant to DOE objectives and is obviously a significant input into the H2@Scale effort.
- The overall goals of the project have the potential to provide significant impact. However, given the noted focus on analysis of fossil-fuel-based hydrogen demand, which is arguably the most easily characterized, it seems that the project in the past year did not provide as much impact as it potentially could. Future work in the project should focus more on the areas where more new knowledge and insight will be generated.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed future work does show signs of moving toward the areas of potentially greater need and greater impact. The work proposed would be breaking new ground in analysis of potential applications of hydrogen. In addition, the regionalization would be a very powerful addition to this work, as it is for the overarching H2@Scale work.
- The proposed future work on environmental life-cycle analysis (LCA) on e-fuels and steel refining processes is excellent. The team should consider the potential demand for low-cost renewable hydrogen blending into existing natural gas pipelines. This could potentially be the "low-hanging fruit" in the decarbonization effort of U.S. energy systems.
- The proposed future work on additional sources of demand ties well into the current work. Other noted future work (LCA, supply chain) is relevant to the H2@Scale initiative, but it is somewhat unclear how this work relates to the current analysis of demand.

- Regional analysis is of interest for future work. The price of hydrogen needs to be considered as part of the regional analysis. It is not just matching supply with demand but rather matching supply at needed price with demand.
- Future work should not focus yet on LCA; it is too early in the development to create detailed LCA of the process. Pathways such as e-fuels are not clearly advantageous and should be validated with industry through workshops before starting an LCA. Additional markets and "advanced" storage and distribution methods and technologies should be considered only at the national level and not in detail for the next phase of the project. Future work should focus on regional aspects of the analysis. The analysis should consider a detailed assessment of the interaction of regions. There are several questions to consider:
    - How much hydrogen moves from the southern or eastern regions into the western region
    - Whether the fertilizer used in California's Central Valley or Oregon's and Washington's eastern fields is sourced from the United States or represents imported "hydrogen" demand that might benefit from the development of significant hydrogen generation capacity in the western region
    - Whether foods and fuels compete or complement when hydrogen energy is more ubiquitous
    - Whether existing regional production (Midwest), substantial wind power sources (Midwest), and hydrogen energy use (California) utilize an existing supply chain system whereby hydrogen already moves from east to west

Project strengths:

- This project does a very good job developing the underlying macroeconomics of hydrogen demand. This enables a deep conversation about the macroeconomic strategy at the national and regional levels. Additionally, the work is credible and well presented, making it easy to access and easy to find key points, and it reduces the likelihood of mistakes in general assumptions formed by the macroeconomic picture. The researchers state the assumptions clearly.
- The principal investigator appears to be executing the project in a very clear, supported, and professional manner. The project appears to draw in the necessary data sets (from collaborators and government databases). This project would fall apart without relevant data, and the team appears to have successfully gathered those data.
- Strengths include the rigorous analysis of the hydrogen demand drivers in refining and ammonia production.
- The strength of the project is the use of historical consumption data for the big existing hydrogen markets.
- The project's greatest strength is the detail exhibited in considering the hydrogen demand pathways. The level of detail shown in the fossil fuel refining and ammonia production analyses needs to be replicated for all applications.

Project weaknesses:

- The hydrogen supply curve should be tabulated and summarized so that the relative hydrogen supplies from each market can be compared. (This is a suggestion, rather than a true weakness.)
- The investigators would be well served by a diverse group of industry participants. While energy providers may be best positioned to advise on the data and data analysis and economists are good as peer reviewers, the team must consider others. Original equipment manufacturers, traditional hydrogen users, and new hydrogen energy users should be allowed to provide perspective to the overall project.
- The weaknesses are the lack of industry collaboration and the focus to date on applications that may not have presented as large a set of unknowns. Analysis of the remaining applications that are more future-oriented is likely to provide the greater impact.
- A cost-competitiveness assessment is lacking for e-fuels and hydrogen for steelmaking (these seem to be technical potential analyses only). The summary table did not present specifics on other sources of demand (vehicles, methane, natural gas replacement), so that portion of the work cannot be evaluated.
- One weakness of the project may be the lack of clear distinction of the source of energy/hydrogen for the assumed market demand, especially for the e-fuels market.

Recommendations for additions/deletions to project scope:

- The team should consider carefully the e-fuel concept. It is speculative and not well validated. It is very difficult to comment on e-fuels and place those next to ammonia or refinery consumption, as the two are very different. Perhaps the team should consider several new and alternative pathways from which it may select a "leading candidate," then present a scenario with that candidate as a surrogate for higher-potential outcomes. Meanwhile, the team should focus on changes in established demand and emerging markets where proven performance is already established.
- The project should consider looking at transportation applications with greater granularity. This could be different types of medium- and heavy-duty applications. The project could also look at different use cases and operating modes for light-duty vehicles, highlighting demand differences between privately owned vehicles, taxis, ridesharing, carsharing, ride-hailing, autonomous vehicles, and other potential applications.
- The project should consider detailed analysis of hydrogen blending to existing natural gas pipeline infrastructure. The team should identify opportunistic low-cost and renewable hydrogen production scenarios, with no storage requirement, along the infrastructure. The market size can be significant and achieved relatively easily.
- It would be good to see the full demand curve generated and discussed (although perhaps this is done under other tasking).
- There are no specific recommendations.

2019 – Safety, Codes and Standards
Summary of Annual Merit Review of the Safety, Codes and Standards Subprogram

The Safety, Codes and Standards (SCS) subprogram supports research and development (R&D) that provides critical information needed to define requirements and close gaps in safety, codes and standards to enable the safe use and handling of hydrogen and fuel cell technologies. The subprogram also conducts safety activities focused on promoting safety practices among U.S. Department of Energy (DOE) projects and the development of information resources and best practices. The SCS subprogram includes research on liquefied and cryogenic hydrogen release physics, contaminant detection and sensor technology, and quantitative risk assessments and consequence analysis. The subprogram also focuses on domestic and global codes and standards harmonization to enable large- and small-scale hydrogen applications.

Summary of Safety, Codes and Standards Subprogram and Reviewer Comments

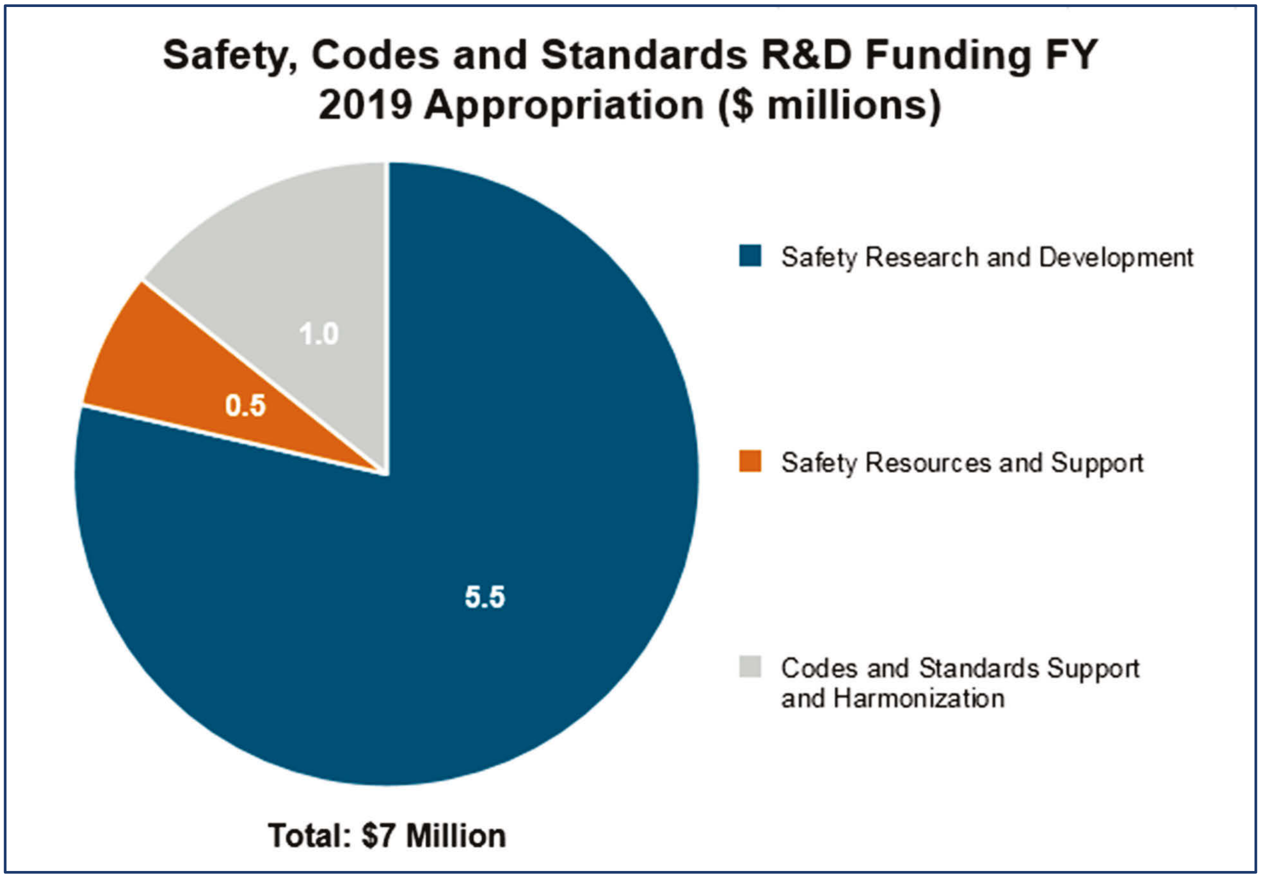
Hydrogen and Fuel Cells Program reviewers were highly supportive of the SCS projects and noted that the work of the SCS subprogram enables accomplishment of the broader goals of DOE and the Fuel Cell Technologies Office. Reviewers recommended further inclusion of a safety element across all subprograms. Reviewers applauded the subprogram for its alignment with industry and stakeholder needs and stated that SCS work is an essential framework for hydrogen and fuel cell activities. Reviewers encouraged the subprogram to identify means of increasing industry stakeholder participation in SCS activities. Reviewers praised the subprogram's increase in international engagement activities and particularly applauded the contribution of the subprogram to organizations such as the International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE). The reviewers also noted the importance of continued SCS participation in international regulations, codes and standards forums.

Key accomplishments identified by reviewers include the launch of the Center for Hydrogen Safety (CHS) and the R&D feedback to enable a significant reduction in the separation distances for bulk gaseous hydrogen storage in the National Fire Protection Association (NFPA) 2 Hydrogen Technologies Code. Reviewers felt that the CHS addressed a critical need for stakeholders in terms of safe deployment of hydrogen and fuel cell technologies. Reviewers continued to praise the science-based approach and the provision of feedback to code development organizations and standards development organizations. Key recommendations for SCS R&D include expanded quantitative efforts and data dissemination. Reviewers praised R&D efforts to enable cost reduction and encouraged the subprogram to balance experimental activities with analytical and computational efforts. Reviewers also recommended that materials R&D be expanded to disseminate materials selection guidance and lessons learned.

Nine projects were reviewed, receiving scores ranging from 2.85 to 3.7, with an average score of 3.43. Each of the individual project reports in this section contains a project summary, the project's overall score and average scores for each question, and the project-level reviewer comments.

Safety, Codes and Standards Funding

The fiscal year 2019 appropriation for the SCS subprogram totaled $7 million. The funding was focused on safety R&D, and the breakdown is shown in the following figure. The funding is expected to provide continued support of SCS R&D and efforts on domestic and international collaboration and harmonization of codes and standards. Future work in the subprogram is expected to focus on facilitating reduced regulatory barriers, such as by providing scientific anlaysis for revised bulk liquid hydrogen separation distances.


Safety, Codes and Standards R&D Funding FY 2019 Appropriation ($ millions)
1.0
0.5
5.5
Safety Research and Development
Safety Resources and Support
Codes and Standards Support and Harmonization
Total: $7 Million

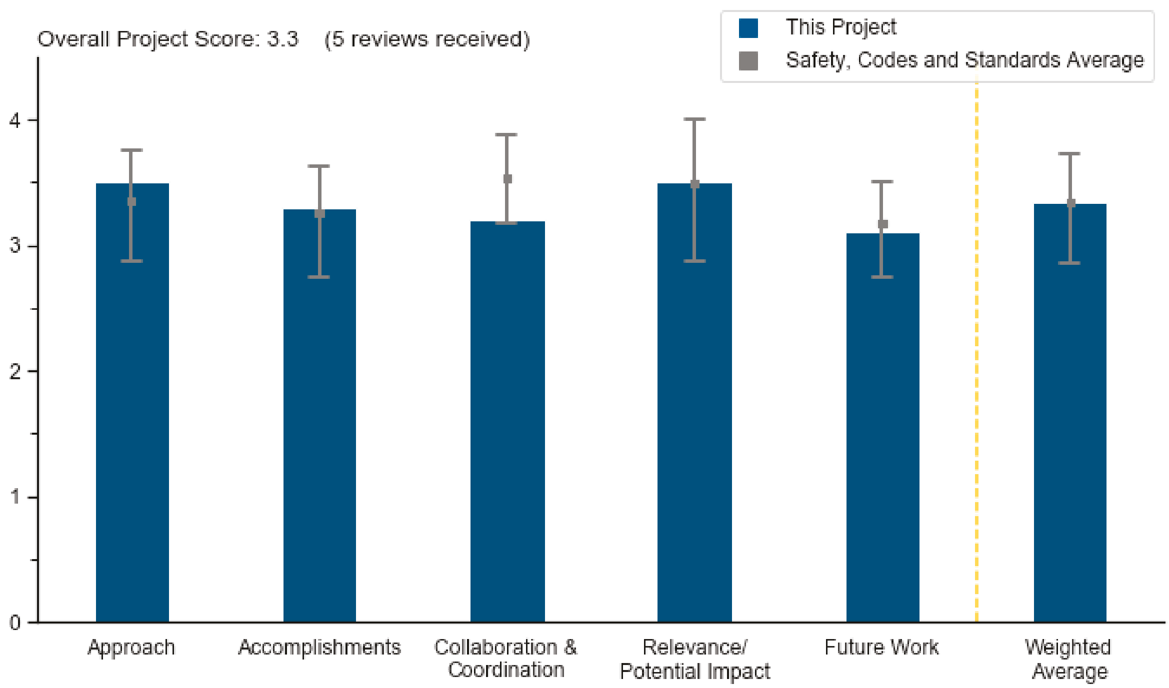
Project #SCS-001: National Codes and Standards Deployment and Outreach

Carl Rivkin, National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to further the deployment of hydrogen fuel cell technologies with particular focus on the infrastructure required to support fuel cell electric vehicles. This outreach and training project supports technology deployment by providing codes and standards information to project developers and code officials, making project permitting smoother and faster.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project accomplishes what it set out to do: work to provide to the standards development organization (SDO) and code development organization (CDO) community with technical data and analysis that will help to build a consistent set of regulations, codes, and standards. This is done by participation in the code and standard writing process; the principal investigator (PI) chairs National Fire Protection Agency (NFPA) 2. By working with other research entities, this project ensures that relevant research in the community, such as in other national laboratories, is efficiently communicated to the SDO and CDO communities and with each other. This is done through the Inter-Laboratory Research Integration Group (IRIG). This project also has branded an iterative process for code development called Continuous Code and Standards Improvement (CCSI). CCSI is intended to easily describe the iterative process for code development that embraces deployment, field performance, research and engineering analysis, and finally modification or development of codes. This methodology for code development brings all the relevant pieces to the development table. In today's science-based code development process, this iterative process is very good.

- The project's approaches include collaborating with stakeholders, leveraging of existing resources, and developing safety requirements, which should be effective for the objective of the safe deployment of hydrogen technologies.
- The approach with the CCSI and IRIG is well-thought-out and can serve the Safety, Codes and Standards community very well.
- The accomplishments for this project are a moving target. NFPA 2 is on a code cycle and will require several generations to optimize the recommendations. Still, the progress to date has been notable.
- The overarching plan and the specific iterative practical accomplishments of this project support real and sustained progress. Embracing the concept of continual refinement in light of field experience, technological evolution, and market dynamics is relevant but also balanced by specific, identifiable, logical, and progressive outcomes in this review period. Engagement and leadership are both integral parts of the approach, and both are essential for progress in codes and standards. It would be beneficial to maintain a more disciplined focus on differentiating tangible accomplishment of important outcomes from activities when reporting accomplishments. For example, presentations such as the one made for the Canadian code committee demonstrate good collaboration and engagement and might support future harmonization; ongoing work with Sandia National Laboratories to address setback for liquefied systems is also important. Both of these have merit and can support future outcomes of note; however, these are not themselves significant accomplishments (as they have been presented). The methods for presenting the newest tangible work products produced by the project are in some cases unclear and somewhat confusing. Going forward, the project should continually refresh the content on accomplishments to be clearer about what specifically was done (e.g., papers and reports published) in the immediate past year, rather than lacking precision about when accomplishments were made over the course of numerous years. It is recognized that technical work products might take several years to result in an identifiable code or standard revision. However, the project should focus on reporting relevant accomplishments in the previous year and dismiss past outputs from the reporting, such as paper publications from numerous years ago.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Chairing the Hydrogen Technologies Task Group for the NFPA 2 Hydrogen Technologies Code is an important role to advance evolving code requirements that are appropriately based on foundational safety concepts. Because of NFPA scheduling reallocations, fiscal year 2018 included the second draft meeting and corollary actions to support the finalization and publication of the much-needed next edition in 2019. Also, the Permit Checklist Task Group, chaired by the National Renewable Energy Laboratory (NREL), developed a standardized approach for permitting stations with gaseous/liquid storage that should promote more rapid approvals and allow for relaxation of safety setback distances while still providing for safe deployment.
- Much progress has been made, which includes the standard permit for gaseous/liquid hydrogen fueling stations, the proposal to reduce safety setback distances, component failure analysis, and so on. These accomplishments and progress all go toward the objective of safe deployment.
- The accomplishments for this project are a moving target. NFPA 2 is on a code cycle and will require several generations to optimize the recommendations. Still, progress to date has been notable.
- All of the accomplishments on slides 8 and 12–17 are valuable and useful. On slide 18, coordination is seen between the NFPA, the International Organization for Standardization (ISO), and the Canadian Hydrogen Installation Code (CHIC). This activity is live now, but the individual performing this activity is leaving, and it is unclear if there is a plan in place to account for that departure. The accomplishments on slides 9, 10, and 11 are surprising; the language is quite strong that the NREL directed the production of 2020 NFPA 2 and its task forces. This is an industry consensus code, and as such, the NFPA Hydrogen Technologies Technical Committee "directs" the changes; the chair is supposed to facilitate the discussions that happen in that process. Slide 19 states that the NFPA 2 technical committee voted not to include the document in the appendix of NFPA 2. With regard to the standard permit checklist, that is not a product or deliverable. As a member of the technical committee and a member of that task force, this reviewer's knowledge of that document is that there was an NFPA 2 supplemental ballot back in March, and there has not been any

further information from then until this poster (i.e., the technical committee has not been made aware of the status or any progress on the standard permitting checklist).

- The IRIG ranking of safety projects seems a little weak to deserve the level of credit that the PI is giving it; however, the leadership and work on NFPA 2 with the five task groups (Emergency Response, Storage, Equipment Enclosure, Permit Checklist Task Group, and Alternative Fuels group) deserve much credit and are very good. This work resulted in a significant reduction in some significant separation distances in the 2020 edition of NFPA 2 compared to the previous version; this is excellent. The development of a standard permit for hydrogen storage will also be extremely helpful in reducing cost and time for permitting; this is also excellent. The development of the component failure analysis for facility owners is very good and should help a great deal in learning about systematic failures in the field for similar systems. This project scored a 3.0, not a 4.0 or 3.5, because the accomplishments for the IRIG were not as strong as expected. It would have been good to see not just a ranking but a true working group among the members, which does not seem to have happened. This needs to be much more than simply NREL polling the national laboratories to rank order priorities. A true working collaboration on projects was anticipated—for example, a working group collaboration on the component failure that would involve a true collaboration with Sandia National Laboratories (SNL) and NREL. It might exist but was not seen in the presentation. The impression is given that the analysis on the failure is not done in a collaborative manner but rather in a stove-piped manner; the part is sent to SNL for materials analysis, but the analysis does not include SNL in the front-end failure determination. The analysis is done in series, not collaboratively in parallel.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- Collaboration and coordination are emphasized in this project. Industrial gas companies, SDOs, DOE national laboratories, regional fire and building officials, and regional hydrogen advocacy groups are involved in this project and have specific different divisions of labor.
- Standards and codes are by their inherent nature collaborative, involving many different parties, and in that sense, the project includes robust collaboration. While there is value in being engaged in a standards development process, the project should focus on enabling or catalyzing new results. Being strategic and focused on identifying, enacting, and reporting on specific collaborations toward outcomes that might not occur, might not occur as soon, or would not otherwise occur would be an appropriate objective and benchmarking process for this project. Coordination among codes and standards is an area of specific and ongoing need for hydrogen technologies, and this project can play a more prominent role in identifying and closing those gaps among codes, standards, and geographies. Some of that work has been initiated, and it should be maintained and amplified.
- This presentation is addressing a myriad of tasks. The collaboration is appropriate for each task. The coordination appears appropriate.
- The only thing on the list of collaborations that can truly be named a collaboration is the partnering with a collaborator to measure leak rates at the facility. Having other entities sit on the same committee as NREL does not itself constitute a collaboration. The fact that NREL, SNL, Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory, and Los Alamos National Laboratory all sit on the NFPA task force groups does not mean they are collaborators. If, however, NREL and SNL collaborate on a failure analysis that occurred in the field and collectively wrote the report to present collectively to the relevant NFPA task force, that would constitute a collaboration. Providing information and performing outreach events does not constitute collaboration; it is outreach but not a collaboration. Providing input to help develop state regulation is not collaboration. If, on the other hand, NREL worked closely with the state regulators in the development of the regulations (i.e., sat on their committees), that would constitute collaboration and/or coordination. NREL has worked with station developers on the component failure project and developed permitting tools; this is a collaboration and/or coordination.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The overarching project intent related to refinement and advancement of hydrogen safety codes and standards remains relevant. The outcomes accomplished in this review period on codes and standards are very good, in light of the impending publication of the 2020 edition of NFPA 2 and its new content, driven in part by the project.
- The potential impact of this project is large. Just liquid spill mitigation is a home run. Component failure modes are also of high value.
- All in all, this project is very relevant and has already shown significant impact in the dissemination of information; possibly most important is the work on NFPA, all task forces, and in particular the resulting reduction in separation distances.
- There is no doubt that the content of this project will have significant impact on hydrogen technology deployment.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project's proposed future work for supporting codes and standards for H2@Scale is relevant. A more specific roadmap would help ensure the project would facilitate deployment of H2@Scale. The project would benefit from more specific planning in preparation for upcoming NFPA 2 and other revision cycles. "[Continuing] to identify the needs of safety information users and provid[ing] information to meet those needs in the most accessible and intelligible form possible" can certainly have value in some cases but is quite amorphous. The project should either define more clearly what that would constitute that is not being accomplished by other entities (such as the Center for Hydrogen Safety), or supplant that work with specific tangible efforts, such as codes and standards, gap analyses, and gap closure. The component failure analysis effort can provide a rich basis for transforming field experience into targeted, substantiated codes and standards proposals for continued enhancement of requirements. This does not seem to have yet occurred, and as presently laid out, the plan to accomplish that is not entirely clear. The project would benefit from a clearer articulation of the specific actions that will result in the fault analyses and how they will be used to surgically elevate the safety requirements. The project would also benefit from clearer bidirectional coordination with the NREL National Fuel Cell Technology Evaluation Center efforts, including the safety aspects of the Hydrogen Fueling Infrastructure Analysis, to minimize redundancy and optimize outcomes. Sharing findings and data with the Hydrogen Risk Assessment Model (HyRAM) is logical and appropriate, but the plan for that to have a clear impact on codes and standards needs to be clarified or the projected outcomes might need to be re-evaluated in this regard. As the permitting checklist was an important outcome for this review period, more actions to address the rollout would be beneficial. This includes promoting awareness of the new tools through mechanisms such as webinars. Furthermore, planning to engage with regulators and other stakeholders to determine whether the tools are as effective as intended, as well as to find specific areas for improvement while preparing for the next edition of NFPA 2, would be relevant.
- The proposed future work is an evolutionary extension of the current effort, which is fine, but there should be a revolutionary proposed next step, maybe proposing efforts to advance hydrogen use in very nontraditional applications, such as in airplanes or in maritime settings onboard ships.
- The proposed future works are specific and will be effective in addressing the key issues.
- The project should continue down the current path.
- It is unclear what is meant by "Structure hydrogen vehicle fueling requirements to better match infrastructure projects." Additionally, "Publish Hydrogen Fueling Station Permitting Guide" is listed as part of future work, but the previous accomplishment slides make it seem like it is published.

Project strengths:

- The project has a strong value proposition in terms of promoting continual refinement of hydrogen codes and standards. Leading work on the impending next edition of NFPA 2 and the permitting checklist comprise practical, effective advancement. The staff executing the project has been well connected with relevant stakeholders in the community to promote ongoing collaboration.
- The project's strengths include the ability to leverage existing resources and the ability to conduct testing at the fueling station; that, along with input from industry experience, feeds into the code development process.
- The issues under this project are very important for the safe deployment of hydrogen technology; the accomplishments and progress are on a good path.
- This is a very important activity with demonstrated value to the community.
- The project's strengths include its plan and new leadership.

Project weaknesses:

- The project's weaknesses include the heavy influence in/on the NFPA 2 process, particularly with the standard permitting checklist process. There is no argument that this kind of document will be helpful; it was more the way in which the process was executed.
- Aside from the direct actions related to codes and standards development, the project does not seem clearly focused on specific actions leading to tangible outcomes. There are opportunities for improvement in striving for catalyzing new outcomes in hydrogen codes and standards that would not otherwise occur, rather than solely being a committee participant. Recognizing that codes are on a cyclic schedule, there does not seem to be a staged plan of planned actions for progress over multiple cycles. The outreach aspect of the project is ambiguous and might be best fulfilled by other entities in practice. A clearer plan is needed for using component failure analyses to drive specific codes and standards proposals. It seems that in some aspects, the project is resting on accomplishments from several years ago, rather than the immediate past, and overvaluing activities as accomplishments in some cases. Leadership roles in code activities have played a large role in successes in the past year, and continued success may be linked to staff maintaining those leadership roles (especially in the present construct).
- NREL should work to develop activities, partners (like the IRIG members) with whom to truly collaborate. It should be that both parties contribute to the root cause of a failure, both parties contribute to the analysis, and both parties contribute to the report. NREL making a presentation at a CHIC meeting is not a coordination; however, NREL coordinating the requirements of NFPA 2 with CHIC and ISO 19880-1 is.
- The project should be aware of tunnel vision and vested interests from advisers.
- The path proposed is not very specific about the hydrogen safety issues identified in the range of applications dictated by H2@Scale.

Recommendations for additions/deletions to project scope:

- As the hydrogen market and community continue to evolve, reconsideration of the coordination and most impactful and specific future work plan would be beneficial. Optimizing and articulating coordination with other work, such as the Center for Hydrogen Safety and the National Fuel Cell Technology Evaluation Center, will help minimize redundancies and best promote impact. With respect to collaborations and coordination, being more focused in general would be beneficial. Standards and codes are by their inherent nature collaborative, involving many different parties. Being strategic and focused in identifying, enacting, and reporting on specific collaborations would be appropriate for the project. Coordination among codes and standards, especially as they evolve on different cycles by the actions of different standards organizations, is an area of specific and ongoing need for hydrogen technologies. This project can play a more prominent role in proactively identifying and closing those gaps. Especially with the cyclic nature of code development, it would be helpful to have an active plan to identify the issues that will need to be addressed in future editions and then plan in advance to build the necessary materials in the intermediary periods.

- The project team should maintain NREL as a resource, for example, for station validation exercises that allow for the advancement of the technology, rather than try to be an influencer in the same capacity as industry or an industry association, like the Compressed Gas Association, for example.
- Years ago, NREL was evaluating a relief valve failure and dropped the evaluation after duplicating the failure. The team should consider reassessing the project. NREL has a test protocol and a test vehicle (the failed valve). The next step would be to substitute other materials for the wetted components and test per the previous test plan. Several assemblies could be tested simultaneously.

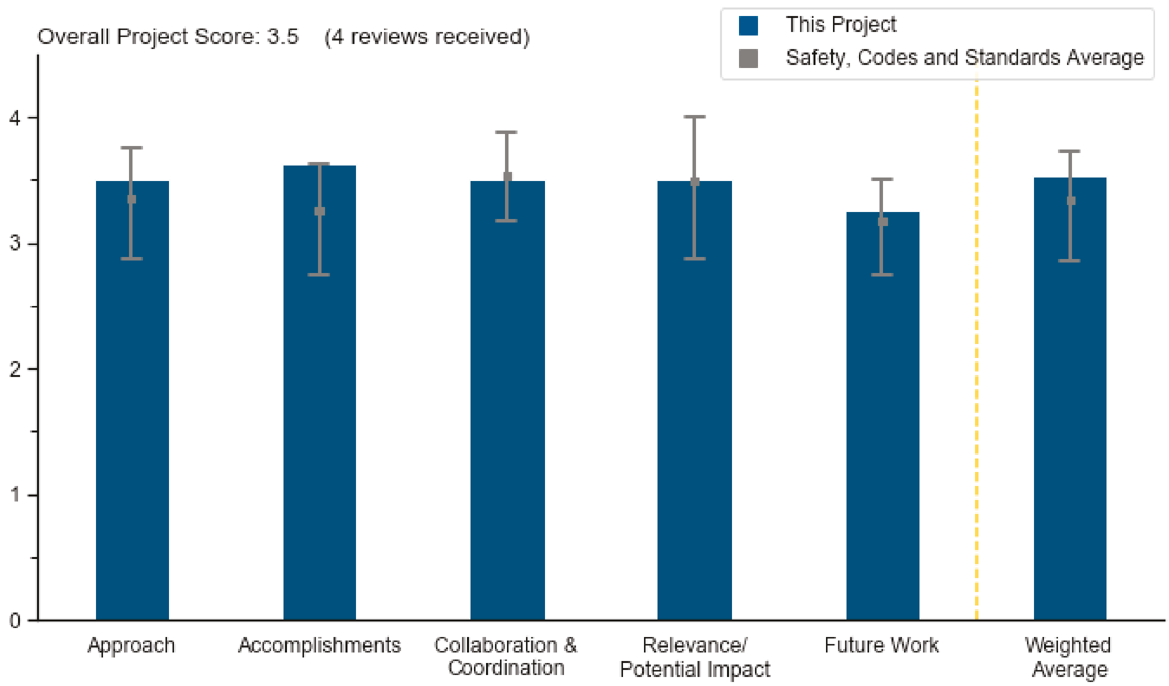
Project #SCS-005: Research and Development for Safety, Codes and Standards: Materials and Component Compatibility

Chris San Marchi, Sandia National Laboratories

Brief Summary of Project

The main goal of this project is to enable technology deployment by providing science-based resources for standards and hydrogen component development and to participate directly in formulating standards. The project will (1) develop and maintain a materials property database and identify materials property data gaps, (2) develop more efficient and reliable materials test methods in standards, (3) develop design and safety qualification standards for components and materials testing standards, and (4) execute materials testing to address targeted data gaps in standards and critical technology development.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach uses a sound physics-of-failure basis for considering the critical attributes and assessments for materials in hydrogen service. Using both design principles and performance principles, tailored to specific applications, is reasonable and will promote different valid options to be explored.
- This project continues to advance the development of science-based codes and standards that are required for commercial hydrogen storage and transport applications. Highlights are capabilities to perform measurements in high-pressure hydrogen, the strong international collaborations, and the development of consensus leading to new American Society for Testing and Materials codes and standards. The approach for use of wet air as opposed to wet hydrogen needs verification. Regarding the aluminum alloys, there may be a need to evaluate oxide surface scales as a function of gas conditions and stress state.
- The approach for this work is excellent. The end goal is to incorporate the data into the ASME Pressure Technology Code, making the data accessible worldwide.

- The approach addresses the technology barriers. It has been in progress for a number of years, and reviewer comments from prior years are addressed in a considerate and objective manner.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The Sandia National Laboratories Hydrogen Effects Database (Granta MI) is accessible to the public. Identifying the critical limiting behavior of fatigue performance has supported specific protocols to be focused and advanced, contemplating a conservative safety factor. Efforts on stationary pressure vessels have demonstrated advancement, including approval of ASME Code Case 2938 (which will be effective upon its impending publication) and design curves addressing options for high-strength steels. A proposal for a standardized international approach on materials compatibility testing has been developed, but agreement is still in progress. Work to address complex geometries and welds is ongoing, but its completion will be essential moving forward.
- Significant accomplishments include the approval of ASME Code Case 2938, which is a direct result of the work funded by the DOE Office of Energy Efficiency and Renewable Energy.
- The progress to date is impressive. The results will ultimately reduce costs and improve safety on hydrogen infrastructure projects.
- The overall project goal is not well defined. Material performance in various hydrogen environments could be researched through never-ending combinations of conditions and materials. However, good progress in some areas has been made to date, and integration with various databases and other efforts has been considered.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- International collaborations in both Asia and Europe are a highlight of this work. Partnerships have been established with leading institutions such as Kyushu University in Japan (and the Japanese National Institute of Advanced Industrial Science and Technology [AIST]) and appear to be truly working relationships with important deliverables on international codes and standards.
- The project incorporates effective collaborations with industry, academia, and standards development organizations to advance the practical outcomes of the project's work. Collaboration spans geographies in the Americas, Asia, and Europe. Connections with the Hydrogen Materials Compatibility Consortium (H-Mat) are identified appropriately and are being addressed.
- The collaboration/coordination/partner list is extensive and international. Additional U.S. companies and researchers might be appropriate.
- Other interested institutions and stakeholders have been identified, and collaborative efforts are under way. Maintaining that collaboration and obtaining consensus may be difficult barriers that were not identified.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The issue remains relevant, and the project is showing real advancement in addressing the issues in moving from a science-based foundation to practical protocols that are affecting, and will continue to positively affect, the hydrogen community. Work to scale solutions globally is relevant and in progress.
- This project makes significant impacts by bridging the scales from the basic science of fracture mechanics to the implementation of applicable codes and standards.
- The project is very relevant and could have a significant impact.

- This activity is highly relevant. A little more focus on tungsten inert gas and metal inert gas field welding might be in order. These welds will most likely be issues.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The planned future work to address welds and aluminum is appropriate and well framed. The feasibility of ongoing revision of technical references rather than planning for fiscal year 2020 should be considered.
- The project scope is good, but plans and future work beyond 2019 are unclear. Note that the project end date is 2022.
- The proposed work appears appropriate.

Project strengths:

- This project constitutes relevant work that is using a physics-of-failure approach to leverage science into practical design and performance criteria, differentiated based on applications. The project has an effective network of global partners and collaborators. These have resulted in tangible and significant advancements.
- The project scope, collaboration with other institutions and stakeholders, and attention paid to past criticisms and suggestions are all project strengths.
- The team (collaboration), test staff, goal focus, and application are project strengths.

Project weaknesses:

- Continued future progress on some aspects, such as further acceleration of fatigue testing, might not be practically possible without breakthroughs in other efforts such as H-Mat.
- Based on the information presented, one weakness of the project seems to be plans for future work beyond 2020.
- There is plenty of European and Asian input but seemingly no input from U.S. academic researchers.

Recommendations for additions/deletions to project scope:

- Consideration of the practical execution of the performance testing is not explicitly addressed but would be beneficial to ensure the highest penetration of the solutions. Validation testing of the protocols using known valid and vulnerable designs, to the degree possible, is not essential but would be instructive.
- Gaps in the existing data should be defined. There should be an explanation as to what “science-based codes and standards” and “science-based test methodologies” mean in the context of this effort.

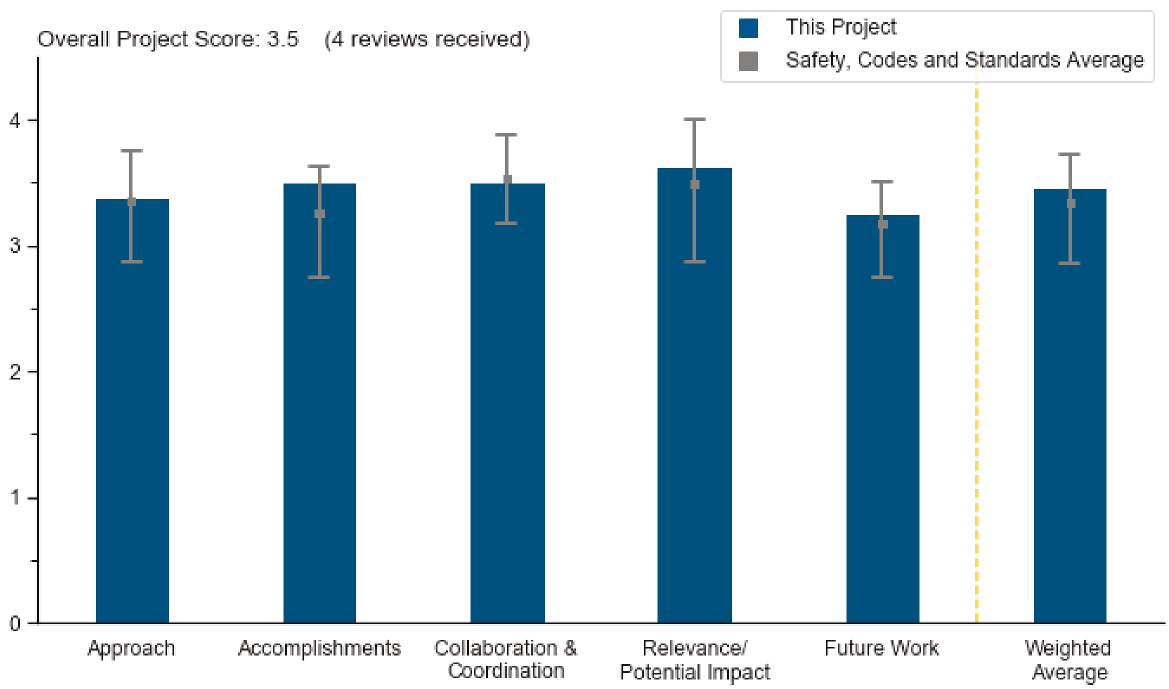
Project #SCS-007: Fuel Quality Assurance Research and Development and Impurity Testing in Support of Codes and Standards

Tommy Rockward, Los Alamos National Laboratory

Brief Summary of Project

The objectives of this project are to (1) focus on polymer electrolyte membrane fuel cell testing and collaborations and work with the American Society for Testing and Materials to develop standards and (2) develop an electrochemical analyzer to measure impurities in the fuel stream. The analyzer will be inexpensive, will be sensitive to the same impurities that would poison a fuel cell stack, and will support quick responses to contaminants.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The project's approach is well thought out, the execution is excellent, and the overall technology used for the detection of contaminants is excellent. The research team addresses problems in a systematic and appropriate technical manner. The team quantifies the results before moving on. This is a very nice project.
- Overall, this project continues to make good progress. It has taken some time, but it is nice to see the hydrogen contaminant detector (HCD) analyzer being validated at a commercial hydrogen refueling station (HRS). Even though the focus on CO makes sense, the detection of other impurities needs to show further development and flexibility.
- There is a minor error on slide 1: the Project 2 end date is September 30, 2022 (not September 30, 2012). There are HCD fuel quality analyzers for offline (Project 1) or in-line analysis (Project 2). Project 2's approach seems to have improved based on feedback from Project 1. The approach now includes partnership with a small business to commercialize the technology, which is very promising. It is a bit concerning that there are significant unverified changes between Project 1 and Project 2 in order to achieve

true in-line testing. While some results are promising, others indicate the need for further changes to meet the requirements of in-line fuel monitoring. It is not clear that the technology is ready for commercialization, although it is needed in the field now.

- The approach is sound and yielding results. It is unclear how the lack of humidification or how the corrosive effects of H_3PO_4 are being addressed, or how the moisture being released by the electrolyte is affecting the water threshold.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project is meeting its milestones. It takes the current state of the art and advances it incrementally to achieve the desired product. The project team has developed polybenzimidazole (PBI)-based and tin pyrophosphate (TPP)-based HCD technology that performs as the previous version but without the need for water, which is perfect. This will also reduce system complexity and cost and, most importantly, will possibly be able to operate in-line. The initial results are very interesting. Both the PBI and TPP membranes show very good promise in producing a HCD that shows promise of developing a technology that will work in this application. Work still needs to be done in increasing understanding of CO and H_2S poisoning for the PBI system. The assembly of the TPP composite membranes needs to be finished. The steady progress this project has accomplished is largely impressive.
- The project's progress is as should be expected. It is unclear how the performance is to be temperature-compensated, whether this is a software correction or a change in material selection. Slide 8 suggests a software tweak. The PBI results are an extender. H_3PO_4 has a vapor pressure that is very low, but measurable. This would slow the evaporation of the electrolyte, which would be a good thing. It is unclear whether the evaporation can be stopped (which would be the better thing) or if this is a case of "better" being the enemy of "good." It is also unclear whether TPP is viable. It seems 1,2-pentanediol may be a contaminant in and of itself. Both ethylene and propylene glycols are catalyst toxins.
- A significant accomplishment is the development of the wicking scheme that solved the hydration issues of dry hydrogen gas. The application of prototypes into real-life stations has resulted in meaningful improvements to the technology. The main concern is the rate of progress, as there has been no testing of the range of contaminants of interest, and improvements are still needed on the response time for CO detection. It is still too early to tell whether the project will ultimately be successful.
- The project has made good progress in the last year, mainly driven by the ability to validate the analyzer under real-world conditions.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- The collaborators on this project are perfect: H2 Frontier, Inc., is a no-cost field test site; Skyre, Inc., is a support activity under the Small Business Voucher (SBV) program and collaborates with the National Renewable Energy Laboratory (NREL) on HCD development; and Los Alamos National Laboratory (LANL) provides support to Southwest Sciences, Inc. (SSI) in HCD development. These collaborations are very good and help the development community make use of LANL's capability and expertise; however, it is not clear what LANL gets out of these. This project did not score a 4 because, while these collaborations and coordination should continue, LANL needs to get something tangible out of the effort.
- The presentation did not get into detail regarding how well coordinated the partnerships and collaborations might be, although the collaboration on DOE Small Business Innovation Research (SBIR) and SBV proposals for the technology commercialization partner is noteworthy. The project partners are all suitable collaborators, including H2 Frontier, Inc., Skyre, Inc. (formerly Sustainable Innovations), SSI, NREL, and Bill Buttner. It would be beneficial to see collaboration with SAE International in some way, as well as with the California Fuel Cell Partnership, or one or more partners that work with fuel cell electric vehicles.

- This is an excellent team. Doug Wheeler might be a helpful consultant. He has phosphoric acid fuel cell (PAFC) experience.
- The project demonstrated great collaboration and coordination with other national laboratories and appropriate industry stakeholders.

Question 4: Relevance/potential impact

This project was rated **3.6** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- There is no doubt that an HCD is critical to the successful deployment of HRSs, now and in the future. The fuel quality delivered to the vehicle must be guaranteed to meet the SAE International and International Organization for Standardization (ISO) standards for contaminant-specified levels, or this technology will fail in deployment. Having HCDs at the fueling station, and more importantly at the nozzle, is critical to the success of fuel cell technologies.
- This activity is highly relevant. Assuming that the trials are successful, it would be beneficial to know if the product will be listed or if, at a minimum, it will be tested for ATEX (International Electrotechnical Commission [IEC] 60079) or the North American equivalent. This should be the final hurdle to commercialization.
- Depending on how the field trial finishes up, the project team should work with the Fuel Cell Technologies Office on how to best transition the technology and support a glaring need at HRSs. There was mention of partnering with a company, but if the Technology Commercialization Fund opportunity does not happen, there should be a plan for the next step.
- It is excellent that a commercialization partner has been identified so that the resulting technology may be able to get to the marketplace. There is concern about the pace of the progress being made.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed technology transfer activities are a very good and necessary role for the national laboratories. The proposed future work is very good. Continuing the development of PBI and/or TPP is appropriate. The proposed future technical work in this area is systematic, well thought out, and based in fundamentals; this is perfect. The project has a focus on commercialization; this will keep the team focused on the endgame.
- The steps defined in the presentation for Project 2 appear to be very basic first steps that will take a minimum of four years to develop into a product that, if successful, may have commercial relevance. The project team should develop a PBI-based analyzer (lower-technology-readiness-level work started in October 2018, based on the four-year proposal).
- The membrane development and evaluation are important, but it is uncertain what happens next. It would be good to see a Gantt chart showing the intended next steps and the final endgame.
- The proposed future work is acceptable.

Project strengths:

- This is a very important activity. It is founded in fundamentals and has extremely talented personnel and excellent facilities, which are applied to LANL’s technologies as well as competing technologies from other entities through outside avenues (e.g., the SBV program). This is a perfect role for a national laboratory.
- The project’s strengths include its team. Doug Wheeler may be a reference for PAFCs and derivative membranes.
- The project has good collaboration with its partners and is doing important work.

Project weaknesses:

- Slow progress is being made toward the availability of a useful product that can be reliably deployed. There is no guarantee that the project will result in the development of an in-line hydrogen analyzer suitable for commercial refueling stations.
- The team has spent too much time focusing on CO, even though CO can be seen as a canary species.
- The end game and the definition of “success” are unclear.

Recommendations for additions/deletions to project scope:

- The team should make an attempt to identify another partner that could help speed up the development of the PBI-based analyzer.
- The project team needs to define the steps to commercialization.

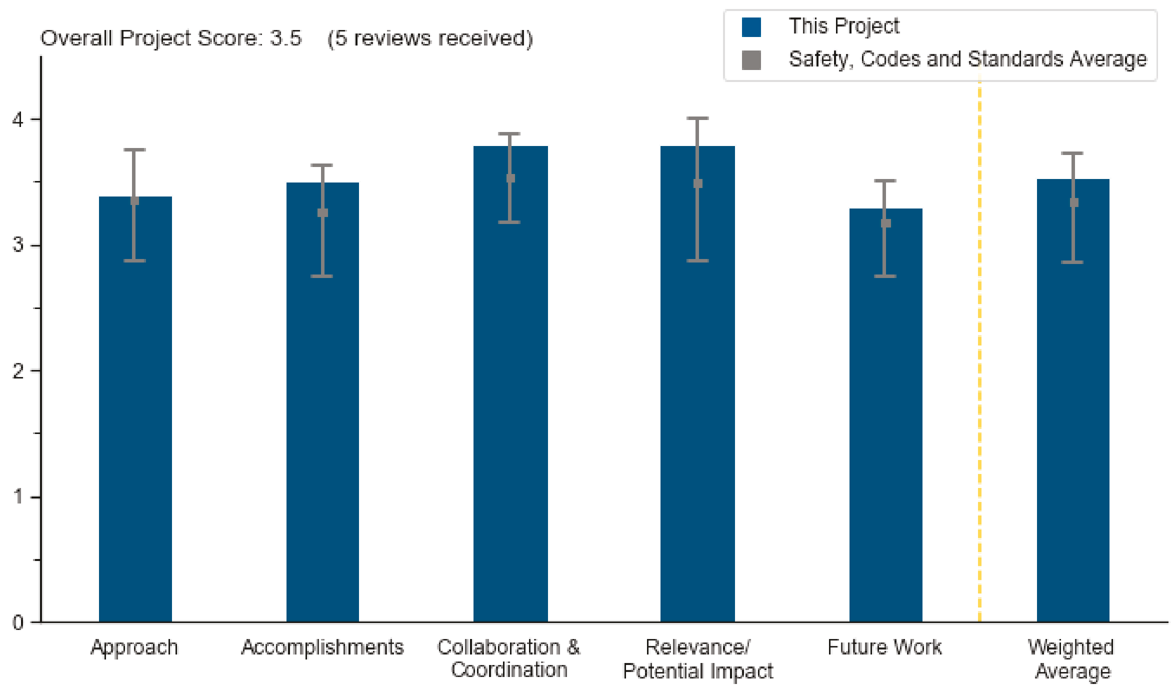
Project #SCS-010: Research and Development for Safety, Codes and Standards: Hydrogen Behavior

Ethan Hecht, Sandia National Laboratories

Brief Summary of Project

The project's purpose is to perform research and development (R&D) to provide the science and engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of uses (including high-pressure and cryogenic). The research includes model and tool development to facilitate the assessment of the safety (i.e., risk) of hydrogen systems and enable use of that information for revising regulations, codes, and standards (RCS) and for permitting stations. Sandia National Laboratories (SNL) is working to address the lack of safety data and technical information relevant to the development of safety, codes and standards (SCS) by (1) providing a science and engineering basis for understanding the release, ignition, and combustion behavior of hydrogen across its range of use (i.e., high-pressure, cryogenic), (2) generating data to address targeted gaps in the understanding of hydrogen behavior physics (and modeling), and (3) developing and validating scientific models to facilitate quantitative risk assessment of hydrogen systems and enable revision of RCS to accelerate permitting of hydrogen refueling. The project began in 2003.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The approach used was multifaceted and involved not only this project but project SCS-011, Hydrogen Quantitative Risk Assessment (reviewed in 2019), and project SCS-025, Hydrogen Infrastructure through Science-Based Codes and Standards (not reviewed in 2019). Coordinating with these other activities, as well as developing and executing experiments for predictive modeling, combines for excellent research. Getting to worst-case scenarios will help in the predictions. Comments on the 2022 edition of National Fire Protection Agency (NFPA) 2 will be needed before long.

- SNL's approach to R&D for SCS is very sound. The team has an impressive pedigree of previous success. There are no issues here.
- This is an excellent approach that addresses all barriers via an intelligent pairing of controlled laboratory experiments with outdoor, real-equipment releases.
- The approach presented is detailed, pertinent, and focused on accomplishing the objective.
- The approach for the specific tasks is good. For the analysis on the non-circular cross-sections, the project team should consider a cross-section that is not planar but radial in nature to simulate a circumferential leak from threads or a crack. This would have the effect of possibly diffusing the leak in different directions as opposed to in one direction. For the truck vent releases, it is not clear whether this is for actual analysis of this activity or only for validating the model. Validating the model seems appropriate because of the variability of that activity. Presumably, the flow rates will be well documented for model comparison.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project has made outstanding progress that answers a number of critical questions related to cold hydrogen behavior. In particular, the project team has shown that a circular release orifice can be used as a representative orifice for modeling and predicting heat fluxes from all possible shapes of ignited leaks, and that a lower hydrogen temperature leads to higher thermal flux from ignited plumes of the same flow rate. These contribute to a more accurate analysis for hazard distances associated with venting or leaks of cold hydrogen gas.
- The open-source release of the modeling is terrific; however, it will open the door to further inquiries that will need responses. It is suggested that the project team consider having a "frequently asked questions" page on the Hydrogen Risk Assessment Model (HyRAM) and Center for Hydrogen Safety (CHS) websites so that some common questions could be answered without taking up valuable resources. It is unclear whether moving the information from HyRAM to the CHS will allow the progress of the project's work to continue to be available at no cost. It is suggested that the project team consider a model that accounts for different temperatures in order to measure the flame length and heat flux. The work planned for Lawrence Livermore National Laboratory (LLNL) is exciting; hopefully the project team will see the proper weather conditions for the releases.
- The accomplishments of the specific tasks are good and useful. Progress has been made in these areas. However, other useful work is needed. The project team made mention of NFPA 2 and separation distances. There is still limited progress in the area of liquid hydrogen (LH_2) to recommend revised separation distance tables for exposures based on experimentation or the use of validated models. One goal mentioned is to affect NFPA 2 for 2022. The time frame is likely for the 2023 edition, but that will require submitting information no later than the spring of 2021. This is a tight timeline, but there is not a corresponding schedule that shows the ability of this project to meet the required dates.
- The reduction of siting burdens is a critical factor that is preventing the proliferation of large hydrogen fueling stations (with on-site storage that can hold thousands of kilograms). There is an issue with one of the statements made by the presenter: the premise that liquid ground storage was the only way forward for large fueling stations. This premise is incorrect in light of recent press releases from companies, such as the Nikola Motor Company, that plan to use on-site generation and compressed hydrogen storage for up to 32 tons/day.
- The project's accomplishments and progress are very good. However, it is not clear whether these accomplishments are the best way or method to meet the goals. For instance, it is unclear how worst-case scenarios will be determined and evaluated.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The project has outstanding collaborations with other national laboratories (including the National Renewable Energy Laboratory and LLNL), as well as in the international hydrogen safety community (including the Pre-normative Research for Safe Use of Liquid Hydrogen [PRESHLY], funded by the Fuel Cells and Hydrogen Joint Undertaking, as well as the HySafe Research Priority Workshops and the International Conference on Hydrogen Safety).
- The project's collaboration with outside companies (Linde, Shell Oil Company, and others), NFPA, the Compressed Gas Association (CGA), and partners outside the United States looks to be outstanding.
- The collaborations are outstanding and numerous. The project team should keep up the great work. Continued active participation with NFPA 2 is necessary so that the code can be updated to include science-based information.
- There is good collaboration with NFPA, CGA, and European projects such as PRESHLY.
- The project's collaboration with other organizations is effective, in both technical content and experience.

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The work is very relevant and can affect hydrogen fueling stations in a positive way by reducing the footprint and lowering setback values for LH_2, etc. The timing to coordinate with the NFPA 2 Technical Committee (TC) in order to advise the committee is well planned. The modeling and data from the experiments (and the scaling for actual vent stacks) will be critical.
- The project has very high relevance and impact, as the project results are critical for the wide market deployment of a hydrogen fueling infrastructure and public acceptance of fuel cell electric vehicles and other technologies using LH_2 in non-industrial settings.
- Separation distances are critical to safety and also to the deployment of hydrogen into areas where it has not traditionally been installed.
- The R&D work correlates directly to DOE targets, namely by identifying ways to reduce siting burdens that prohibit the expansion of hydrogen fueling stations. It is very important work.
- This project is critical not only to the DOE Hydrogen Fuel Cells Program but also to commercial partners and the safety of the general public.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The proposed future work is very nicely presented for the remaining fiscal year (FY) 2019 and FY 2020. The data generated from the other crack patterns of the releases will be interesting. The critical path will be in completing the modeling and experiments in time to have solid data for the NFPA 2 TC to consider for the 2022 edition. The 40% reduction in station footprint is exciting and could be a real game changer.
- The proposed future work is outstanding, keeping the balance between laboratory experiments, computational fluid dynamics modeling, and outdoor, cold-hydrogen-venting non-ignited releases. The contribution to CGA of ignited experiments on liquid tanker venting is also important.
- The project team has good plans for future work that is key to meeting DOE goals and supporting the industry. Perhaps some efforts should be directed toward testing to validate the use of walls for optimizing separation distances.
- The schedule for the LH_2 separation distance work continues to slip, and there are not definitive timelines for this work to be completed and/or to meet the timeline of NFPA 2. The project needs a detailed schedule for when validation of the LH_2 model will be completed and when testing can be completed. The analysis of the releases for depressurizing tankers is relevant only to the validation of the model. The main area of

concern would be inadvertent releases and failures. These are the primary scenarios for which separation distances are required. One of the primary issues with NFPA 2 has been mitigation via barrier walls. A gap that exists between NFPA and common practice is the use of four barrier walls for gaseous hydrogen and three to four barrier walls for LH_2. Analysis on the impact of these additional walls, either via modeling or experimentation, would be useful to the NFPA committee. This would have high relevance to NFPA and the resolution of some alternative means and measures that are commonly used. In addition, the use of barrier walls is not permitted for some of the separation distances that are more difficult to meet. It would be helpful to understand the impact of these walls and their height on these separation distances.
- The presentation does not make clear how the various large-scale spill experiments relate to the eventual planned customer facilities.

Project strengths:

- The work was nicely presented, including the project's objectives, relevance, work to date, goals, barriers, and project partners. Having this work presented and ultimately accepted into the next edition of NFPA 2 will be very meaningful for the hydrogen industry.
- The project team has strong knowledge and expertise in measurement techniques and modeling capabilities, as well as strong industry ties, national laboratory collaborations, and active participation in relevant international activities.
- This work has direct influence on NFPA separation distances. The work is required for the NFPA TC to make informed decisions.
- The project has great focus on R&D to serve DOE goals and to meet the needs of siting large-storage hydrogen fueling stations.
- There are two overall project strengths: the critical relevance of the project and the technical expertise of SNL, including the partnership and synergy with LLNL.

Project weaknesses:

- There are not many project weaknesses; the project team seems to cover all the bases. It is perhaps advised that there should be slightly more recognition of equipment and practices that are relevant to the real world.
- It does not seem certain that there is adequate funding for this project to accomplish everything necessary. While there are many partners, it may be that the project team should collaborate with these organizations to make the information more broadly available to stakeholders.
- The timeline continues to slide, and it is critical not to miss important submission deadlines for NFPA documents. The lack of large-scale release testing is being addressed with the development of a project to perform these tests, but the schedule is vague and needs to be accelerated.
- There are two main weaknesses: the project schedule for future work is somewhat vague (without very many milestones), and future funding seems variable and uncertain.
- The presentation did not speak directly to NFPA 2 footprint reduction.

Recommendations for additions/deletions to project scope:

- There are no recommendations for additions or deletions; the current plan is excellent. As a suggestion for the planned cold hydrogen venting at LLNL, the project team should compare a typical vent stack termination with a T-shape (that has bull horns) to the single-outlet termination that is currently planned. This should contribute to a better understanding of the effect of wind and other weather conditions on the dispersion of the cold hydrogen plume.
- One of the primary issues within NFPA 2 has been the mitigation via barrier walls. A gap that exists between NFPA and common practice is the use of four barrier walls for gaseous hydrogen and three to four barrier walls for LH_2. It would be useful to the NFPA committee if analysis were done on the impact of these additional walls, either via modelling or experimentation, and what configurations might be effective and safe. This would have high relevance to NFPA and the resolution of some alternative means and measures that are commonly used.
- The project should perhaps do testing to validate the use of walls in measuring and optimizing separation distances.

- It is recommended that the project team more thoroughly consider weather conditions and future hydrogen facilities (e.g., size, materials, and operating conditions).

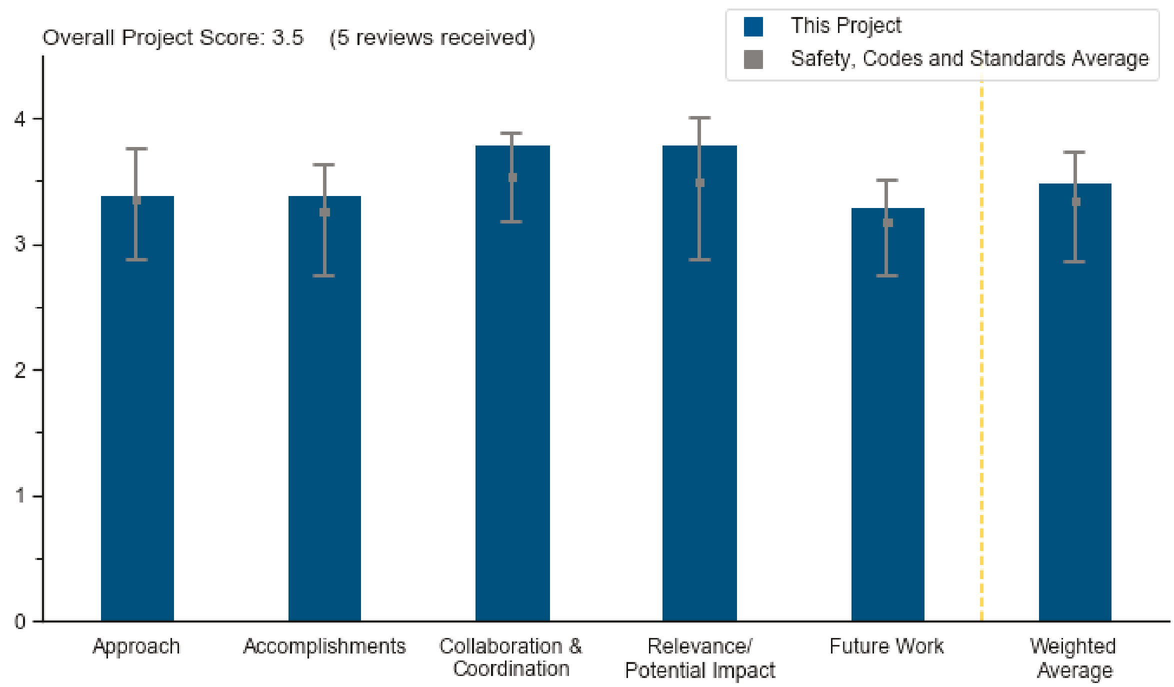
Project #SCS-011: Hydrogen Quantitative Risk Assessment

Alice Muna, Sandia National Laboratories

Brief Summary of Project

The primary objective of this project is to provide a science and engineering basis for assessing the safety of hydrogen systems and facilitate the use of that information for revising regulations, codes, and standards (RCS) and permitting stations. Sandia National Laboratories (SNL) will develop and validate hydrogen behavior physics models to address targeted gaps in knowledge, build tools to enable industry-led codes and standards revision and safety analyses, and develop hydrogen-specific quantitative risk assessment (QRA) tools and methods to support RCS decisions and to enable a performance-based design code compliance option.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Over the long history of this project, the data-and-analysis-based evaluation of risk modeling has been excellent. This is work that would be difficult for an industry member or industry trade association to do, and the credibility and longevity of the project, as well as the model development in the laboratories, has been key to the work's success and impact.
- The first comment on slide 12 is still relevant. It was surprising to hear that the Hydrogen Risk Assessment Model (HyRAM) is oriented for station analysis and that tunnel information will be incorporated next. It would be beneficial to know what other scenarios are planned for future focus, as well as how HyRAM can be used for general analysis.
- This project has been very responsive to the needs of the industry and in addressing the issues that are present in the deployment of infrastructure.
- The displayed approach continues SNL's excellent work to systematically address and overcome barriers.

- Overall, the project has a good approach, but there could have been more technical information added to the main presentation.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The project's accomplishments are many and positive. As to the expansion of HyRAM beyond hydrogen, it would be beneficial to better understand the need for the other alternative fuels. However, this does make the playing field more "even," as it does not put hydrogen in the spotlight for safety, so this could be a positive thing.
- The project continues to provide the basis for developing and validating the safety standards for stations and other hydrogen applications. The recent work on liquid hydrogen (LH_2) and tunnels has been instrumental in developing a pathway to introduce these technologies in the field.
- The HyRAM team made significant progress in expanding the toolkit capabilities by enhancing the fault tree analysis in the QRA module, as well as enhancing models of physical effects. This allows for a broader use for HyRAM beyond hydrogen fueling facilities.
- LH_2 storage is key to hydrogen infrastructure. The characterization of hazards arising from liquid leaks and cold plumes is critical. QRA will be deficient until such hazards data can be added to HyRAM. The work completed is solid, but more progress is needed.
- Good progress has been made. However, it would be good to see more progress with respect to the LH_2 activity.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The HyRAM team continues an outstanding effort, collaborating with a wide range of North American and global stakeholders. The plans for the release of an open-source version 2.0 will allow for even more engaged participation from the international hydrogen safety community, further enhancing HyRAM capabilities.
- This project has excellent collaboration and coordination. This is highlighted especially by the support of all the cooperative research and development agreements and the impact on codes and standards development.
- The collaboration and participation by laboratory experts and industry representatives have been excellent, as good as with any DOE project.
- The list of collaborators is long, signaling that excellent feedback and input is going into the project.
- The external collaborators have excellent reputations, but how they have contributed is not completely clear from the presentation; slide 13 notes their "roles."

Question 4: Relevance/potential impact

This project was rated **3.8** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project represents exactly the type of project that DOE should have in its portfolio. It addresses an important, relevant topic that calls for the independent and credible participation of laboratory staff, and it has the longevity needed for safety, codes and standards work. It would be difficult, if not impossible, to enter new markets or bring new technologies to market without this type of work being done in support.
- This project's results are critical for broad market deployment of hydrogen infrastructure and public acceptance of fuel cell electric vehicles and other technologies. HyRAM has already contributed to the significant reduction of separation distances in NFPA 2 and NFPA 55 related to bulk compressed

hydrogen, and the modeling is expected to have a similar impact on the existing separation distances for LH_2.
- This work is critical to a proactive execution of codes and standards, and it will become even better appreciated when the infrastructure applications move from experimental and trial usage to the mainstream.
- This project is one of the most relevant, if not the most relevant, to the industry and issues of the day.
- This project is relevant and has a high level of impact to support commercial rollout.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future work looks impressive. The only potential oversight is in the lack of resources associated with the release of the open-source version 2.0. It is reasonable to suggest that the international community will receive this release with great enthusiasm, and hence will be willing to engage in enhancing HyRAM capabilities, which is the intent. This, in turn, may require some "babysitting" of potential interface or interoperability issues that may arise between the core HyRAM code and external models. It is thus advisable that the HyRAM team be prepared to deal with this appropriately.
- The Fuel Cell Technologies Office is encouraged to prioritize and focus heavily on completing the LH_2 leak scenarios to provide input for the code, as well as to support the modeling of specific tunnels so as to aid in the discussions with the authorities having jurisdiction in those jurisdictions. The non-destructive tank inspection methodologies are also interesting, and necessary, but not as high of a priority at this time.
- The future work shown is an extension of the ongoing work related to LH_2 and tunnels; formalizing these results into usable tools and methodologies for these applications is appropriate.
- The project team should include a work item that would evaluate how a more general QRA can be applied to help users address scenarios outside of the main focus to date.
- A more detailed future work strategy would be appreciated. The information provided seemed too high-level.

Project strengths:

- Overall, the project has achieved excellent results. HyRAM has gained broad international recognition and is referenced in International Organization for Standardization (ISO) 19880-1, the international standard on gaseous hydrogen fueling stations. If the aftermath of the release of an open-source code is handled adequately, it can become a global platform of choice for hazard and risk assessment of hydrogen facilities and applications.
- The project couples SNL's experimental and modeling capabilities with industry experience to address codes and standards development. The QRA tool and applied datasets give systems developers an agreed-upon basis for addressing safety requirements directly. This is critical where there is no experience for rolling out hydrogen infrastructure.
- The project's impact, longevity, and response to industry needs have all been excellent. The team is highly collaborative and supportive of short-term, high-priority requests and of interfacing with regional policymakers and stakeholders.
- There is excellent interaction with stakeholders and response to the needs of the community; the project has demonstrated quality deliverables and relatively quick turnaround, which is critical for addressing real-world needs.

Project weaknesses:

- If it can be viewed as a weakness, HyRAM was going through "growing pains," which of course are natural. Some chosen physical effects models (e.g., for enclosure dispersion and overpressure) are limited to very specific boundary conditions, yet the models could be used beyond their original limiting parameters. Thus, it could be desirable to provide a warning to the user if the model is being used outside its validated range.

- Though it is not so much a weakness of the project as it is a resources issue, the LH_2 experiments need to get completed in time to get the information to the NFPA 2 task force and get a proposal into the next version of NFPA 2. This could require some creative funding solutions.
- A larger effort is needed. At the funding levels available, the team can address issues only in a measured way. Addressing the needed cryogenic hazards data is involved and requires time, but the QRA models are needed as soon as possible.

Recommendations for additions/deletions to project scope:

- This project continues on a good path. No significant changes are recommended.
- The project team needs to address how systems developers can use existing data in HyRAM to address general scenarios involving other applications, systems, and components.
- The project team should have a plan to support the open-source code version 2.0.

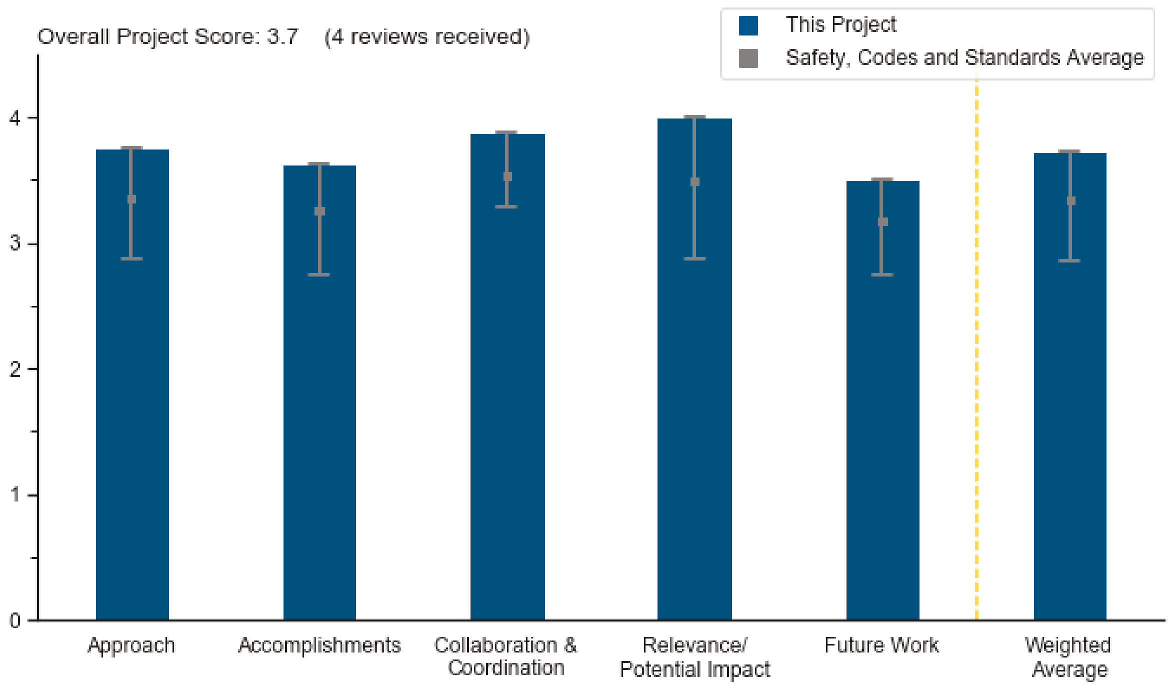
Project #SCS-019: Hydrogen Safety Panel, Safety Knowledge Tools, and First Responder Training Resources

Nick Barilo, Pacific Northwest National Laboratory

Brief Summary of Project

This project provides expertise and recommendations through the Hydrogen Safety Panel (HSP) to identify safety-related technical data gaps, best practices, and lessons learned, as well as help integrate safety planning into funded projects. Data from hydrogen incidents and near-misses are captured and added to the growing knowledge base of hydrogen experience to share with the hydrogen community, with the goal of preventing safety events from occurring in the future. The project also aims to implement a national hydrogen emergency response training resource program with adaptable, downloadable materials for first responders and training organizations.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.8** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project is really an assembly of three distinctly separate tasks: the HSP, outreach (Hydrogen Tools [H2Tools]), and emergency training. All three of these activities are well thought out, well planned, and well executed. Each of the activities scores a four in this category. The HSP has been challenged in the recent years because of the need to grow and change direction a bit. The principal investigator found a very creative solution, one that will turn out to be extremely good for the panel and the U.S. Department of Energy Hydrogen and Fuel Cells Program (the Program) at large. The creation of the Center for Hydrogen Safety (CHS) under the auspices of the American Institute of Chemical Engineers (AIChE) promises to be an excellent move. The increased exposure to a much larger relevant community and having a much larger community to draw on to support outreach and other such activities (e.g., workshops and educational and safety-related activities) will be very good. In addition, the exposure to a relevant community that is different from the traditional hydrogen community will prove to be an excellent move. The international

community has expressed concern more than once about competing with other established entities (such as the International Association for Hydrogen Safety [HySafe]). Time will tell, but this concern has been recognized, and the desire is clearly to collaborate with HySafe and grow the mutual activities, learning and leveraging from each other.
- The approach is definitely logical, and there are clear lines that can be drawn between the objectives, the barriers addressed, and the individual tasks of this project. In addition, the approach of this project is exemplary in the way that it responds to stakeholder needs and has found a solution to one of the most pressing reviewer concerns from the previous year.
- The stated approach (priority, attention, and visibility) is a good statement of the need. The team should consider how the transition to the CHS will maintain or enhance this approach.
- The project's approach is to use the HSP for the team's eyes, the responder's training for the team's voice, and the knowledge tools for the team's collective knowledge. HSP's doing reviews for the state is concerning. Up until this point, the team shared knowledge and best practices. It should be determined whether this is morphing into formal, state-mandated approvals and, if so, whether the team members are licensed practicing engineers for each state where reviews are being conducted and, if an incident occurs, where the legal liability falls: the team member, the customer, or the state.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The HSP continues to be one of the gems of the Safety, Codes and Standards subprogram. The move to AIChE should prove to be an excellent opportunity for the safety community, and specifically for the HSP, by exposing this resource to a broader community and providing the HSP with expanded resources. Here is just a sampling of accomplishments to demonstrate this point: 499 safety reviews, 388 projects, more than 100 publications, 25 panel meetings, 10 white papers, and four investigations. A site visit to the U.S. Navy site in Keyport, Washington (Naval Undersea Warfare Center Keyport Division) was performed; a task group on mobile applications was formed (funded by the California Energy Commission [CEC]); a testimony letter was sent to the City of Walnut Creek in California; and a station review was completed by HSP during the California Program Opportunity Notice application. With respect to the H2Tools portal, excellent progress continues to be made in this part of this project. The portal has clearly demonstrated its value to the hydrogen community, internationally and domestically. It contains 2,944 pages, 2,297 bibliographic references, 217 "lessons learned" pages, and 142 best practices; 56% of the pages reviewed are outside of the Americas. The first responder training was well received in the Northeast (United States). Every aspect of this project is excellent.
- There has definitely been excellent progress, although the objectives that this project addresses are a bit more difficult to evaluate in a quantitative manner (there are not really enumerated targets for this project to meet). However, the team found an elegant solution to a pressing problem that previously existed by moving to AIChE to ensure the longevity of the project while maintaining much of the expertise, capability, transparency, and public availability.
- This long-term project counts significant accomplishments over many years in making safety plan reviews the norm, providing resources for a variety of stakeholders, and culminating in the transition to the CHS: a transition from a government-led activity toward an industry-driven resource.
- Partnering with AlChE is another way to reach out and share lessons learned with designers. AIChE should have mechanisms in place to partially protect the team from liabilities.

Question 3: Collaboration and coordination

This project was rated **3.9** for its engagement with and coordination of project partners and interaction with other entities.

- This project in particular interfaces with stakeholders consistently, almost out of necessity. Through these collaborations, the project is having a direct impact on the deployment of hydrogen applications. In

addition, because of the activities that it has taken on, the project is helping to inform and improve the capabilities of technical staff industry-wide.
- The HSP has done a great job of collaborating with local, state, and federal government, as well as industry and other organizations, to take advantage of a broad array of expertise and to disseminate information.
- The team make-up is fine. If any additional current or former fire marshals for states or major cities could contribute to the team, that would be helpful. It is suggested that the project recruit fire marshals from East Coast cities (New York, Boston, Chicago, or Atlanta). The National Association of State Fire Marshals may be a path to obtain the recruits.

Question 4: Relevance/potential impact

This project was rated **4.0** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This is one of the highest-impact projects within the Program, and it has clear impact on hydrogen deployment in California today. It is good to see that the project is also looking to other regions, such as the Northeast, as other places to focus its efforts. This will be absolutely necessary and likely only to expand as other regions of the country begin to more seriously adopt hydrogen and fuel cell electric vehicles.
- There is no doubt that this work has contributed immensely to the impact on the community, the safe execution of DOE projects, and the safe deployment of hydrogen technologies (e.g., hydrogen fueling stations). The emergency responder training is always well received and appreciated. The project's relevance to the hydrogen community and the impact on helping to enable safe hydrogen deployment is extremely high.
- Safety needs to be front and center in this industry. For building confidence with stakeholders and authorities having jurisdiction (AHJs), the tools deployed by the HSP are a critical part of this "safety culture." Although it is still sometimes difficult to get data from private companies when an incident occurs, the HSP allows for as much information as possible to be collected, and the safety review process helps instill the expectation that safety will always be a primary design element for any hydrogen project.
- The relevance is obvious. However, some of these tasks should start to be moved to licensed professionals within their respective states.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The proposed work is very good, particularly with regard to the creation of the CHS.
- The proposed future work is fine. It would be nice to start migrating these tasks (i.e., inspection, review, and training) to the proper authorities at the state and major city levels. Database management and document distribution might better be addressed by AIChE and the National Fire Protection Association.
- The project does have much remaining and continuing work left to complete, and all of this was appropriately identified in the future work that was discussed. However, it would be good for this project to begin to look beyond these most immediate needs. Especially with the resources available through the new structure and home at the CHS, the project should begin to scope out the future needs that it will have to address. This should especially concentrate on the regionalization of information-sharing and analysis and the evaluation of designs and concepts for deployments in different regions. In addition, the team should begin to anticipate the expanding scope of potential applications for which the CHS will need to be able to act as an expert.
- The transition of activities to the CHS will require some adjustment, but it will allow for focus on the core activities needed to support the DOE, CEC, and outreach activities. At this point, it appears that a focus on outreach in the Northeast will be critical to be successful with AHJs there and to establish the routine permitting of hydrogen stations in the United States.

Project strengths:

- This project is, and has been, a gem of the Program. With the creation of the CHS, the excellence is expected to continue.
- The project's strengths include the depth of expertise represented by the HSP and the established processes for design reviews, plan reviews, site visits, and incident fact-finding, analysis, and support.
- The project's greatest strengths are its direct applicability and the impact that it is having in launching hydrogen deployment.
- The project's strengths include the team's focus and dedication to the task.

Project weaknesses:

- No particular project weaknesses were identified.
- The project should consider whether it is time to start migrating some of these tasks to other individuals and organizations.
- A weakness for the project is the difficulty in getting detailed information about safety incidents and near-misses that occur in private industry.

Recommendations for additions/deletions to project scope:

- The project should begin to anticipate the future needs to help spread hydrogen to new regions and into new applications. Planning appropriately for this expansion will be crucial to ensuring the longevity of the project's efforts in their current form at the CHS.
- At this time, it makes sense for the HSP to complete the transition of activities to the CHS and get settled into the new routine that the move may entail before considering any additions to scope.
- The team should consider how the HSP will move to the CHS.

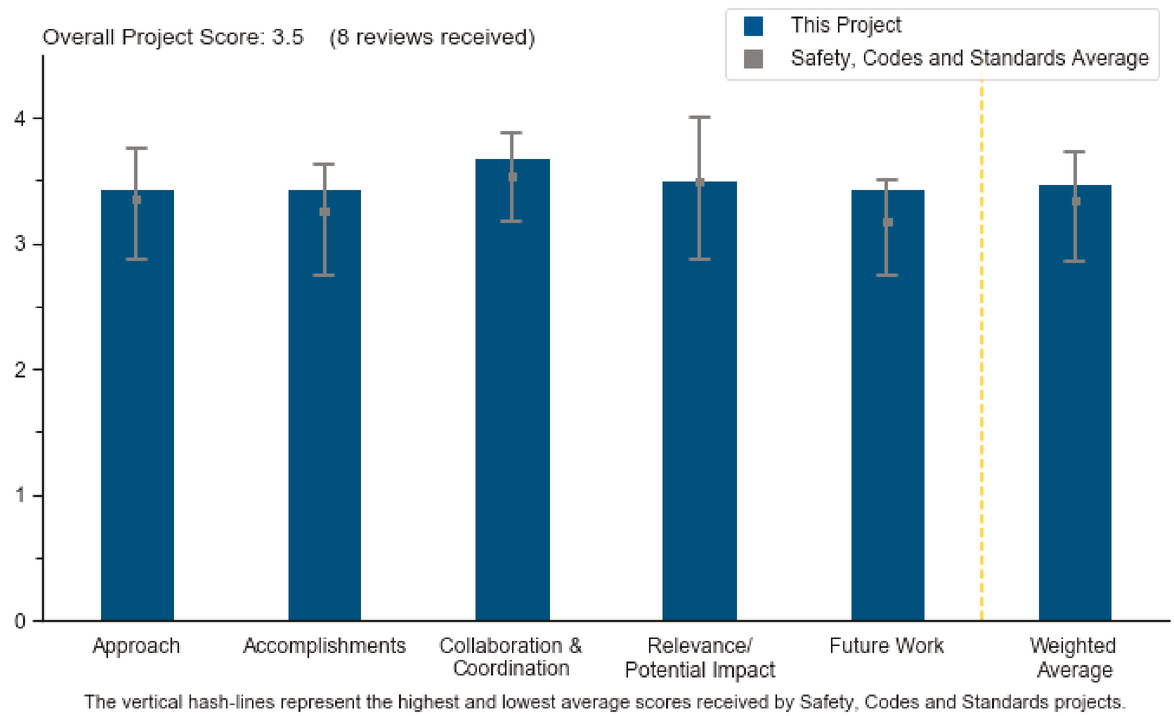
Project #SCS-021: National Renewable Energy Laboratory Hydrogen Sensor Testing Laboratory

William Buttner, National Renewable Energy Laboratory

Brief Summary of Project

Sensors are a critical hydrogen safety element and will facilitate the safe implementation of the hydrogen infrastructure. The National Renewable Energy Laboratory (NREL) Sensor Testing Laboratory tests and verifies sensor performance for manufacturers, developers, end users, and standards-developing organizations. The project also helps develop guidelines and protocols for the application of hydrogen safety sensors.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- This project has matured, and continues to mature, from testing individual sensors to understand the performance of sensors, to implementing an array of sensors to create a "wide-area monitoring (WAM) system," and then to making sensors an integral part of an integrated safety system approach to reducing risk at a deployment site (such as a hydrogen fueling station). This approach of making sensors an integral part of the safety system to actively contribute to the design and risk mitigation effort is very nice. This could be a game-changer in the approach to mitigating risk in these systems. This principal investigator (PI) is very rigorous in his approach, combining detailed laboratory work with that of field deployments (including indoor, outdoor, and medium-to-large facilities to understand hydrogen release behavior). This PI makes sure that the information generated is available to the appropriate customer. This project does, at times, work on and produce output that needs to be protected intellectual property (IP). The project has been criticized in the past because of the need to protect IP; this is necessary at times, but this PI works hard to distribute the knowledge gained from this work appropriately.

- The approach to the work has been finessed over the years of the laboratory's existence. While the laboratory continues to evaluate the performance of sensors for industry, more research is being conducted to help with characterizing hydrogen behavior for the purposes of affecting safety and reducing the hydrogen station footprint.
- This project continues to support the industry in the area of hydrogen detection. It was good see a stronger link to the hydrogen release and quantitative risk assessment (QRA) work at Sandia National Laboratories (SNL). In addition, the focus on WAM is important, especially for the work looking at sensor placements in enclosures.
- The approach makes sense and addresses the needs of the hydrogen community. The sensor evaluation work is ongoing. The new efforts include the evaluation of sensor position in various scenario applications and the use of sensor data to feed into QRA.
- The project team is focused on meeting specific needs for sensors. The approach is well defined to meet these needs while remaining flexible enough to address emerging technologies and applications.
- This project has done well in its collaboration for the vehicle sensor component in the development of the SAE International (SAE) document.
- There are two ways to look at the approach: proactive and reactive. From a reactive point of view, the approach has been to support all requests. This is helpful and useful. However, there does not seem to be much proactive direction or research to improve future detection technology and deployment. This is a gap in the project.
- The approach is sound. It is unclear why a number of CO detectors that trip on exposure to hydrogen are not being screened. The detectors usually have product safety listings, production lines, sales channels, and name recognition.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Many accolades are due to the NREL Sensor Testing Laboratory for the publication of the SAE J3089 technical information report (TIR) for onboard vehicle sensors, and for meeting the United Nations Global Technical Regulation (GTR) requirements. The Sensor Testing Laboratory always seems to have student internships that benefit both the student and the industry. It is easy to imagine that the students enjoy working with Dr. Buttner, and it seems they are given great experience for their next career moves. Other projects may have interns assisting in the research work, but this project continues to showcase the student research assistants.
- The publication of the SAE TIR is a noteworthy achievement. The GTR-13 verification work seems to be starting off well. The guidance on indoor sensor placement work is at early stages, but it looks promising. The hydrogen WAM (HyWAM) modeling progress is good.
- Good accomplishments and progress have been made. It is not always obvious, but the work found within this project supports a wide range of codes and standards development for the vehicle, refueling, and infrastructure.
- The team is congratulated for publishing SAE J3088. Perhaps there is a CSA Group (CSA) version to address the limitations of, and compete with, the existing Underwriters Laboratories 2075 or the International Organization for Standardization document.
- There is a clear demonstration of commitment to this project.
- There is no question that this work has helped advance DOE goals for other projects where sensors are a key parameter for completion. However, this project primarily supports other projects, and this project does not have a clear objective as to what it is supposed to deliver. This is a gap, moving forward. This might be expected of any 10-year-old project.
- DOE goals are being met; however, the accomplishments were modest because of the late receipt of funding.

Question 3: Collaboration and coordination

This project was rated **3.7** for its engagement with and coordination of project partners and interaction with other entities.

- This PI is very proud of the project's collaborations and coordination with entities outside of NREL, and he should be. This project has had a quite impressive list of collaborators, from a very productive laboratory-to-laboratory relationship with the JRC on sensor performance evaluation, to a true collaboration with A.V. Tchouvelev & Associates (AVT) to understand sensor placement for various positions and release scenarios for indoor releases, to mentoring young researchers. This project engaged in true collaborations with other entities (such as AVT) to make the project more impactful than it would have been without the collaboration. There are some who think that making a presentation at a meeting is a collaboration; this PI understands what it means to collaborate, and he engages and embraces the collaborative nature of research. This is very nice.
- This project is well connected to national and international key players: SAE, Prenormative Research for Safe Use of Liquid Hydrogen, AVT, SNL, Lawrence Livermore National Laboratory, the Compressed Gas Association, the National Fire Protection Association (NFPA), and others. Frequent outreach and engagement with industry has been demonstrated.
- Excellent collaboration is demonstrated with the WAM work, which examines hydrogen release in industry containments, supports modeling efforts, and coordinates findings with standards requirements. This project features good coordination between partners and other institutions.
- The project's collaboration with industry, government, academia, and original equipment manufacturers enables the research and allows the project to expand its impact. The project's participation with SAE, NFPA, and the GTRs will help support work in codes and standards.
- Collaboration and coordination has always been strength of this project, especially with the mentoring of students from the Colorado School of Mines.
- There are many collaborators, and it was made clear that the extent of collaboration is also significant.
- The list of organizations is impressive, but it should be updated annually on such a long-running project. This is less a "project" than a "continuing support" that is funded annually. The "collaboration" is more a list of organizations that are supported, as opposed to the traditional approach of organizations that are assisting DOE in achieving the DOE objective. It is not clear how projects and support are prioritized.
- The collaboration list is long on national laboratories, Colorado universities, and very small companies. It is unclear why some of the industrial and home CO sensor manufacturers are not at the table, including the Mine Safety and Health Administration, Detector Electronics Corporation, Kidde-Fenwal, Inc., First Alert, etc.

Question 4: Relevance/potential impact

This project was rated **3.5** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The performance of sensors (original effort) is critically important to (1) satisfy code requirements, (2) ensure the highest possible level of risk mitigation (WAM), and (3) support the new thrust of aggressively pursuing sensors as an integrated part of risk mitigation strategy; this makes this activity very relevant and impactful to the safe deployment of hydrogen technologies. This project is critically important.
- Doing basic research, modeling, and practical experiments to facilitate the risk-informed determination of the placement of hydrogen sensors has the potential to contribute to the improved safety of future installations. The main effort verifies the performance of sensors to increase confidence in their use and thereby increase safety. The liquid hydrogen (LH2) release work is important and timely.
- The need for the Sensor Testing Laboratory to support safety research is critical. The potential impact is being seen in the results of SAE J3089 TIR and HyWAM. This laboratory is a resource to the hydrogen community.
- It is important to support the hydrogen sensor industry with a neutral test capability for evaluating new sensor technologies. Additionally, it is important to provide definitive information on how to use and place sensors in common applications. Both of these activities will support the hydrogen community.

- There is a need for accurate hydrogen sensing, regardless of application. A low-price, robust, accurate, and reliable design will find a market. The team should speak with existing CO sensor manufacturers.
- As the project continues, it will be important to evaluate the progress and how the progress relates to the development of H2@Scale. It will be important to evaluate some of the other sectors, such as industrial usage, grid integration, electrolyzers, etc.
- The support provided is relevant, but there are two comments: (1) It is not clear how this support is prioritized or what metrics are being used to decide what to support. (2) The HyWAM seems to be a system that has a series of point-detector locations for supporting testing, as opposed to a device, system, or technology that could be more easily deployed in an actual field site or system. In that regard, it is not clear that the system is a tool and not a product. Making a low-cost and effective technology for mass deployment might be a useful objective.
- The vehicle sensor work is very relevant; however, other areas (outdoor sensors, for example) may not be as critical, given that other methods of detection are being employed in other projects. While the collaboration in Europe is positive, perhaps the United States should work to influence the focus. It is suggested that the project team re-evaluate the targets.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed work for active monitoring as a mitigation strategy to help with the LH2 setback distances is worth the price of admission. Station footprint reduction in the next NFPA Hydrogen Technologies Code (NFPA 2) is critical; this sensor laboratory work coordinates well with other projects. There are many aspects of this work and equipment that can be commercialized.
- The future work addresses lowering costs for facility integration and further development of research tools to support developing codes and standards; Task 3 (Hydrogen Contaminant Detector [HCD]) also addresses on-site HCD systems. There is a critical need for work on LH2 facilities, so it is very good to see that present in the plans and integrated with NFPA 2 activities.
- The project's movement into using sensors as part of a risk mitigation strategy is excellent and a game-changer.
- The continued work on hydrogen deployment and the proper use of hydrogen sensors is critical.
- The inline fuel quality work is very necessary and timely.
- All of the proposed subsequent work appears rational.
- In terms of future work, much of fiscal year 2019 is reactively supporting other DOE and industry projects. It would be helpful to develop an overall objective for the project and then a subset of specific items to support that objective. The objective could be structured so that many of the existing activities are included, but with additional ones that would advance the technology in a positive direction. In particular, HyWAM needs more definition as to what it is and what it is intended to do.
- For the short term, the project has good direction, but it is encouraged to look more outward and to its impact on the sensor targets.

Project strengths:

- This is, has been, and remains a gem of the Program. Even when the laboratory was being moved and was not functional, this PI continued to contribute to this space by staying active and publishing in open literature. This work is really appreciated.
- The NREL Sensor Testing Laboratory has developed a strong collaboration network throughout the years, and its coordination with the national and international community is a huge asset. The laboratory continues to see interest at SAE, NFPA, and the GTR committees. The work with student interns is mutually beneficial for the hydrogen and alternative energy industry. The opportunity for new market applications (e.g., shipping, rail, marine) provides great potential. The collaboration with SNL (involving Ethan Hecht) on LH2 behavior is exciting news and can help with the NFPA 2 updates for LH2 station footprint reduction and science-based setback distances.

- Bill Buttner is very clearly the right person for this project, as he has a real vested interest and seems to very much enjoy the work. There are some really good things that have come out of this project, along with other things that seem more like busy work. All in all, it is a strong project.
- The project is making clear progress in the development of more reliable, lower-cost sensors, as well as methodology for sensor placement. The HyWAM work and the plans to study LH2 release behavior are areas needed by industry, and they are natural additions to build upon the work done to date in this project. NREL's history and future plans for working with industry to commercialize new technologies are certainly strengths.
- The laboratory has good leadership, and it is productive and engaged with good partners.
- The diverse set of partnerships covers a wide range of capabilities.
- Furthering sensor technology is important, as is supporting other projects with sensor technology.
- The project's strengths include the knowledge and dedication of the research team.

Project weaknesses:

- This is more of a need than a weakness, but the project needs the development of an outward strategy as it pertains to H2@Scale—for example, in heavy-duty vehicles and industrial applications.
- The cause of the continued "funding uncertainties" is not well understood. There is much technology transfer and commercial work; it seems this project is perhaps becoming self-sustaining. The comment that "the royalties from SAE J3089 will keep a teetotaler in beer" did not go unnoticed (and was appreciated). The team should consider how this might change so that more stakeholders might be interested in the good work being done with this project.
- The weakness is in the inconsistent DOE funding, which is not a fault of the laboratory.
- The project's weaknesses include the HyWAM project. While it is true that there is no good guidance from the manufacturers on sensor placement (what area one sensor covers, for example), it seems that with 20+ years of sensor use at various facilities, there are learnings that can and should be collected to create some best practices on sensor use. This can and should also be given back to industry for industry use and/or published as guidance or as reference for industry customers.
- While it is clear that optimizing sensor placement will increase safety and minimize costs, it would be beneficial to see more emphasis in the project on reducing costs for sensors, including capital costs and operation and maintenance costs.
- There is a lack of objective; the project needs an overall objective. Lacking an objective, the project is wandering and somewhat reactive. Perhaps those projects that request support should fund that support. There is also a loss of focus on new technology sensors. There seems to be less of a focus on the development of new types of sensors that otherwise improve upon the behavior of those that already exist. It is stated that sometimes sensors work, and sometimes they do not. It is not clear what is being done to directly improve that performance and perception. There is also a weakness in the HyWAM definition; this has exciting potential but needs better definition. There is a reference to "standoff" devices; this is the technology that could provide a breakthrough, but there is very limited information provided on this potential.
- There is a lack of major sensor manufacturers involved with the team.

Recommendations for additions/deletions to project scope:

- The team should continue with the plans given in the presentation.
- The team should perhaps consider validating HyWAM on future projects that are under review by the Hydrogen Safety Panel.
- The team should add an overall objective for the project. The team should also develop a method to prioritize requests for support and proactively develop new activities to further the technology of sensors. The team needs to list specific priorities for technology advancement, better define HyWAM as either a tool or a product, and evaluate the next steps for the technology. While it can be used to support NFPA research, it is not clear that it is a product that can be used effectively as a mitigation tool at this point.

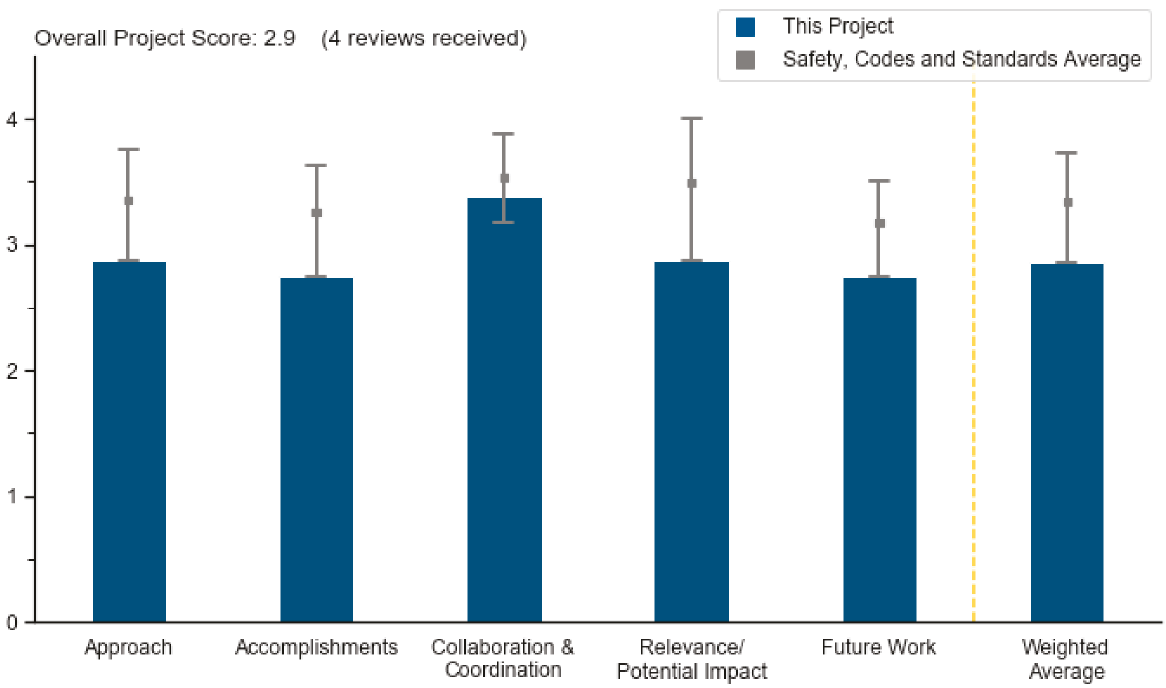
Project #SCS-022: Fuel Cell and Hydrogen Energy Association Codes and Standards Support

Karen Quackenbush, Fuel Cell & Hydrogen Energy Association

Brief Summary of Project

The goal of this project is to support and facilitate development and promulgation of essential codes and standards to enable widespread deployment and market entry of hydrogen and fuel cell technologies and completion of all essential domestic and international regulations, codes, and standards (RCS) by 2020. The Fuel Cell and Hydrogen Energy Association (FCHEA) participates directly in key domestic and international RCS technical committees and encourages its members to participate directly in technical committees, working groups, and discussions. FCHEA also develops and enables widespread sharing of safety-related information resources and lessons learned with first responders, authorities having jurisdiction, and other key stakeholders.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **2.9** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- Overall, the approach is sound and well reasoned for its intended purpose. Three FCHEA working groups provide industry feedback on new RCS, with outside experts invited to contribute as needed. Diagrams and bullet points facilitate the conveyance of information. The presenter had in-depth knowledge of the industry and the relevant stakeholder groups. Coordination, outreach, and resolving technical challenges were identified as focus areas consistent with the mission of the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (the Program). It is suggested that the team include a page that defines all of the acronyms used in the presentation.
- Overall, the approach for the project seems reasonable and logical, but it does seem to lack an ability to be nimble. In addition, for a facilitation role, the approach seems to rely a bit more on stakeholders approaching the project for involvement than might be expected. This is especially true given that one of

the barriers identified for this project to address is the limited business participation in code development. Furthermore, it is unclear whether the working groups are limited to FCHEA membership. Many times, smaller business stakeholders, who may not have budgets for memberships, have important, real-world feedback for things like safety, codes and standards (SCS), and it was not clear that these members of the business community were being reached. This would likely require proactive engagement in this project; even though FCHEA staff run the project, they would have to proactively seek input outside their members.

- Standards and codes are important enablers of technologies, including hydrogen systems. Private-sector participation in standards development activities, especially from industry, is generally funded by the industry. The specific standards development organizations identified would all offer the opportunity for membership and/or input (e.g., proposals or comments) from the industry through various avenues. It is not clear why the industry requires DOE funding in order to be engaged in standards development activities that directly affects industry. Aside from standards meeting attendance, the activities identified comprise teleconferences, meetings, working groups, and posting of summaries, which are all done via simple communication or can be accomplished that way with minimal effort.
- The project approach has merit in assisting the development of codes and standards, although the effectiveness of creating separate working group forums is unclear. It would seem that if an FCHEA member has the time to attend these working group meetings, then that member could attend the codes and standards meeting directly and influence the direction of a standard directly.

Question 2: Accomplishments and progress

This project was rated **2.8** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- The team noted appropriate progress in the presentation, with respect to information sharing and data exchange among industry stakeholders to facilitate a collaborative process within the working groups.
- The project's progress is difficult to measure, based on the nature of the project's goals and the fact that some of the ultimate outcomes are dependent on other individuals and organizations. However, it is important that the project has established working groups for coordinating among several varying stakeholders.
- The explanation of the project's accomplishments does not clearly map to tangible outcomes that are moving toward DOE goals, but rather seems to consist of activities. The benefits of the project in accomplishing outcomes, or in promoting advancement that would not otherwise occur through ongoing standards development activities, are not clear. The publication of the Hydrogen and Fuel Cell Safety Report provides information about field experiences.
- The specific accomplishments of this project are vague and difficult to quantify. The project has activities such as monthly meetings and bi-monthly safety reports, but it is unclear if these are actually making a difference to advance codes and standards. The slides appear to be similar to those from previous years, and the progress from the past year could have been further clarified.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- RCS development, review, and prioritization is a key focus of the collaboration. The project's collaborative efforts involve a very wide cross-section of the industry that includes universities; government laboratories and agencies; trade associations; manufacturers of fuel cell materials, components, and systems; hydrogen producers and fuel distributors; utilities; and other end users.
- The collaboration for this project is assumed to be high, based on the nature of the activities and number of FCHEA members. The main focus of this project is on providing collaboration and coordination between FCHEA members and the various standards organizations.
- Aside from the issues noted in a prior response from stakeholders outside of FCHEA, it was a logical and intelligent choice to begin establishing working groups that leverage the organization and relationships provided by the existing FCHEA organization.

- The collaboration with Oak Ridge National Laboratory is noted. By their inherent nature, standards and codes are collaborative and involve many different parties, and in that sense, the project includes collaboration. Industry associations, similarly, inherently exist to be a platform for collaboration among industry. However, the team does not note any specific collaborations that unlock outcomes beyond simply participating. While there is value in being engaged in a standards development process, the project should focus on enabling or catalyzing new results. It would be an appropriate objective and benchmarking process for this project to be strategic and focused in identifying, enacting, and reporting on specific collaborations toward outcomes that might not occur, might not occur as soon, or would not otherwise occur.

Question 4: Relevance/potential impact

This project was rated **2.9** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- The work that is being addressed by this project is clearly important and must be done. The work also has great potential for impact. However, it does not yet seem that the project has had enough time to demonstrate the full potential impact it could have, especially with regard to international harmonization. It is recommended that the project take a more active role in seeking input and identifying needs, rather than waiting on industry representatives to identify issues and come to the project. Based on prior experience and for RCS concerns in particular, industry often appears to be more reactive and focused on short-term pain points, rather than long-term codes and standards development efforts that might be needed.
- The relevance of the work was provided in sufficient detail and was significantly augmented by the speaker's knowledge and experience. The speaker provided detailed answers to questions; however, it is suggested that the team more specifically cite in the slides what affected the industry when addressing potential impacts.
- The project has a good overall objective to support the development of essential codes and standards for hydrogen and fuel cell technologies. The alignment of the impact to the Program's goals could be improved since the project discusses a wide variety of applications beyond transportation, such as stationary, portable power, and drones.
- The publication of the Hydrogen and Fuel Cell Safety Report is noted as a mechanism to communicate about incidents. Other than information sharing, translating this data source to the advancement of specific codes and standards has not been established. The team had not established the relation and bidirectional coordination of the Hydrogen Fuel Cell Safety Report with the NREL National Fuel Cell Technology Evaluation Center efforts, including the safety aspects of the Hydrogen Fueling Infrastructure Analysis, to minimize redundancy and optimize outcomes. This project's impact on specific codes and standards development has not been made clear.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The presentation provided significance and a take-home message to reinforce important accomplishments and highlight the progress that is under way. The project's output included monthly discussions and bimonthly reports.
- Addressing the transportation aspects of micro fuel cells in airline carry-on bags and luggage presents a legitimate technical concern. Ultimately, these policies are addressed by the United Nations, International Civil Aviation Organization, etc. Additional information would be needed to determine whether this is or will be happening at a frequency that would merit prioritization of the standards effort to overcome a significant barrier. If the market expectations support a significant impact, then the project group can consider the question of whether to fund an industry organization to convene an International Electrotechnical Commission working group. The comments about continued task group work for the 2020 edition of National Fire Protection Association (NFPA) 2 are unclear, as it is in the final stages of publication by the NFPA; as of August 2019, new additional input will not be allowed, and no action should be required to "complete the revision cycle." "Review" of a published NFPA standard—that the

industry participated in developing with funding under this project—does not comprise an appropriate aspect of funded future work. Similarly, continuing to review standards is an ambiguous basis for future work.
- It seems unclear what the project staff's role is for the remaining work, especially for the coordination with international standards. There is mention of industry partners putting in effort to ensure harmonization, but it is unclear whether the staff is looking to be an active part of that. It is not evident that the project staff is carrying out proactive facilitation of U.S.-based and foreign-based individuals.
- The proposed future work seems generic and could be improved with specific items. The effort in portable power, in terms of checked baggage, does not necessarily align with the Program's goals. DOE funding should encourage this project to focus on the Program's goals, rather than on a variety of applications.

Project strengths:

- The project achieved its goals and continues to provide a key role in the harmonized development of RCS.
- The strength of the project is in its structure for leveraging partnerships and collaboration through the already existing FCHEA members in order to get a participation base for the tasks being executed.
- The strength of this project is the number of FCHEA members and the project's collaboration with this membership.
- The publication of the safety report provides incident information to the community.

Project weaknesses:

- The need, value, and outcomes for funding industry group participation in codes and standards development are not clear; this seems best addressed by the private sector. For most of the defined standards work, specific advancements and outcomes are not clearly identified. The project seems to be overvaluing activities as accomplishments. Much of the defined work seems to consist of meetings, teleconferences, information dissemination, etc., which can be accomplished effectively through the use of communications and work-sharing technology. On the topic of incident reporting, optimizing and articulating coordination with other work, such as the Center for Hydrogen Safety and the National Fuel Cell Technology Evaluation Center, will help minimize redundancies and best promote impact. The proposed future work plan needs significant development to substantiate relevant, significant outcomes.
- The team is likely overlooking other business entities who could have pressing SCS needs or who could provide valuable insight, but who are being overlooked simply because they are not FCHEA members. This is especially a problem given that one of the barriers that this project intends to overcome is the lack of business participation.
- The weakness with this project is that, while many activities are occurring, its specific contribution is not clearly communicated. The scope of this project is too broad and is not focused on the key areas.
- A project weakness is the inability to independently track, measure, and evaluate results and outcomes against DOE and industry goals.

Recommendations for additions/deletions to project scope:

- The codes and standards matrix is interesting, although it is just being used for comments regarding the status of documents. This document could be expanded to capture critical issues with each standard and include the project's contribution. A recommendation is to reduce or eliminate activities in this project that are not directly aligned to the Program's goals. The FCHEA website could be improved to help the industry, especially in the area of tracking the codes and standards, which is currently disabled.
- While it may not have been relevant so far in the project's lifetime because of the schedule of code cycles, there did not seem to be much work directed toward heavy-duty applications, including vehicular, marine, and other applications. Given the growing momentum around hydrogen in these applications, activity in this area may need to be increased.
- It is suggested that the team provide more details about the challenges of implementation, techniques for accelerating deployment, and lessons learned, as well as an assessment of the project's current standing compared to the amount of work remaining. This can be done either graphically or diagrammatically, when applicable.

- This project needs the addition of value-adding work that will substantiate specific outcomes that would not otherwise be accomplished.

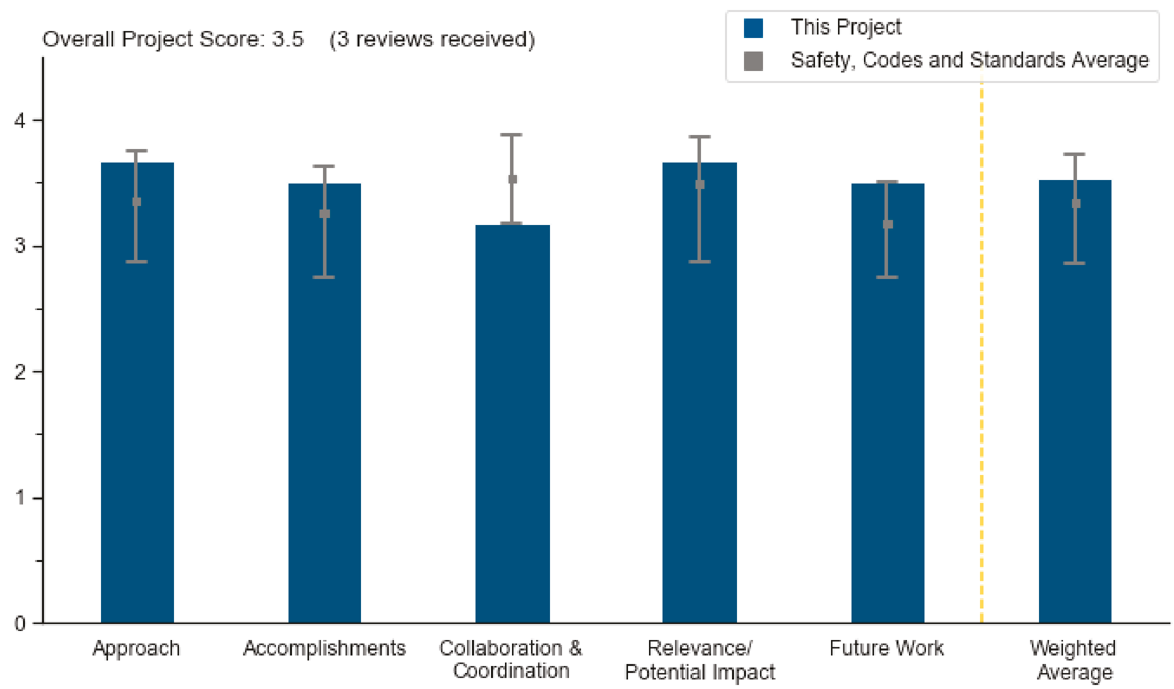
Project #SCS-026: Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Polymers

Kevin Simmons, Pacific Northwest National Laboratory

Brief Summary of Project

The project objective is to fill a critical knowledge gap in polymer performance in hydrogen environments. Investigators are gathering and assessing stakeholder input about the challenges, materials, and conditions of interest for hydrogen compatibility. Findings inform the project's development of standard test protocols for evaluating polymer compatibility with high-pressure hydrogen, characterizing polymers, and developing and implementing an approach for disseminating the information.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Safety, Codes and Standards projects.

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing barriers, project design, feasibility, and integration with other relevant efforts.

- The combination of analysis that is followed by model development, followed by test method development, followed by validation is excellent. The difficulty of bringing the number of materials and the number of conditions of interest down to a manageable level is daunting, but in general, the initial selection (commonly used materials) and the defects and failure modes that were selected for analysis make sense.
- This project covers a large number of related activities, including the study of degradation, modeling, the identification of suitable formulations, and materials for cryogenic hydrogen service. Early engagement with relevant stakeholders is demonstrated. Direct inroads to the development of the Compressed Hydrogen Material Compatibility (CHMC) 2 standard are clear.
- The approach seems well thought out and effective. A challenge that is acknowledged is how to address the wide variety of non-metallic materials. The presentation did not state whether a prioritization based on commonly used materials has been completed.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals.

- Obtaining the stakeholder feedback and distilling that into a prioritized matrix of materials and failure conditions to test is a worthy accomplishment. It is recommended that the principal investigator(s) do a sense-check on that matrix to make sure that they agree that no high-priority materials or failure modes have been omitted. Likewise, the initial tribology studies and the initial work on the test methods document represent significant accomplishments in the first year of the project.
- The project's progress is good; the published database is highly anticipated, but that appears to be a fiscal year 2019 objective.
- The project is in the early stages. Engagement with relevant stakeholders was performed early to inform the effort. The prioritization of failure mode and effects analysis was essential to ensure that industry priorities are being addressed.

Question 3: Collaboration and coordination

This project was rated **3.2** for its engagement with and coordination of project partners and interaction with other entities.

- The project has excellent multi-laboratory and industry collaborations. There is great early engagement with stakeholders. NASA was engaged early in a call but had very little to share regarding polymers. It is noteworthy that NASA is interested in this project's work.
- The team should consider whether it would it be helpful if there were additional materials or seal manufacturers directly involved as partners.
- Other than the listing of the laboratories participating in the Hydrogen Materials Consortium, there was not much discussion of the collaboration. It would be helpful to know, for example, who the stakeholders are who were surveyed in developing the list of materials and failure modes.

Question 4: Relevance/potential impact

This project was rated **3.7** for supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan.

- This project is foundational for the goals of DOE and industry, as it will underpin the design and deployment of safe hydrogen systems, and it will also play a key role in improving the reliability of systems and equipment, such as hydrogen dispensers and compressors.
- The early results are promising. The tribology study report is in publication. Having cutting-edge research data available will aid confidence in design. The work on CHMC 2 is relevant. The work already led to discovering plasticizers that can migrate to the crack edge following exposure to hydrogen.
- Extensive information is available on metallics, but it is needed for non-metallics as well.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The future work is well scoped for the resources of the project and for the fact that it would be pretty easy for the scope to grow too far, given the number of materials that could be considered and the daunting task of developing both models and test protocols for a wider range of failure modes.
- The project has a good plan.
- The project is just getting into the heart of the research.

Project strengths:

- This work is critical, as understanding non-metallic material compatibility with hydrogen is a significant, long-standing knowledge gap. Collaboration with DOE, multiple laboratories, and Ford Motor Company instills promise that the work will be directly relevant to current industry needs and will facilitate the development of CHMC 2, the new, developing standard on hydrogen compatibility with non-metallic materials.
- This is a well-organized project, with clear focus on issues critical to the safety, reliability, and cost of hydrogen production, transport, and dispensing.
- Providing knowledge on non-metallic materials will be helpful to the industry. The project seems to have an ordered approach and has sought extensive stakeholder feedback.

Project weaknesses:

- This is more of a challenge than a weakness: there is not much previously published information available upon which to build.
- It would be beneficial to more clearly see who the industry collaborators are, what the range of materials and failure modes submitted in the questionnaire were, and how the priorities were chosen.
- The project’s weakness is in being able to address multiple materials and variations of the same material from different manufacturers.

Recommendations for additions/deletions to project scope:

- The project has a potentially very broad scope already, so additions are not necessarily recommended, but it would be helpful if it were possible to state the goals in terms of something like “for applications such as sealing a ball valve under 700 bar hydrogen pressure, we recommend material X.”
- The team should expand from “cryo-compressed” to liquid hydrogen and perform testing down to 20 K. It is not clear that testing at temperatures this low is being considered, but it is necessary as part of the material properties.
- Perhaps in the future, formal collaboration with international research entities could be considered.

2019 Hydrogen and Fuel Cells Program Review Summary

This Appendix shows the results of the Hydrogen and Fuel Cells Program-level peer review for the 2019 Annual Merit Review (AMR), including feedback from a subset of the reviewers attending the AMR. A total of 132 Program-level reviewers were invited to provide feedback, and 29 reviewers responded.

1. Program Reviewer Fuel Cell Expertise Selection: Are you a reviewer with general Hydrogen and Fuel Cell Program expertise, Solid Oxide Fuel Cell (SOFC)-specific expertise, or expertise in both program areas?

(Your response to this question will change the set of questions that you are asked to evaluate below. You will have the option to skip any questions you do not feel qualified to answer).

General Hydrogen and Fuel Cell Program Expertise (Limited or no Solid Oxide Fuel Cell Experience): 22 reviewers
Solid Oxide Fuel Cell Program Expertise Only: 3 reviewers
Both Solid Oxide and General Hydrogen and Fuel Cell Program Expertise: 4 reviewers

2. The Hydrogen and Fuel Cells Program has a mission and strategy that are clearly articulated and has appropriate goals and milestones, as well as quantitative metrics that are SMART (Specific, Measurable, Actionable, Relevant, and Timely).

Please comment on the overall Hydrogen and Fuel Cells Program (including activities in the U.S. Department of Energy [DOE] Fuel Cell Technologies Office, Office of Fossil Energy, Office of Science, Office of Nuclear Energy, and ARPA-E), as well as each subprogram/activity area, as appropriate. (Note: Hydrogen delivery is now included under the Hydrogen Infrastructure [Research and Development] R&D area. Technology Acceleration includes the prior-year subprograms Technology Validation, Manufacturing R&D, and Market Transformation.)

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

	Hydrogen and Fuel Cells Program Overall Rating	Hydrogen Production R&D Subprogram Rating	Hydrogen Storage R&D Subprogram Rating	Hydrogen Infrastructure R&D Subprogram Rating	Fuel Cell R&D Subprogram Rating	Technology Acceleration Subprogram Rating	Safety, Codes and Standards Subprogram Rating	Systems Analysis Subprogram Rating
Average Score	8.9	9.1	8.2	8.7	8.9	8.6	8.6	8.8
Number of Responses	22	20	20	20	20	20	20	20

Comments:

- It is great to see an increased emphasis on reliability and cycle life of the proposed technologies, even for early-stage (low-technology-readiness-level [low-TRL]) programs. Technologies need to be evaluated on a regular basis based on both the initial and end-of-useful-life performance. Statements of project objectives should include highly accelerated life testing protocols, early in the development, to eliminate solutions that do not meet the life targets.
- The Program has produced a wealth of significant results. It explores in depth the most important research topics. It has clear goals and horizons. Its budget is well distributed across sectors. Consortia have an

important impact—they mobilize the expertise needed to explore new avenues and advance the frontiers of technology. Investigating theory-guided applied materials R&D has growing importance.

- The Program as a whole is highly evaluated not only for advanced technology R&D but also for its work in safety codes and standards, cost analysis, etc.
- The subprograms are strong overall. Oral presentations and, for the most part, poster presentations showed that principal investigators (PIs) receive clear instructions and are aware of Program requirements.
- The general focus of the activities is aligned well with industry's long-term needs for developmental objectives.
- Yes, this was repeatedly and clearly emphasized in statements and presentations.
- Communication of Program priorities is excellent, as are Program management and leadership. The Program should be commended for transparency and clear articulation of goals and milestones. The AMR is among the best program reviews in the government. It serves a critical role in communication of priorities and also significantly enables engagements across the international hydrogen stakeholder community. The Program should consider expanding priorities to include activities that are not technology-specific. One example is a need to ensure participation of diverse groups in science and engineering. The lack of diversity is particularly pronounced within the hydrogen community, and lack of diversity is correlated with less creative solutions to complicated problems. The Program should articulate goals around diversity. The Program should also consider developing specific goals to ensure a balance of investment in various stakeholders, including small business, university, large business, and national laboratory. The current portfolio appears heavily weighted toward large business and national laboratory, even in early-stage research activities in which universities should play a more pronounced role. The Program should also articulate quantitative safety-related goals within each Program element. Currently very few programs have any safety goal, despite the stated importance of safety among all stakeholders. Safety needs to be considered and incentivized at all stages of technology development and deployment.
- The plenary presenters articulated the Program-wide targets for hydrogen cost per kilogram, energy efficiency, and durability unambiguously and with explanatory context. The 2019 AMR plenary speakers presented and explained the related dependencies and assumptions. They also described the status of "where we are" in reaching "all of the above strategies." The Hydrogen Production R&D plenary presentation, however, could have been more successful had less material been presented. Hydrogen Production R&D is an extremely important area, but because of the accelerated, packed presentation (too fast and too much material to be practically presented), some information about the Hydrogen Fuel R&D subprogram's SMART metrics was lost. Therefore, a lower rating, compared with others, is given. In addition, most of the section leaders of the Program who presented at the 2019 AMR plenary were too humble to take credit for the progress in hydrogen R&D across sectors in H2@Scale. Perhaps they can be coached on taking credit, speaking about tangible benefits, and speaking about their vision, as leaders. As follow-up to the 2019 AMR plenary presentations, it would be good to consolidate and publish the techniques used to meet the DOE targets across the entire Program. The purpose is so that others may apply the same techniques. Also as follow-up, it would be good to know what companies and organizations are doing to reward employees/researchers for meeting the Program targets. Perhaps the 2020 AMR can explain which organizations met the targets and the impacts of not meeting the targets. It would also be good to know what would happen to the U.S. energy industries and energy users if a lesser number of hydrogen and fuel cell projects meet targets. The community would benefit from "missed target" information, and perhaps new directions can be established.
- In general, mission, strategy, and goals are clearly articulated and appropriate. Based on the plenary, consortia, and other overview presentations, milestones (what must be realized when) and metrics (which performance/specification must be met under what conditions) seem to be less developed and consistent. Hydrogen Infrastructure R&D, for example, has no separate target for distribution and dispensing. There is only a target including production ($7/kg). Metrics and milestones are most elaborated for Fuel Cell R&D

and Hydrogen Storage R&D. They largely seem to be lacking for Technology Acceleration; Safety, Codes and Standards; and Systems Analysis, which may be due to the diverse nature of the topics.

- It would be good to see two changes as metrics/adjustments to targets. The first is that so many of the targets and therefore the Program efforts are geared toward cost. This is especially true of the Fuel Cell R&D subprogram. However, pure cost (of manufacture or other general economic/business activity) seems too restrictive a metric for a technology that will likely be introduced in phases or waves and is looking to serve a variety of use cases. For example, strict cost targets for price parity with conventional (hybrid) vehicles ignores the aspects of potential consumer adoption. Early adopters may have more price elasticity. They may find value in fuel cell electric vehicles (FCEVs) because of capabilities. There are many other metrics. While we know consumers are influenced by purchase price, translating that into strict cost targets across all Program areas may be too restrictive. Indeed, it may end up pushing research to focus too heavily on more difficult, longer-term research projects that pull needed effort from programs that makes advances sooner—advances that could still translate into value propositions for the ultimate customer. The second suggestion is related. The Program targets are not really addressing the timeliness of needed advances. With momentum building nationally for zero-emission vehicles, and the amount of market- and mind-share that battery electric vehicles have captured in the public and among decision-makers, it seems that this Program is not yet realizing the urgency of advancements, demonstrations, and transitions to commercial products that are needed. This may be true of the FCEV and hydrogen industry broadly, but perhaps the Fuel Cell Technologies Office's (FCTO's) programs could be a strong catalyst for pushing for faster timelines.
- It seemed that decarbonization priorities, especially in terms of greenhouse gas (GHG) emissions, were not coming through strongly enough during the plenary presentations.

3. The Hydrogen and Fuel Cells Program is well focused and managed, and is effectively fostering research and development (R&D) to enable innovation and advance the state of technology for hydrogen and fuel cell technologies to be competitive and achieve widespread commercialization and deployment by industry.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

Average Score	**8.8**
Number of Responses	22

Comments:

- The extent to which the Program is well focused and managed has impacts on the entire industry. Fortunately, the Program is well focused and well managed (said wholeheartedly). The focus on cost reduction of hydrogen fuel, storage tanks, electrolyzers, and fuel cells is integral to the success of hydrogen refueling for light-, medium-, and heavy-duty FCEVs. The focus and success on technology transfer from the national laboratories to the field is also crucial. Advanced onboard hydrogen storage, flexible hydrogen dispenser hoses, and electrochemical compression are just a few examples of research presented at this AMR that are needed in the short term for already installed hydrogen refueling stations and in the longer term for stations that are planned and not yet operational. No matter what the pace or sequence of applications, development in hydrogen at scale across sectors remains a key factor in cost reduction of the fuel and the equipment. In 2018, hydrogen supply limitations resulted in fuel shortages and customer impacts. The Program focus on problem-solving equipment that will lead to more reliable, redundant, and resilient supply is needed. The Program is leading the energy industry to hydrogen production at scale, which the industry needs.

- It is impressive how the Program "walks the talk" of thoroughly informed decisions and consideration of feedback for setting priorities and making adjustments.
- The Program was able to obtain premier speakers from around the world in important Program areas.
- Seen from the outside, this reviewer strongly agrees concerning focusing and managing R&D to enable innovation and advancements in the state of technology for hydrogen and fuel cell technologies and acceleration of the uptake/transfer of advances to industry. The Program structure, consortia, and other collaboration instruments seem to make this possible. Whether the Program enables competitiveness and widespread commercialization remains to be seen. This depends on creation of markets, which is outside the scope of the Program. Without solving market failure, conventional use of fossil fuels will likely continue to dominate in the foreseeable future. Widespread commercialization requires more than basic and applied R&D.
- The Program is extremely well managed. The work of DOE's teams is impressive. Developing closer links to industry needs is advisable. The Program is focused more on technology than on industry targets. Research-wise, it is excellent, but the road to widespread commercialization is not apparent. The horizons are excellent, but it seems that more interaction with industry would accelerate the deployment of hydrogen technologies.
- Overall, the Program has clear and well-thought-out objectives and milestones. It is especially beneficial that DOE focuses on the early-TRL R&D-stage technologies that are too early for the private sector. That said, active engagement of industry in the subprogram technology teams and/or projects is likely to help the focus and progress of research in the right direction.
- The Program management is excellent and is a model of effective management among the federal agencies. The subprograms consistently enable hardware innovation and addressing commercialization problems that industry does not address. The portfolio could be strengthened with regard to computing enabled innovation and software development.
- The competitive and widespread commercialization push does not seem strong enough in the overall Program, especially when considering timeliness. Having said that, there is good management practice evident across the Program, and many advances are being made. However, the ability for these advances to have real impact on vehicle deployment nationally is not as clear.
- The Program should continue fostering collaboration with national laboratories, universities, and industry. Duplication with other agencies within or outside DOE should be avoided.
- Industrial partners' more frequent participation in project activities would accelerate the uptake of developed technological solutions and would ensure the alignment of activities with industrial objectives.
- Regarding fuel cells, the Program is very much focused on basic research, and so commercialization seems to be many years ahead.

4. The Hydrogen and Fuel Cells Program's portfolio of projects is appropriately balanced across research areas to help achieve the Program's mission and goals.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

Average Score	**8.3**
Number of Responses	22

Comments:

- The Program portfolio reflects many energy sectors; this is highly appropriate and useful. The portfolio reaches across many early-stage research areas to achieve cost reduction of technologies and systems, improved durability of the technologies and systems (realistic cycles of use), and competitive component and system development from a number of stakeholders. The emphasis on consortia and projects funded through funding opportunity announcements (FOAs) yields highly focused projects. Several presenters explained the breadth of the stakeholders under consortia arrangements and the ability to leverage and share expertise among stakeholders. The consortia approach is a smart way to address the collection of needs for a broad portfolio of energy projects. The only issue is how to connect consortia to consortia.
- With California's experience showing that station deployment gets vehicles on the road, it seems like the Program should shift more of its funds to the Hydrogen Infrastructure R&D subprogram. In addition, because the customers interface constantly with hydrogen fueling, they are constantly face-to-face with the cost of hydrogen. This is not currently a barrier, thanks to original equipment manufacturer (OEM) subsidies, but this will not always be the case. Low-cost hydrogen is a near-term priority for continued expansion of hydrogen networks. Therefore, hydrogen production and distribution funding should be increased.
- Although the Program diversifies, it still leans heavily on basic research. Better understanding of the basic principles may guide finding better (laboratory-scale) solutions but is not yet a guarantee for adequate performance under practical conditions. Consideration could be given to strengthening the pilot and demonstration component to complement basic research with more "learning by doing" (a good example is the hydrogen station data collection and analysis).
- The portfolio is fairly well balanced, but going forward, it is clear that low-cost electrolysis (low electrolyzer capital cost) is key to large-scale integration of hydrogen, as a low-carbon energy carrier, into the national energy system. It would be good to see increased emphasis on projects that help move electrolyzer technology to lower cost and larger manufacturing scale.
- More emphasis on manufacturing and less on new fuel cell catalysts should be considered. Industry needs more support with industrialization of the technology. The Hydrogen Storage R&D and Hydrogen Infrastructure R&D subprograms seem well balanced, although compression technologies could be looked at more intensively.
- The Hydrogen Materials—Advanced Research Consortium (HyMARC) is not well coordinated. There is too much focus on very specific materials, which does not seem so promising. The work seems to focus mostly on $Mg(BH_4)_2$—these materials have serious recycling costs and logistics problems that are not being accounted for. Almost all of the consortia members work on this material, which does not make sense. The subprogram should have begun by down-selecting the materials after deciding on the criteria for good hydrogen storage/carrier characteristics. Most of the more mature projects are very organized and constructed to reach the goals set by the FCTO, specifically the Electrocatalysis Consortium (ElectroCat) and the Fuel Cell Consortium for Performance and Durability (FC-PAD). FC-160 achieved the goals set in terms of activity and went beyond them, showing remarkable progress in platinum-group-metal-free (PGM-free) development and performance in membrane electrode assemblies (MEAs). It seems the most important challenge is to increase the atomically dispersed iron content and catalytic site density. There are still open questions regarding durability and degradation mechanisms. These topics are currently the biggest hurdle in the field and should be given more emphasis in the future.
- Two comments on Program portfolio balance. First, the Safety, Codes and Standards portion of the budget has been flat for years; this is a significant decrease in net spendable dollars year over year and urgently needs to change. Both cost and safety continue to remain highly verbalized priorities by DOE and by stakeholders, yet year after year, cost reduction and technology development receive nearly 10 times the funding of safety. Second, the portfolio is heavily focused on hardware and materials research, with a

largely experimental focus. A more balanced portfolio would include more analytical and computational activities and system-level research.

- It seems that the decarbonization dimension does not necessarily come through in a prominent way, especially for the projects dealing with infrastructure and systems related to H2@Scale activities. Some very low-TRL activities, such as photoelectrochemical water splitting or development of hydrogen storage materials, will likely not have a significant impact on the Program's targets in a foreseeable timeframe.
- Ideally, achieving greater commercial industry participation in some of the developmental areas would be helpful.

5. The Hydrogen and Fuel Cells Program's R&D aligns well with industry and stakeholder needs, and is appropriate given complementary private sector, state and other non-DOE investments. Please comment on the overall Hydrogen and Fuel Cells Program as well as each subprogram/ activity area, as appropriate.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

	Hydrogen and Fuel Cells Program Overall Rating	Hydrogen Production R&D Subprogram Rating	Hydrogen Storage R&D Subprogram Rating	Hydrogen Infrastructure R&D Subprogram Rating	Fuel Cell R&D Subprogram Rating	Technology Acceleration Subprogram Rating	Safety, Codes and Standards Subprogram Rating	Systems Analysis Subprogram Rating	Fossil Energy Solid Oxide Fuel Cell Subprogram Rating
Average Score	8.7	8.5	7.7	8.6	8.2	8.7	8.6	8.8	8.8
Number of Responses	21	20	20	21	21	21	21	21	4

Comments:

- There is excellent alignment between the big picture (hydrogen economy) and specific technologies/ capabilities needed to achieve it.
- Work on electrolysis is important, world-leading research.
- The industry perspective enhances alignment of Program goals with industry objectives and timelines.
- Excellent systems analysis work has been done over the past several years under the H2@Scale initiative. This work should continue, with engagement from hydrogen industry experts and potential users, where possible. Perhaps the Program should also look at broader value chains: e.g., the value of the oxygen co-product; the value of renewable hydrogen in various applications, given current incentives such as the California Low Carbon Fuel Standard; where renewable hydrogen presents a logistics challenge; and where renewable hydrogen presents an advantage in terms of production rates, buffering, and distribution.
- Non-DOE investments complement the projects presented at this AMR. However, there is a difference between the two vantage points. DOE national laboratory staff conduct work from a vantage point that achieves innovative solutions for systems analyses of hydrogen production, storage, infrastructure, and technology acceleration. Perhaps non-DOE-funded projects also achieve this, but the proprietary nature of non-DOE work may preclude public reporting of their work products. The DOE systems analyses are useful in that they are highly technical and, sometimes, theoretical. The more technical and theoretical analyses show insight, experience, and new ways to approach these complex problems. One question is whether more effort can be placed on connecting the output of the AMR process to non-DOE-funded

projects to benefit both types of projects. Perhaps a panel at the next AMR could report on this connection: "How we applied the DOE systems analyses in our environment and how this helped us achieve our stated goals."

- Industry and stakeholder participation is considered an important indicator to assess whether the Program aligns well with their needs. Regarding Hydrogen Production R&D, the presentation materials indicate significant industry participation in electrolysis production projects but much less participation in high-temperature thermochemical production and photoelectrochemical production. Industry and stakeholder participation in Hydrogen Storage R&D seems even less, or is not indicated well enough. Fuel Cell R&D shows a varied picture with considerable participation in projects for "Fuel Cell Performance and Durability" and "Catalysts and Electrodes" but clearly less involvement in, for example, "Membranes/Electrolytes" and "MEA, Cells and other Stack Components." In general, the Hydrogen Infrastructure R&D presentations indicate considerable industry and stakeholder participation, with five out of nine presentations presented by industry representatives. The same holds for "Technology Acceleration," which may be explained by the fact that it covers activities that are closer to the market. Finally, activities on Safety, Codes and Standards and Systems Analysis align very well by nature with industry and stakeholder needs because they provide an essential framework for product development and hydrogen and fuel cell activities in general. Assessment of differences in industry and stakeholder participation in various parts of the Program might be used to improve focus and alignment with industry and stakeholder needs.
- The focus of the R&D subprograms at DOE is well aligned in general with industry needs and objectives. It would be better if there were even more participation and/or inputs from commercial companies.
- It is difficult to see how the Fuel Cell R&D subprogram is really reacting to industry needs. In addition, while it is logical to look at storage mediums other than compressed gas because of insurmountable physical limits, it seems that the Hydrogen Storage category is focusing too heavily on materials storage, when industry stakeholders have not indicated a willingness or readiness to transition their development plans away from gaseous storage. Indeed, gaseous storage on today's vehicles often provides sufficient range for drivers' needs. This may indicate that either automotive OEMs are finding other system-level ways around the physical limitations of gas storage, which would indicate that new storage mediums may not be necessary, or that the technology targets simply are not in line with more recent understanding of consumers' needs. Re-evaluation may be necessary, with guidance from industry. The needs and impacts on station operators and the hydrogen production/distribution community should also be considered. A paradigm shift to a different storage medium could have far-reaching ripple effects on these industries' costs and plans, and their long-term plans and needs must be accounted for as well.
- Most of the research is performed together with industry partners. Given the targets of the Program, the Program portfolio is appropriate given complementary non-DOE investments. However, the Program could have more impact on the economy if the Program targets were discussed jointly with industry, in particular the energy and transport industries.
- The focus on solid-state hydrogen storage is closer to fundamental research than to industrial/market applications. Electrolyzer research should have a stronger focus on polymer electrolyte membranes (PEMs).
- The Fuel Cell R&D subprogram is focused on basic research, while the other subprograms allow for applied research and are more directly related to industry needs.
- Given DOE's objective of achieving "cleaner," or low-carbon, fuel and the insignificant market share of non-fossil-based hydrogen, the current resources allocated to hydrogen production are not sufficient. Integration with low-cost renewable energy is critical R&D that needs more attention. Boosting resources associated with Safety, Codes and Standards is appropriate and requires international engagement.
- Although ElectroCAT has been making very good progress, it seems to neglect work on Pt, which is the industry choice. Hence, more basic work is needed on Pt-based catalysts to provide new designs.

6. The Hydrogen and Fuel Cells Program is funding high-impact projects that have the potential to significantly advance the state of technology for the hydrogen and fuel cells industry. Please comment on the overall Hydrogen and Fuel Cells Program as well as each subprogram/activity area, as appropriate.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

	Hydrogen and Fuel Cells Program Overall Rating	Hydrogen Production and Delivery R&D Sub-Program Rating	Fuel Cell R&D Sub-Program Rating	Hydrogen Storage R&D Sub-Program Rating	Technology Acceleration Sub-Program Rating	Safety, Codes and Standards Sub-Program Rating	Fossil Energy Solid Oxide Fuel Cell Sub-Program Rating
Average Score	8.8	8.5	7.8	8.8	8.5	8.8	8.8
Number of Responses	21	21	21	21	21	20	4

Comments:

- Achieving infrastructure R&D targets is essential; energy efficiency, integration, and cost reductions in hydrogen and fuel cell technologies, especially, are high-impact projects. Projects that expand R&D beyond light-duty vehicle (LDV) fueling operations to medium- and heavy-duty vehicles (MDVs and HDVs) will “push” MDVs and HDVs beyond the “start-up” period the LDVs experienced. As a result, time and resources will be saved. Testing actual MDV and HDV fueling in the field is needed to support industry expansion into hydrogen MDVs and HDVs and complement the LDV rollout. The work in HydroGEN on fuel production also has the potential to advance today’s processes. The Hydrogen Materials—Advanced Research Consortium (HyMARC) also advances the state of the art. These consortia should continue.
- The number of results produced by HydroGEN is overwhelming. Data management will be crucial. The consortium has well identified that cost reduction and technology remain key metrics. HyMARC research on storage is important. Their approach is very good: “design rules” are needed to guide materials discovery. The development of models and the analysis work is a strong component of DOE’s Program. Fuel Cell R&D is well focused; it is a very strong subprogram. Cobalt may not be a good replacement for platinum. Safety, Codes and Standards is an excellent subprogram providing important results. The creation of the Center for Hydrogen Safety will play a major role in helping industry to develop hydrogen technologies.
- Many of the independent fuel cell companies lack the ability to make advanced R&D investments and tend to have shorter-term focus. The DOE-funded R&D provides key forward-looking investment that will be essential to the ultimate hydrogen and fuel cell commercialization, adoption, and commercial applications.
- The Fuel Cell R&D subprogram is very focused on basic research, so the impacts might be in the long term. H2@Scale activities already have impacts and are attracting strong interest from around the world. Also, the Systems Analysis subprogram provides guidelines to the global community.
- The Program should continue work on heavy-duty trucking sector analysis and work on energy carriers such as ammonia and methanol. It would also be interesting to understand what renewable hydrogen can do

to lower the GHG footprint of existing U.S. corn ethanol (both through fertilizer pathways and possibly as a feedstock for liquid fuels for farm machinery).

- The Program's project integration and coordination with other government agencies and industry is the standard for DOE and the nation.
- The projects are evaluated highly since they focus on high-impact technologies. They are also evaluated well when they set cost targets clearly.
- The Program seems to set well-informed R&D priorities with a mix of high-risk, novel, potentially game-changing R&D.
- Systems analysis and hydrogen infrastructure-related topics seem to be the areas where the Program shines the most in this regard.
- In general, this statement is quite true, although there are a few projects that do not seem to show prospects. Specifically, in FC-170, the path to the development of Mn-N-C—the why and how—is not clear. Some of the data interpretation does not seem to be accurate, and most of the conclusions are based on electron microscopy. The concept must be re-evaluated. In general, some fuel cell R&D projects do not follow the DOE testing conditions and accelerated stress test (AST) protocols, which makes it very hard to analyze and compare results between projects. All must adhere to the same conditions and protocols. The hydrogen storage analysis was very important and very well done, breaking the chain into parts and explaining what needs to be done to lower prices in the future. ST127 places too much emphasis on specific materials that do not seem to be very promising. In addition, when selecting and studying such materials, full life cycles should be considered, not only theoretical hydrogen storage, which may be exaggerated in some cases. Efficiency and safety are also neglected.
- The reviewer tends to agree with this statement, considering the importance of the vast majority of the topics that are addressed. However, it is difficult to assess to what extent the totality of project results contributes to improving the state of the art of the various technologies and, for example, what the relation is between the project results and the detailed cost analysis for fuel cells systems and storage tanks. The coherence between these activities could perhaps be improved, while similar (detailed cost) analysis might also be worthwhile for other technologies and systems, such as different types of electrolyzers. Indications/summaries of the state of the art of electrolyzers and the progress therein through, for example, successive spider web diagrams (as for storage tanks) might also be helpful.
- Data collection, validation, dissemination, and analysis are under-used in multiple aspects of the Program. Knowledge exchanges, analysis, and policy activities should also be seen as high-impact activities. The activities in Safety, Codes and Standards are mostly qualitative, expert-based, and somewhat incremental; this subprogram needs a larger budget to be able to make more meaningful advances. Data collection activities need to be accompanied by data dissemination activities; otherwise, the data remain behind national laboratory firewalls.
- Industrialization of hydrogen production should be looked at more intensively. Maybe through systems analysis, there would be some space to include more specific technoeconomic studies.
- Based on talking to several PIs during the poster session, it seems as if they have to prioritize technological advances over fundamental understanding. This may not the most prudent approach in the long term. (This does not seem to be a universal sentiment among PIs.)
- This question is strongly related to the previous one. It is difficult to foresee a clear future path for activities focused on a very low TRL.

7. In your opinion, what were the most significant accomplishments within the Hydrogen and Fuel Cells Program during the past year? Please consider the entire AMR content and entire DOE portfolio, including poster sessions, rather than the plenary talks alone.

Please respond for any subprogram/activity area as appropriate (e.g., hydrogen production, hydrogen storage, hydrogen infrastructure, fuel cells, technology acceleration, safety, codes and standards, solid oxide, ARPA-E, Basic Science, etc.).

Comments:

- There are a number of significant accomplishments: PGM-free electrodes demonstrating reasonable current densities in MEAs at typical cell operating voltages; one of the first MEA demonstrations of PEM-based water electrolysis with PGM-free oxygen evolution reaction catalyst at practical operation conditions (Argonne National Laboratory); demonstration of continued performance improvement for completely PGM-free anion exchange membrane electrolysis (Northeastern University); encouraging 2.5x improvement of PGM-free fuel cell catalyst, although it is still almost a factor of 3 away from the target; progress in development and understanding of MEA fabrication methods; development of Coriolis flow meters that achieve 2% accuracy during SAE J2601 fills; validation/experimental verification of a pressure consolidation strategy for hydrogen filling stations with an outlook for significant cost reduction; and completion of rigorous safety analysis, leading to an outlook for significant reduction (20%) of safety distances for hydrogen filling stations, to be formalized through implementation in National Fire Protection Association (NFPA) 2 (Sandia National Laboratories and the National Renewable Energy Laboratory).
- This AMR included a significant number of ongoing, practical cooperative research and development agreement (CRADA) projects. This includes developing costs per kilowatt-hour and kilogram across the H2@Scale sectors to provide a better perspective for hydrogen and fuel cell stakeholders. The Center for Hydrogen Safety kicked off and anticipates increased proliferation of safety practices in new areas. The HyMARC material compatibility test and evaluation with hydrogen is needed. This includes the embrittlement work for storage vessels, which are presently expensive components, and assessment of overall station life expectancy due to obvious and nonobvious materials used in components. Some hydrogen refueling station developers state their plans for stations that will last 10 and 20 years, and what is needed are tests that help the investment community and public funding agencies understand whether the stated life expectancies at the beginning of projects, or even prior to funding, are realistic.
- The activities of Systems Analysis and Technology Acceleration (H2@Scale in particular) define a background against which benchmarking business cases becomes possible. The subprograms' role in providing a tool for measuring progress in market development is also extremely relevant. Regulations, codes, and standards (RCS) activities and Hydrogen Materials Compatibility Consortium (H-Mat) activities are extremely important, at not only at a national but an international level, for accelerating and enabling widespread penetration of hydrogen technologies.
- The H2@Scale analysis is a significant accomplishment -- it has made great progress over the past year, and there is much more to be done. Ideally, this analysis, including a look at the policy landscape, will serve as the foundation for roadmap work and feed into Program priorities and target-setting. The success of fuel cells in material-handling equipment over the past decade is encouraging, and the Program contribution to that success is evident. Further systems analysis can help to answer the questions of what is next, when, and how big the prize is.
- The hydrogen production and storage cost analyses are critical for industry, and good work has been done there to help decision-makers in industry. ElectroCat has been showing new activity records while getting closer to understanding and mitigating durability issues. The recent progress in the development of new catalysts is one of the most significant accomplishments during the past year. Another important

accomplishment is the study of corrosion-resistant materials, including synthetic routes such as ceramic aerogel materials.

- In considering the biggest Program accomplishments during the past year, three points come to mind: (1) the successful rollout of the H2@Scale initiative, (2) DOE's (in particular the FCTO director's) strong coordination and support for the industry-led U.S. Hydrogen Roadmap study, and (3) the new initiative on "e-fuels" since there is a strong, but often ignored, link between CO_2 conversion and availability of low-cost "green" hydrogen that needs to be fully explored.
- In general, the Program management systems seem comprehensive and very well managed to keep the Program relevant and value-added year after year to very diverse stakeholders. Specifically, the magnetocaloric liquefaction of hydrogen clearly has huge potential benefits.
- The innovative intelligent networks project by Ivys, the magnetocaloric liquefaction project at Pacific Northwest National Laboratory, and the advanced mobile fueler developed through Electricore seem like potentially high-impact projects from this year's Program.
- The announcement of the Center for Hydrogen Safety is a significant step forward toward addressing a major need for all stakeholders in all of the hydrogen-related technology spaces. The extensive interagency activities are commendable.
- Accomplishments include progress in exploring the potential of non-PGM fuel cell catalysts and progress in reducing costs of hydrogen production.
- Accomplishments include progress on the applications enabled by DOE investment over the years. The Program is striving to maintain U.S. participation in the hydrogen revolution worldwide.
- There was a clearly deliberate focus on durability projects across the portfolio. This topic is critical to developing technology that will be commercially applied.
- The R&D consortia are producing remarkable results. They have a major impact on the organization and the optimization of research efforts. This is one of the best uses of national laboratories.
- There has been remarkable progress in quickly setting up H2@Scale.
- Progress and accomplishments on codes and standards were great; completing changes to the upcoming NFPA was key to enabling more deployments and locations of hydrogen infrastructure. Continued advancements in roll-to-roll are also very good, but more industry participation is needed.
- All aspects of the Hydrogen Production R&D and Hydrogen Storage R&D subprograms seem to be doing well. In particular, the work on $Mg(BH_4)_2$ -> MgB_2 appears to have progressed nicely. Safety, Codes and Standards might need more guidance, but it was difficult to get feedback from many PIs at the poster session (posters in general were not always attended).

8. Early-Stage Research and Development: The Hydrogen and Fuel Cells Program is focused on early-stage R&D as aligned with Administration objectives for federal research funding. Please provide suggestions for early-stage R&D that the Hydrogen and Fuel Cells Program should consider for promoting its goals and objectives.

Comments:

- The focus of the Program is consistent with current administrative priorities, as required.
- There is a need for emphasis on early-stage R&D aimed at reducing the costs of electrolyzer designs and operations (for all sizes of electrolyzers) so the energy industries can increase electrolyzer use. Other suggestions include:
    - Early-stage R&D to develop more resilient hydrogen production systems. This would include autonomous and continuous operations supported by software that anticipates maintenance, carries out the maintenance, and logs maintenance.

  - Early-stage R&D that decreases the cost of renewable hydrogen production by generating hydrogen through ancillary services that optimize electrolyzer applications and complement the grid at the same time.
  - Work on electrolyzer configurations and footprints that provide flexibility to fit the equipment into small physical spaces.
  - Innovation in early-stage hydrogen energy carriers and the most viable applications that will work across industrial sectors that use hydrogen as an energy carrier.
- Research activities related to circular economy, reduction of raw materials, and materials footprint could be introduced/strengthened. These activities could potentially play a role across sectors and technologies and encourage the development of a more mature value chain (if this qualifies as early-stage). Manufacturing activities for hydrogen technologies could be further improved (if this qualifies as early-stage). Development of durable low-PGM catalysts for electrolysis and fuel cells is already happening and, because of its importance, could be further strengthened. Hydrogen production through advanced bioengineering solutions could be further explored, too.
- Given the early-stage research focus, more involvement of universities seems necessary in the H2@Scale and infrastructure and systems R&D activities. The Program should expand the early-stage R&D activities, which currently focus on materials engineering research and technology development tasks. Early-stage research also includes theoretical, computational, communication, and analytical research activities, which are not well-represented in the Program portfolio.
- Electrolyzer technology, in both design and manufacturing, seems immature in comparison to fuel cell stack work. At the same time, dramatic drops in solar and wind capital costs are making electrolysis more and more relevant. DOE should continue to fund work on electrolysis concepts, as well as work on novel alternatives (direct solar water splitting), if they can show promise in competing with electrolysis.
- Exploring new storage strategies is needed, as compression is limited and cryogenic storage even more so. Scientific understanding of manufacturing issues for fuel cells, electrolysis, and compressors is required to enable industrialization and supply chain development, ultimately for product cost reduction and reliability.
- Several PIs, especially for the Hydrogen Fuel R&D subprograms mentioned that the milestones are still too technical, given the state of the field. More early-stage research/structure–property investigations are needed.
- Although studied for many years, alkaline fuel cells have shown significant improvement in recent years. Together with new findings related to the durability of these cells, this technology seems to deserve more attention.
- One suggestion is a project focusing on lifecycle GHG emissions analysis of various scenarios of e-fuels pathways and plausible hydrogen sources.
- High-temperature electrolysis, maritime, and rail sectors have high potentials. These sectors would need significant increase in early-stage R&D.
- The Fuel Cells R&D subprogram might investigate the impact of manufacturing processes on fuel cell performance and degradation behavior.
- Membrane and MEA durability improvements and onsite hydrogen production costs are possible early-stage R&D topics.
- Cryocompressed hydrogen storage vessels is a suggested topic.
- Larger-scale storage and transportation are suggested.

9. Energy Materials Network (EMN) Consortia: Do you have any comments or recommendations on the Hydrogen and Fuel Cell Program's EMN consortia approach? Please state what is working effectively and areas that may benefit from further improvement.

Comments:

- The EMN is an effective approach for connecting a core consortium team's R&D and experimental work with materials used with hydrogen systems. The work includes storage systems that are often purchased as an afterthought. The EMN requires strong leadership, which it appears to have. The EMN is a good work effort and program that looks at the long-term viability of materials. Perhaps it would be possible for more hydrogen stakeholders to provide input to the EMN consortia. The input could be as simple as tracking the correct and incorrect uses of materials in field installations. Other input could be on hydrogen-related safety events due to the use of incompatible materials in a hydrogen system. The trust in the technology is bolstered by increased knowledge and confidence in the selected materials, and these consortia will contribute to both.
- The EMN concept is a good platform with the potential to drive discovery and collaboration on multiple applications that require advanced material development. However, the stated measures of success are not as clear and sometimes appear to reward mere collaboration or "contact" with another national researcher more than results. Perhaps the governance structure could be refocused a bit to make it less constraining to the researchers and give them more leeway so they could focus on actual deliverables.
- The concept of using the consortium approach seems logical and well structured. It also seems to be providing opportunities for more efficient utilization of cross-laboratory capabilities and knowledge transfer. One potential point of improvement could be developing a greater distinction between FC-PAD and ElectroCat—or at the very least, considering why there need to be two separately defined consortia for the overall goal of low-cost, high-performance, highly durable fuel cells.
- The overall consortium approach in materials has many advantages by providing better focus and enabling faster commercial adoption.
- The EMN seems very well organized. It seems a good support structure for the research and should continue to yield benefits, adding to the Program's success.
- The size of the EMN network is impressive. Data production is intensive. The EMN has high potential, but consortia need to identify their targets in close collaboration with industry to be successful.
- The activities of some consortia seem to be historically focused around the same cluster of topics and issues (especially certain material classes). Reprioritization should be encouraged and fundamental research discouraged if, after a certain amount of time, no results that can be brought to a higher TRL are achieved. Clear go/no-go processes could be established with guidelines and participation at a Program level.
- Method(s) should be developed to easily assess the significance of project results against a benchmark (state of the art) and targets so that results can be compared easily.

10. H2@Scale: What are the strengths and weaknesses of the H2@Scale initiative? Do you have any recommendations for other H2@Scale research topics or recommendations to enable the scale up and value proposition of H2@Scale (e.g. a region with low electricity prices, excess curtailment, and hydrogen supply opportunity along with a co-located demand for hydrogen, etc.)? Please provide any other recommendations on H2@Scale.

Comments:

- H2@Scale remains invaluable. From a communication perspective, the value of the "image" of the model is excellent and useful when communicating how scale matters. When someone faces the question of how costs will decrease, the image works. The only recommendation for H2@Scale is the development of case studies that show the impact of scale on a multi-sectoral business application. The study could include the "before" and "after" economics, addressing questions such as when scale "kicked in." There is a need for more people who can teach H2@Scale theory and when and how scale matters. Also, perhaps a case study of utopia could be added, i.e., "This is how H2@Scale would work in the best case scenario," followed by a discussion of how utopia seems impossible and the changes to H2@Scale that result when utopia is not met. There are plenty of hydrogen refueling stations that can be used to explain the impact on those stations when hydrogen production is scaled up through shared and co-located business opportunities. As far as electricity prices, it would be good to know how H2@Scale can be reverse-engineered to show utility providers the impact on hydrogen refueling with price changes. A management question is how this model will be maintained. A rhetorical question is what could possibly be better than this model.

- H2@Scale provides a holistic solution for the hydrogen economy, from energy harvesting to hydrogen production and use. It is well organized, and the FCTO is doing a very good job identifying and developing new programs (such as HyMARC and H-MAT) while maintaining the older and much more developed programs. These new programs, together with cost analysis of hydrogen production, storage, and use on a large scale, are definitely in line with the initiative goals. One recommendation for the use of fuel cells in private homes is for the development of reversible fuel cells. These can serve as buffer systems that can store energy and generate it on demand, depending on price and need.
- The H2@Scale concept is beneficial in that it provides researchers and technology developers the opportunity to integrate with different hydrogen sectors and potentially save on the cost of development. However, to be more useful, H2@Scale needs to develop a deep-dive version with targeted and more practical value propositions. Here are a couple of potential topics to consider: (1) another H2@Scale scenario based on technologies with compatible TRL levels, maybe +/-1 or, alternatively, based on near-term and long-term time horizons; and (2) hydrogen sector integration opportunities based on region or subregion, e.g., the U.S. Gulf Coast region. Also, given that 95+% of current U.S. hydrogen comes from fossil-fuel-based sources, it is critical to have meaningful projects that explore the benefits of incorporating carbon capture and sequestration (CCS) to reduce the carbon footprint of large-scale hydrogen supply.
- H2@Scale is an important program. The results presented at the AMR allow one to have a vision of future hydrogen deployment in the United States. The coherence of the efforts is impressive. The study of the transition to equilibrium should be the next step. Investors interested in the hydrogen sector need guidance on the profitable investments needed to accelerate the deployment of hydrogen technologies.
- Hydrogen availability governs the principal enabling of fuel cell deployment and adoption. The initiative is extremely important to overcoming the current limitations due to either geography or the cost of the hydrogen needed to enable FCEVs and other fuel cell applications.
- H2@Scale shows a strong commitment to the world. This is globally very motivating. The initiative should aim at global alliances and international collaboration.
- The strength is that H2@Scale involves as many stakeholders as possible.
- In the discussion of the market potential for H2@Scale, there seemed to be a surprising amount of focus on the fossil fuel market as a hydrogen consumer. While there is not really any getting around the reality that fleet turnover will be slow and fossil fuel refining will be a major part of the fuel system for some time, it seemed the market potential still dominated too much, given the several legislative and executive actions taken at the state level. To this same point, it seemed that, overall, the analysis did not consider technology-forcing actions in place and that could be in place in the future, and the HDV hydrogen consumption analysis seemed off. There also seems to be a good deal of focus on industrial uses of hydrogen when the H2@Scale market studies themselves show these as certainly the smaller potential future markets. However, the H2@Scale project as a whole is a great example of a timely research effort, as governments and decision-makers are calling for a more holistic understanding of the possible role hydrogen can play in the energy future, especially since this seems more fleshed out or easily understood for electricity. One recommendation is to get a fast start on the effort of regionalizing H2@Scale analyses and working with

the regions' state-based stakeholders to develop analyses that not only are projections but that also allow the states to be involved in a more exploratory manner. The topic does not require simply placing charts and numbers in front of decision-makers. This is a complex topic, and the arguments supporting hydrogen have to overcome incumbent biases. Thus, building an H2@Scale research program with a high degree of collaboration with the states will likely be absolutely necessary to spread the concept.

- One recommendation is identification of the most promising regions through a multi-criteria analysis (potential demand, demand density, availability of renewables, availability of infrastructure, energy prices, policy conditions, etc.) to create hydrogen regions (establish complete and various value chains). The idea of excess curtailment is probably not useful—this is not likely to occur unless there is bad planning or overly stimulating policy. It is unlikely that anyone will continue to invest in renewable energy source (RES) generation capacity if periods of curtailment increase and prices decrease as a result. Development of RES potential and hydrogen should go hand in hand. Hydrogen is a means to keep using fossil fuels but in a decarbonized way in combination with storage of the carbon content, and/or hydrogen is a means to capture solar and wind energy and to make this energy available to the energy system in a form that can easily be stored, transported, and used as fuel for applications where batteries or electrification are not possible, insufficient, too expensive, etc.
- Different business models should be reviewed as well. Considering that hydrogen at scale would supply fuel for transportation, it seems one may not rely only on excess renewable. Similarly, considering that electrolysis has a strong dependence on electricity price, an energy company that produces hydrogen would likely invest in its own electricity generation. Therefore, the company's cost of electricity would be different from the utilities' costs. Building more cases for hydrogen utilization only helps validate the H2@Scale initiative. Also, clearly linking the work from HydroGEN and the Advanced Water Splitting Materials Consortium in the pipeline of H2@Scale as a strategy would be very relevant.
- It would be helpful to integrate analyses of lifecycle energy use and emissions more closely with the H2@Scale effort (if it is not already being done). For example, there seemed to be an increased focus on R&D related to liquid hydrogen at this year's AMR. While potentially important to reducing costs and increasing hydrogen's viability across different applications, the use of liquid (rather than gaseous) hydrogen could significantly increase life-cycle energy intensity and emissions, particularly if hydrogen is produced from natural gas. It would likewise be helpful to understand energy losses associated with chemical carriers (e.g., ammonia and methane) from a life-cycle perspective, as new research in this area was discussed at the AMR. One of the biggest benefits of hydrogen and fuel cells is the potential to lower GHG emissions and help states meet air quality goals. Increased attention to the significant variation in energy and emissions profiles for different hydrogen pathways (production, storage, transmission, and use) at this early market stage for hydrogen could have big impacts in the future.
- Strengths include big-picture thinking and potentially transformative impact. Regarding weaknesses, the basis for all activities centers on the national laboratories, with which it is notoriously difficult to partner. This is limiting the engagement of stakeholders beyond national laboratories. The H2@Scale vision may need to become more focused to facilitate achieving its goals through a portfolio of smaller activities over a longer time frame.
- Very good work has been done to date, but this is a complex area, particularly when it comes to interaction with the electric power grid. A good next step might be to build on the Hydrogen Analysis (H2A) type of framework and put together some end-use economic model cases, e.g., hydrogen from solar/wind to interstate truck stop fueling in several parts of the country, hydrogen from wind/solar to fertilizer in the farm belt, and hydrogen from wind/solar to low-carbon methane/methanol production. It would also be good to understand where steam methane reforming with CCS might be a strong option.
- The development of demonstrations, especially in conjunction with utilities, industries, or regions, is encouraged. The actual benefits (environmental in particular) for carbon capture and utilization pathways is a topic that should be further assessed.

- There is potential to have large-scale model validation demonstrations at fixed installation sites. Hydrogen as energy storage for the grid is a prime example.
- There is a lack of targets, and metrics are needed for hydrogen carriers.

11. Collaboration: The Hydrogen and Fuel Cells Program is collaborating with appropriate groups of stakeholders. Please add any additional comments, particularly on which stakeholders (e.g., academia, companies, small businesses, types of industries, etc.) should be more engaged and in what manner.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or N/A if you have no opinion. Please add any additional comments.

Average Score	**8.57**
Number of Responses	22

Comments:

- Working with stakeholders is one of the biggest strengths of the Program. The day-long interagency track showcased the strong engagement across the federal government, as well as with state and local governments. Sector-specific workshops such as H2Rail are appropriately bringing together diverse stakeholders to focus on deployment barriers and solutions.
- The collaborations that DOE takes on through this Program are exemplary.
- Collaboration in the Program is truly amazing—DOE-best.
- The Program has good industry and government engagement and perspective, including international stakeholders, and this should be continued, given the importance of global cooperation and adoption of these technologies. The engagement with industry and with national laboratories is strong. It is unclear to what extent the needs of other stakeholders are being considered (e.g., users and communities impacted by the technology). The Program could articulate who these other stakeholders are and ensure that those needs are also addressed. The Program should engage with academia more directly.
- Interaction with state agencies seems very minimal. There is opportunity to leverage these resources/ initiatives through joint university and corporate projects. The addition of the DOE Office of Fossil Energy's Solid Oxide Fuel Cell subprogram to AMR is working well and allowing for greater interactions.
- Although the FCTO is the most established office in U.S. fuel cell R&D, in recent years there have been large investments and efforts in other parts of the world to develop fuel cells. It is recommended that the Program find ways to open the U.S. programs to international collaboration, which is currently lacking. Such an initiative will benefit all sides.
- A strong and clear engagement with multinationals, such as those who founded the Hydrogen Council, would be desired. However, it is not recommended that the FCTO provide funding to those organizations but rather co-invest through subject matter experts, national laboratories, and academia.
- The constraints of government resources and policies are understandable, but more collaboration and coordination with other government agencies would be useful, e.g., the National Science Foundation (NSF) on EMN-related research or the National Energy Technology Laboratory on CCS-related projects. Such coordination also avoids some overlap.
- It is difficult to get a clear and complete overview from the presentation material. There is certainly a good deal of collaboration happening, especially between national laboratories and universities. It seems that

private-sector participation can be strengthened, especially in H2@Scale and Technology Acceleration subprogram activities.
- There is good collaboration between academia and the national laboratories and, on some specific activities, with industry. There could be more industry participation, but finding willing participants is always challenging.
- More frequent participation of industrial partners (both subject matter experts, where appropriate, and large industries) in project activities would accelerate the uptake of developed technological solutions and would ensure the alignment of activities with industrial objectives. The interaction with other institutional stakeholders seems good.
- Deployment of hydrogen technologies needs acceleration. More collaboration with stakeholders is recommended. The Program is well built in terms of technology but not so well in terms of economics. Increased collaboration between research and industry, in particular with energy operators and automotive industries, would be profitable.
- Military bases around the country are potential customers for validating models through hardware demonstration.
- Perhaps future FOAs could explain that awardees (and non-awardees) can opt to participate in core consortia teams. This approach could broaden the reach of the FOA projects.
- Some types of collaborations seem to be in the initial stages, so it is too early to tell.
- It would be good to see more engagement with industrial gas players.

12. International Collaboration: The Hydrogen and Fuel Cells Program collaborates through a number of international partnerships. For example, the International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE) is an international partnership to coordinate activities on hydrogen and fuel cells across 18 countries and the European Commission. The U.S. assumed the chair role for IPHE in 2018. Please comment on actions DOE in conjunction with IPHE can undertake or activities that are effective/need improvement to accelerate progress in hydrogen and fuel cell technologies.

Comments:

- Several international initiatives are discussing the importance of hydrogen, in particular, Mission Innovation, the International Energy Agency, the Clean Energy Ministerial, and the G20. The actions of DOE in conjunction with IPHE would be important to linking these initiatives to stakeholders in a global action plan. DOE should also continue to contribute to IPHE in the domains of outreach, regulations, codes, standards, and safety. DOE's contributions in these domains are outstanding.
- International hydrogen leadership is crucial for those companies that want to build and market technologies and systems worldwide. This applies to equipment used in hydrogen refueling stations or FCEVs. Players want to design one hydrogen refueling station and system to be used worldwide. The same is true with FCEVs. Perhaps the IPHE could undertake work projects in international best practices for H2@Scale; this would allow hydrogen refueling station developers to apply best practices internationally. Also, companies in "adjacent H2@Scale sectors" could save time by applying others' related best practices. This effort could differ from international standardization in that the effort could produce public best practices with verbiage and examples that do not necessarily lend themselves to international technology standards. As examples, an international project could address optimal approaches to need assessments or risk assessments for hydrogen refueling stations.
- A priority for DOE should be harmonization of international standards and code development. An example is the push for higher-capacity tanks included in the LDV version of J2601, simply because the International Organization for Standardization (ISO) standard moved in this direction. However, in both cases, this seems like a quick, clumsy solution to a short-term problem that would best be addressed

through other standards development means. DOE could help guide the conversations and help provide reasoned analysis for the best paths forward in standards development that avoids such short-term focus. In addition, DOE should collaborate internationally to understand the opportunities for the U.S.-based hydrogen industry to gain financial independence and accelerated growth through export of our technologies/products.

- International work is especially important in establishing common materials, components, and system test protocols; fueling protocols; and safety, codes, and standards. DOE funding of U.S. expert participation in international forums has been extremely helpful to U.S. industry and should be continued.
- It is suggested that the Program work closely with other countries, such as Canada, to align funding cycles to maximize the ability for international collaborations. Maybe a portion of funding should be dedicated to co-funding with other countries. National laboratories are clearly great points of contact for such.
- IPHE is a very important aspect of realizing true commercialization of fuel cell technologies. The presentation by Australia's chief scientist was very informative, and increasing participation by having more international participants present at the AMR would be beneficial.
- There is excellent government-level outreach that is focused and effective. Continued community and student outreach would be welcome.
- There should be a stronger focus on safety in international fora such as IPHE, and the establishment of international workshops is a positive initiative.
- International projects between institutes or companies are still difficult to set up and should be promoted in the future. International collaboration, such as that with IPHE, is very helpful.
- Although officially this collaboration exists, very little outcome is presented in the AMR. It may be that the incentives for collaboration between laboratories are lacking.
- There appears to be an obvious gap in opportunity to collaborate with international auto companies, especially given the clear lead of Japanese autos on hydrogen and fuel cell deployment.
- The Program involves many organizations, including IPHE.
- From the science viewpoint, collaborations are mostly on paper, not true collaborations.

13. Prizes: Agencies have shown interest in implementing prizes and competitions as a mechanism to complement the conventional grant process. Examples include the H-Prize (H2Refuel) for a small-scale hydrogen fueling appliance that complements large retail stations. Please provide comments on the prize/competition approach and provide any suggestions for future prizes or competitions that would align with the goal of accelerating the widespread success of hydrogen and fuel cell technologies.

Comments:

- The Program might consider a competition or prize related to education and outreach. For example, DOE could host a student "hackathon" to develop apps or other tools to assist commercial fleet operators or city managers weighing the purchase of fuel cell trucks, buses, or vocational vehicles (with data from existing tools such as Fleet DNA as the underpinning). A prize to incentivize broad public education on hydrogen could also be useful (e.g., developing a school curriculum or a social media campaign) for a relatively low dollar amount.
- Competitions are recommended in the areas of (1) electrolyzer efficiency advancements and cost per kilogram of hydrogen and (2) achieving stack durability >20,000 hours in automotive applications.
- Prizes are important to identifying leading scientific research groups and acknowledge their importance for the development of the field. The award ceremony is important for the community. A specific prize for the most important result of the year is suggested.

- Prizes are a good way to spur competition and something that corporations and startups can be proud of as they try to disseminate new technology. They usually end up creating multidisciplinary teams at universities—driving distance, for example.
- Prizes are notable. For example, a prize could "sweeten the deal" for a company that did not receive a funding grant. A prize could be given for a company that implements some of the DOE energy efficiency, durability, and cost reduction targets, among others. A prize could be all the encouragement a company needs to apply for a grant and follow through on the execution and completion of the grant. The prize could be for positive impacts from implementing DOE targets. One area where this could be beneficial is in the production of liquid hydrogen.
- Since public awareness and acceptance is so important, there should be an award for best public awareness video.
- A prize around renewable hydrogen production, with emphasis on low capital cost, is suggested.
- It is a very good idea to acknowledge leaders in industry for their efforts and achievements. Companies can leverage these prizes to attract more investments and media coverage.
- There should be competitions, especially if these were open to co-applications with international collaborators.
- Prizes are of questionable value in motivating technology development. Recognition of innovation is important, though.
- Prizes are an incentive that might favor bigger players and therefore suppress the most innovative approaches.

14. Please comment on the overall strengths and weakness of the Hydrogen and Fuel Cells Program and its portfolio of projects. Please provide strengths and weaknesses for each subprogram as appropriate. On which technology areas should the Hydrogen and Fuel Cells Program put more or less focus for future activities?

Comments:

- The concept of seedling projects seems to work quite well in allowing many concepts to be investigated. On a similar note, one strength compared to European funding is that the Program selects several projects per FOA, whereas the European Union typically selects only one. This has the advantage of not "pre-selecting" the winning technology and instead letting the go/no-go criteria do the down-selecting.
- The interagency activities section is an excellent part of the agenda that allows attendees to see the fruits of all the technical work being done. Applications of hardware and additional technical needs are highlighted in this section, further informing the stakeholders.
- H2@Scale is one of the more key aspects because of the global view of hydrogen production. Advanced manufacturing is also key; as we begin to see commercial growth in stacks and applications (FCEVs) this is a key aspect of adoption.
- The increased focus on MDV and HDV fuel cell applications is a Program strength and will be critically important in advancing adoption in these sectors. Particularly key is the Fuel Cell R&D subprogram's work to develop lower-cost (and lower-PGM) fuel cells able to meet the higher power and durability requirements of applications beyond LDVs. Shifting more Program resources toward R&D in these other sectors (MDVs, HDVs, non-road, rail, ports, etc.) with the goal of advancing adoption could also complement growth in battery electric vehicle adoption happening in the LDV sector.
- Many projects and programs do a good job of integrating computational modeling with experimental work.
- The Program is very strong and well managed overall.
- The Program is strong in basic and applied R&D concerning PGM-free catalysts for PEM-based technologies and storage tank R&D. The Program is also strong in analysis-guided target-setting and systems and cost analysis. More emphasis could be put on the Hydrogen Infrastructure R&D subprogram

(e.g., the possibility and impact of hydrogen admixing in natural gas grids), the Technology Acceleration subprogram, and the Safety, Codes and Standards subprogram. Much technology is already available, although not yet perfect. In addition to new technology, optimization through practical experience can also lead to improvement and cost reduction. Furthermore, cost reduction will have to be achieved to a large extent by scaling up (system size and economy of scale). The longer implementation is delayed, the longer it takes before this potential can be used. The Systems Analysis subprogram could focus more on (energy) transition analysis.

- The merging of manufacturing R&D with infrastructure R&D diluted its impact. The Program should build more activities under manufacturing. There is significant need for fuel cell manufacturing, from which results can be applied to electrolysis and electrochemical compression. Quality control R&D requires a good deal of scientific understanding and is a great area for international collaboration. H2@Scale and the HydroGEN consortium are coming across as very strong, especially around electrolysis. Other means for hydrogen production seem secondary in the Program and should be reconsidered to either reduce or increase the intensity of activities. The Safety, Codes and Standards subprogram is strong and would also be conducive to strong international collaborations. The FC-PAD and ElectroCat consortia seem out of phase with industry needs. The relevance to current needs is not clear. The value for future needs is clear, but the intensity of effort in those directions should be reframed.
- The most important strength of this Program is its cumulative memory. The Program must protect that resource and maintain important research fields, even if they do not look very promising in the near future. So far, this Program has been very successful at doing so. One of the biggest weaknesses is lack of adherence to comparable measurable parameters. For example, in the case of hydrogen storage materials, the total energy (well to power and back to well) must be calculated for each material—the full life cycle. Without that, it is impossible to make any kind of comparison. Another example is found in ElectroCat, as not all use the same ASTs and testing conditions; in one specific case, a record in activity was presented, but it was measured at temperature and pressure more elevated than the standard set by the FCTO.
- The Program is very good at developing project portfolios that attempt to address known challenges from a variety of angles, thereby increasing the chance of success. However, it may be time to re-evaluate the structure and framework of the goals themselves. The current targets may need to remain as ultimate goals, but targets that are designed along a transition period may help accelerate deployment of technologies in the short term. There is a risk that the pursuit of longer-term goals may inhibit the pursuit of incremental improvements that could increase near-term technology deployments. Simply put, the FCEV and hydrogen community needs near-term proof of its value in the commercial customer market, and the current targets may be too restrictive to enable a near-term impact on deployment.
- Program strengths include excellent program management, major advances in materials research and in technology development, and interagency activities. AMR is a model activity for promoting communication, stakeholder engagement, review, and more. Program weaknesses include a lack of quantitative metrics for safety and a lack of a high-level champion to increase funding for the programs. In addition, many activities are centered around national laboratories that are difficult to collaborate with and that limit information-sharing.
- The Program seems well balanced. A significant strength is the safety, codes and standards work and the technoeconomic analysis performed. Some activities with a very low technological maturity could be deprioritized or assessed more critically if they are not evolving according to the Program's objectives.
- The only weakness is the apparently decreased effort in hydrogen station technology validation. Perhaps on-board hydrogen storage could be beefed up, and paths/off-ramps for technology transfer could be strengthened. The Program should focus on the end cost of a product in the early research stage and how research directions affect the projected cost of a product. The Program could also set up an online system with cost reduction targets, energy efficiency targets, and durability targets and how the targets could best

be achieved to attract companies and industries to take over once an R&D project reaches completion. The results of the R&D should be applied to save time and money.
- In the poster session, many projects that started at the beginning of 2019 were presented. These projects do not have results at that stage, so it is not really helpful to present them.
- The Program is well balanced. Suggestions include more focus on the maritime and rail domain, as well as heavy-duty transport.
- The Office of Energy Efficiency and Renewable Energy may not be the right place for Hydrogen Infrastructure R&D. Perhaps there is a more appropriate place within the overall funding landscape.

15. Do you have any other comments or suggestions to improve the overall effectiveness of the Hydrogen and Fuel Cells Program or any of its specific subprograms?

Comments:

- The overall effectiveness of the Program is excellent. It is clearly one of the best R&D programs on hydrogen in the world.
- The AMR process, as it is, is plenty effective. The Program might consider holding a series of virtual AMRs that address H2@Scale cost reduction, energy efficiency, durability targets, and technology transfer targets as a result of the early-stage R&D. These sessions should discuss what needs to be done to continue achieving the targets and the impacts of not meeting the targets. Perhaps we can have virtual AMRs that explain the cost of meeting and not meeting energy targets. It would also be good to receive training on how to use the results of early-stage R&D. This may seem like a naive suggestion, but many of us do not work in research but do read about research and want to benefit from the research.
- Overall, the work that DOE is completing is, at the end of the day, invaluable to this community. While some of the framework may be due for a refresh, it is important to acknowledge that so many of the projects completed by DOE have had a role in launching the first FCEV market in the United States. DOE should not think of the current state of FCEVs and their deployment as taking place "eventually" or "slowly over the next xx years"; this simply will not work in the real-world political and retail marketplace.
- Suggestions include developing methods to increase collaboration, building on completed projects, and determining how to advertise success and move technology from the initial stages to deployment. The best way to do this is not obvious, but opportunities to discuss results (such as at the poster session) seem to go a long way toward building connections.
- The willingness to share R&D advancements and progress is great for overall commercialization. It would be even more beneficial to see other countries offer similar opportunities for presentation of their R&D activities and accomplishments.
- The Program should investigate further collaboration opportunities with the Bioenergy Technologies Office, including fertilizer from renewable hydrogen, farm fuels from renewable hydrogen, and oxy-combustion of biomass/waste using the oxygen co-product from large-scale electrolysis.
- The Program could benefit from bringing on board outside researchers or managers to inject fresh ideas. An NSF-style 1- to 2-year sabbatical from academia or industry might be introduced.

Attendee List: 2019 Hydrogen and Fuel Cells Program

Last Name	First Name	Organization
Abbasi	Reza	University of Delaware
Abdul Jabbar	M. Hussain	Nissan Technical Centre North America
Abe	Tadashi	The Association of Hydrogen Supply and Utilization Technology (HySUT)
Abernathy	Harry	National Energy Technology Laboratory
Adams	Jesse	U.S. Department of Energy
Adhikari	Santosh	Rensselaer Polytechnic Institute
Afzal	Kareem	PDC Machines, Inc.
Ahluwalia	Rajesh	Argonne National Laboratory
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Allendorf	Mark	Sandia National Laboratories
Almeida	Steve	Aris Energy Solutions
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Basu	Soumendra	Boston University
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Baturina	Olga	U.S. Naval Research Laboratory
Beckner	Matthew	General Motors
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Bergeson	William	Federal Highway Administration
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Bhambri	Akshi	Shell New Fuels
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Bishop	Sean	Redox Power Systems
Blackburn	Bryan	Redox Power Systems
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Bowden	Mark	Pacific Northwest National Laboratory
Boyce	Kenneth	UL
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Brown	Patrick	Southern California Gas Company
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Chan	Thomas	Southern California Gas Company
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Chen	Mengjie	University at Buffalo
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Danilovic	Nemanja	Lawrence Berkeley National Laboratory
Dattelbaum	Andrew	Los Alamos National Laboratory
Davenport	Timothy	United Technologies Research Center
Davies	Peter	Garrett Advancing Motion
De Castro	Emory	Advent Technologies, Inc.
De Guire	Mark	Case Western Reserve University
De Valladares	Mary Rose	International Energy Agency, Hydrogen
Delay	Tom	Cimarron Composites
Deng	Chenxin	Case Western Reserve University
DeSantis	Daniel	Strategic Analysis, Inc.
Deshpande	Salil	The Building People
Deutsch	Todd	National Renewable Energy Laboratory
Devlin	Pete	U.S. Department of Energy
Ding	Dong	Idaho National Laboratory
Ding	Hanping	Idaho National Laboratory
Dinh	Huyen	National Renewable Energy Laboratory
Dirschka	Eric	NASA
Dobbins	Tabbetha	Rowan University
Dogdibegovic	Emir	Lawrence Berkeley National Laboratory
Dolan	Gregory	Methanol Institute
Dolci	Francesco	European Commission Joint Research Centre
Dorda	Andreas	Federal Ministry for Transport, Innovation and Technology
Dornheim	Martin	Helmholtz-Zentrum Geesthacht
Dorobantu	Mihai	Eaton Vehicle Group
Dosanjh	Bal	Ceres Power
Doshi	Jayesh	eSpin
Draper	Christopher	Power Innovations
Duan	Chuancheng	Colorado School of Mines
Duh	Steve	Toyota Motor North America, Research and Development (R&D)
Edwards	David	Air Liquide
Ehrhart	Brian	Sandia National Laboratories
Eisman	Glenn	Eisman Technology Consultants, LLC

Last Name	First Name	Organization
Elbaz	Lior	Bar-Ilan University
Elgowainy	Amgad	Argonne National Laboratory
El-kharouf	Ahmad	University of Birmingham
Elrick	Bill	California Fuel Cell Partnership
Emmons	Sara	U.S. Department of Energy (Contractor)
Ertekin	Elif	University of Illinois at Urbana–Champaign
Escribano	Sylvie	Commissariat à l'énergie atomique et aux énergies alternatives (CEA, French Atomic Energy Commission)
Ettie	Gordon	Energy Scienomic, Inc.
Eudy	Leslie	National Renewable Energy Laboratory
Ewan	Mitch	Hawaii Natural Energy Institute
Fairlie	Matthew	Fairfield Group Inc
Farese	David	Air Products and Chemicals, Inc.
Feng	Zhili	Oak Ridge National Laboratory
Fennis	Maria	High yield Energy Technologies (HyET) Hydrogen
Flood	Gary	GSF Consulting LLC
Flotkoetter	Robert	Nissan North America
Flowers	Daniel	Lawrence Livermore National Laboratory
Fontaine	Joseph	U.S. Department of the Navy
Forrester	Nicole	Commonwealth Scientific and Industrial Research Organisation (CSIRO)
Foster	Lee	Cimarron Composites
Fox	Elise	Savannah River National Laboratory
Fox	Melissa	Los Alamos National Laboratory
Francis	Martin	Arcelormittal
Frank	Ed	Argonne National Laboratory
Fritz	Katrina	California Stationary Fuel Cell Collaborative/ National Fuel Cell Research Center (NFCRC)
Frois	Bernard	Commissariat à l'énergie atomique et aux énergies alternatives (CEA, French Atomic Energy Commission)
Frost	Mary	Duke Energy
Furukawa	Takatoshi	Hino Motors Manufacturing U.S.A., Inc.
Furusawa	Koichiro	Honda R&D Co., Ltd.
Gagliano	Joe	United Hydrogen
Gaillard	Nicolas	University of Hawaii

Last Name	First Name	Organization
Galbach	Phillip	FedEx Express
Gambone	Livio	Nikola Motor Company
Ganesan	Prabhu	Greenway Energy, LLC
Gao	Puxian	University of Connecticut
Garche	Jürgen	Ulm University
Garcia-Sanz	Mario	Advanced Research Projects Agency–Energy (ARPA-E)
Gardiner	Monterey	BMW Group
Garfunkel	Eric	Rutgers University
Garland	Nancy	U.S. Department of Energy
Garsany	Yannick	EXCET, Inc./ U.S. Naval Research Laboratory
Garvin	Joshua	U.S. Navy, Naval Surface Warfare Center, Carderock Division
Ge	Ben	China University of Mining and Technology, Beijing
Gearhart	Chris	National Renewable Energy Laboratory
Gebert	Matthias	Solvay Specialty Polymers
Geiman	Laura	W. L. Gore & Associates, Inc.
Gennett	Thomas	National Renewable Energy Laboratory
Gervasio	Dominic	University of Arizona
Ghezel-Ayagh	Hossein	FuelCell Energy, Inc.
Ghosh	Chuni	Fuceltech Inc.
Ghosh	Sujit	U.S. Department of Transportation, Maritime Administration
Gibbons	William	University of Maryland
Gilmore	Dennis	RTI International
Girard	François	National Research Council Canada
Givens	Jesse	U.S. Army
Glover	Austin	Sandia National Laboratories
Goodarzi	Gordon Abas	US Hybrid Corporation
Goodbody	Leslie	California Air Resources Board
Gopalan	Srikanth	Boston University
Gordon	Bryan	Ivys Energy Solutions
Gore	Colin	Redox Power Systems
Gorensek	Maximilian	Savannah River National Laboratory
Gorte	Raymond	University of Pennsylvania
Goto	Risei	Sumitomo Corporation of Americas

Last Name	First Name	Organization
Graetz	Jason	HRL Laboratories
Graff	Michelle	U.S. Environmental Protection Agency
Grassilli	Leo	Office of Naval Research (Consultant)
Green	Johney	National Renewable Energy Laboratory
Green	Malcolm	Taconic
Green	Zachary	Giner, Inc.
Greenbaum	Elias	GTA, Inc.
Greenblatt	Jeffery	Emerging Futures LLC/Lawrence Berkeley National Laboratory
Greenfield	Carl	International Technology and Trade Associates, Inc.
Gregori	Matt	Sempra Utilities
Grein	Alfred	U.S. Army, Combat Capabilities Development Command, Ground Vehicle Systems Center
Groos	Ulf	Fraunhofer Institute for Solar Energy Systems ISE
Gross	Thomas	Energy Planning and Solutions
Grot	Stephen	Ion Power
Groth	Katrina	University of Maryland
Grubel	Katarzyna	Pacific Northwest National Laboratory
Gryniewicz	Anthony	U.S. Department of Energy, Fuel Cell Technologies Office
Gu	George (Zhijun)	Horizon Fuel Cell
Gu	Taoli	Xergy Inc
Guan	Bo	West Virginia University
Gumeci	Cenk	Nissan Technical Center North America
Guo	Jinghua	Lawrence Berkeley National Laboratory
Gupta	Ram	Virginia Commonwealth University
Ha	Mai-Anh	National Renewable Energy Laboratory
Habibzadeh	Bahman	U.S. Department of Energy
Hacker	Viktor	Graz University of Technology
Hackett	Gregory	National Energy Technology Laboratory
Hahn	Michael	U.S. Department of Energy, Fuel Cell Technologies Office
Hamann	Thomas	Michigan State University
Hamdan	Monjid	Giner, Inc.
Hamilton	Jennifer	California Fuel Cell Partnership
Han	Jeongwoo	ExxonMobil Research and Engineering Company

Last Name	First Name	Organization
Han	Jonghee	Korea Institute of Science and Technology
Hancu	Dan	U.S. Department of Energy
Hanlin	Jason	Center for Transportation and the Environment (CTE)
Hardy	John	Pacific Northwest National Laboratory
Harris	Aaron	Air Liquide
Harris	Alexander	Brookhaven National Laboratory
Harris	Kevin	Hexagon
Harrison	Kevin	National Renewable Energy Laboratory
Harrison	William	NanoSonic Inc.
Hartmann	Johanna	Redox Power Systems
Hattrick-Simpers	Jason	National Institute of Standards and Technology
Haug	Andrew	3M Company
Hayasaka	Maki	New Energy and Industrial Technology Development Organization
Hays	Thomas	U.S. Navy, Naval Surface Warfare Center, Carderock Division
He	Cheng	Washington University in St. Louis
He	Yanghua	University of Buffalo
Headley	Alexander	Sandia National Laboratories
Hecht	Ethan	Sandia National Laboratories
Hellstrom	Sondra	Robert Bosch LLC
Heo	Su Jeong	National Renewable Energy Laboratory
Heo	Tae Wook	Lawrence Livermore National Laboratory
Herbert	Thorsten	NOW GmbH (National Organization Hydrogen and Fuel Cell Technology)
Heske	Clemens	University of Nevada, Las Vegas
Hester	Dave	Shell New Fuels
Hibbs	Michael	Sandia National Laboratories
Hickey	Darren	Cummins Inc.
Hickner	Michael	Pennsylvania State University
Hicks	Mike	H2PowerTech
Hill	Laura	U.S. Department of Energy
Hillebrand	Don	Argonne National Laboratory
Hinkley	James	Victoria University of Wellington
Hirai	Shuichiro	Tokyo Tech

Last Name	First Name	Organization
Hiraiwa	Chihiro	Sumitomo Electric
Hirata	Yuko	Daiwa Institute of Research Ltd.
Ho	Donna	U.S. Department of Energy
Hoefelmann	Ole	Air Liquide
Hofmann	Karsten	Continental Automotive GmbH
Holby	Edward	Los Alamos National Laboratory
Holladay	Jamie	Pacific Northwest National Laboratory
Holzmann	Markus	Greenerity GmbH
Hong	Bo Ki	Hyundai Motor Company
Hopkins	Owen	Hexagon
Horita	Teruhisa	National Institute of Advanced Industrial Science and Technology (AIST)
Hornauer	Stefan	ElringKlinger AG
Houchins	Cassidy	Strategic Analysis, Inc.
Hovsapian	Rob	National Renewable Energy Laboratory
Howell	Thomas	Air Force Research Laboratory
Hu	Boxun	University of Connecticut
Hu	Keda	University of Delaware
Huajian	Chang	State Power Investment Corporation Research Institute, China
Huang	Jin	University of California, Los Angeles
Huang	Kevin	University of South Carolina
Huang	Yi-Lin	University of Maryland
Huang	Yu	University of California, Los Angeles
Huezo	Romulo	GB-Technica
Hulvey	Zeric	Oak Ridge Institute for Science and Education (ORISE)/Fuel Cell Technologies Office
Hunter	Brian	U.S. Department of Energy
Hunter	Chad	National Renewable Energy Laboratory
Hurst	Katherine	National Renewable Energy Laboratory
Hussey	Daniel	National Institute of Standards and Technology
Huya-Kouadio	Jennie	Strategic Analysis, Inc.
Huynh	Greg	Los Angeles Department of Water and Power
Hwang	Robert	Sandia National Laboratories
Hwang	Shinjae	Rutgers University
Igarashi	Hiroshi	N.E. CHEMCAT Corporation

Last Name	First Name	Organization
Ihnfeldt	Robin	General Engineering & Research, LLC
Iiyama	Akihiro	University of Yamanashi
Ikeda	Tetsufumi	The Association of Hydrogen Supply and Utilization Technology (HySUT)
Ikehata	Yuta	Toyota Motor North America
Im	Se Joon	Hyundai Motor Company
Impullitti	Joseph	South Coast Air Quality Management District
Inci	Bora	The Chemours Company
Ingram	Brian	Argonne National Laboratory
Ireland	Daniel	Solvay Specialty Polymers
Irvin	Nick	Southern Company
Irwin	Levi	ManTech/U.S. Department of Energy
Isaac	Raphael	University of California, Davis
Ishii	Chiaki	Air Liquide
Ishikawa	Katsuya	KAWASAKI Heavy Industries, Ltd.
Jacobson	David	National Institute of Standards and Technology
Jadun	Paige	National Renewable Energy Laboratory
Jakupca	Ian	NASA
James	Brian	Strategic Analysis, Inc.
James	Will	Savannah River National Laboratory
Jang	Ji-Hoon	Hyundai Motors
Jankovic	Jasna	University of Connecticut
Jansen	Daniel	Robert Bosch GmbH
Jaramillo	Thomas	Stanford University
Jaworski	Casey	Tanaka Kikinzoku International
Jeffers	Matthew	National Renewable Energy Laboratory
Jelen	Deborah	Electricore, Inc.
Jenks	Cynthia	Argonne National Laboratory
Jensen	Mark	Phillips 66
Jesionowski	Gary	KeyLogic Systems
Jia	Hongfei	Toyota Motor North America
Jia	Qingying	Northeastern University
Johnson	Terry	Sandia National Laboratories
Jorgensen	Scott	Hyrax Intercontinental LLC
Jorion	Alexandre	EDF Renewables

Last Name	First Name	Organization
Joseck	Fred	U.S. Department of Energy
Jung	Chiyoung	Korea Institute of Energy Research
Jung	Juhea	Hyundai Motor Company
Kalapos	Tom	National Energy Technology Laboratory, Leidos Research Support Team
Kalimuthu	Vijaya Sankar	Technion–Israel Institute of Technology
Kamguia Simeu	Severin	Argonne National Laboratory
Kanaoka	Nagayuki	Honda R&D Americas, Inc.
Kanesaka	Hiroyuki	Fuel Cell Cutting-Edge Research Center Technology Research Association
Karabacak	Tansel	University of Arkansas at Little Rock
Karkamkar	Abhijeet	Pacific Northwest National Laboratory
Kast	James	Toyota
Katsube	Yasuyuki	Sumitomo Corporation of Americas/Business Development Group
Kauffman	Douglas	National Energy Technology Laboratory
Keeler	Aimie	Anglo American
Keller	Jay	Zero Carbon Energy Solutions
Kent	Ronald	Southern California Gas Company/Sempra Utilities
Khalil	John	United Technologies Research Center
Kidner	Neil	Nexceris LLC
Kim	Hyoung-Juhn	Korea Institute of Science and Technology
Kim	Kiyoung	Ilsung Machinery Co. Ltd.
Kim	Sung Chun	Cambi Korea
Kim	Tae-Young	Korea Institute of Energy Research
Kim	Yu Seung	Los Alamos National Laboratory
Kimball	Brett	Automated Dynamics, Trelleborg
Kimble	Michael	Skyhaven Systems, LLC
Kimura	Koichi	Honda R&D Co., Ltd., Automobile R&D Center
Kimura	Tatsusaburo	Sumitomo Corporation
King	Laurie	Stanford University
Kirby	Brent	Pacific Northwest National Laboratory
Kishimoto	Takeaki	Nisshinbo Holdings Inc.
Klebanoff	Leonard	Sandia National Laboratories
Kleen	Greg	U.S. Department of Energy
Kleinbaum	Sarah	U.S. Department of Energy

Last Name	First Name	Organization
Kline	Gregory	Rensselaer Polytechnic Institute
Knights	Shanna	Ballard Power Systems
Ko	Edward	T2M Global
Kobayashi	Yohei	Honda Engineering Co., Ltd.
Koeppel	Brian	Pacific Northwest National Laboratory
Komatsu	Shinji	DENSO International America, Inc.
Komiyama	Tomonari	JX Nippon Oil
Kondo	Shinji	Sumitomo Corporation
Kongkanand	Anusorn	General Motors
Konzal	Pawel	Chevron
Kopasz	John	Argonne National Laboratory
Koski	Brent	United Hydrogen
Kramer	David	Physics Today
Krause	Ted	Argonne National Laboratory
Kreller	Cortney	Los Alamos National Laboratory
Krishnaswami	Arjun	Natural Resources Defense Council
Kumar	Ashok	Cummins Inc.
Kumar	Rajesh	University of Connecticut
Kumaragru	Swami	General Motors
Kuroki	Rentaro	Toyota Motor North America Inc.
Kurosaki	Daisuke	Chiyoda Corporation
Kurtz	Jennifer	National Renewable Energy Laboratory
Kusoglu	Ahmet	Lawrence Berkeley National Laboratory
Kusumoto	Teruaki	Toyota
LaFleur	Chris	Sandia National Laboratories
Lahjibi	Asma	ENGIE
Lai	Ming-Chia	Wayne State University
Lake	Jeffrey	Doosan Fuel Cells America
Lalli	Jennifer	NanoSonic
LaManna	Jacob	National Institute of Standards and Technology
Lane	Erin	Cascade Associates
Langhorst	Lisa	Carnegie Mellon University
Lany	Stephan	National Renewable Energy Laboratory
Lara-Curzio	Edgar	Oak Ridge National Laboratory
Larsen	Ross	National Renewable Energy Laboratory

Last Name	First Name	Organization
Lawson	Seth	National Energy Technology Laboratory
Le Goff	Soizic	ENGIE
Lee	Byung Gwon	Korea Institute of Science and Technology
Lee	Mathias	Kentec Enviro Solutions
Lee	Samuel	Kentec Enviro Solutions
Lee	Sangwoo	Rensselaer Polytechnic Institute
Lee	Seyeong	Hyundai Motor Company
Lee	Shiwoo	National Energy Technology Laboratory/Leidos
Lee	Won-Yong	Korea Institute of Energy Research
Lee	Yueh-Lin	National Energy Technology Laboratory
Lee	Yunsu	Hyundai Motors
Lehner	William	Independence Hydrogen
Lei	Yinkai	National Energy Technology Laboratory
Lei	Ze	China University of Mining and Technology, Beijing
Leick	Noemi	National Renewable Energy Laboratory
Leighton	Dan	National Renewable Energy Laboratory
Leighton	DeLisa	IGX Group
Leighty	William	The Leighty Foundation
Leshilo	Julian	Department of Science and Technology (DST), South Africa
Levesque-Tremblay	Gabriel	American Institute of Chemical Engineers
Levie	Daniel	National Renewable Energy Laboratory
Li	Dongsheng	Advanced Manufacturing LLC
Li	Jimmy	National Institute of Clean and Low-Carbon Energy (NICE) America Research Inc.
Li	Jun	Kansas State University
Li	Wei	The University of Texas at Austin
Li	Wen	Tianneng Power International
Li	Wenyuan	West Virginia University
Li	Xianglin	University of Kansas
Li	Yue	Redox Power Systems
Lim	Tae Hoon	Korea Institute of Science and Technology
Lipp	Ludwig	T2M Global
Litster	Shawn	Carnegie Mellon University
Litzelman	Scott	Advanced Research Projects Agency–Energy
Liu	Meilin	Georgia Technology Institute

Last Name	First Name	Organization
Liu	Di-Jia	Argonne National Laboratory
Liu	Gao	Lawrence Berkeley National Laboratory
Liu	Hong	Oregon State University
Liu	Hongtan	University of Miami
Liu	Jian	National Energy Technology Laboratory
Liu	Xingbo	West Virginia University
Liu	Zeyan	University of California, Los Angeles
Liu	Zheng	Sinocat
Liu	Zhien	National Institute of Clean and Low-Carbon Energy (NICE) America Research Inc.
Lomax	Frank	Headwaters Solutions LLC
Long	Brian	Fuel Cell Enabling Technologies, Inc.
Long	Jeffrey	Lawrence Berkeley National Laboratory
Longstreth	Benjamin	Natural Resources Defense Council
Louderback	Benjamin	Idaho National Laboratory
Lubawy	Andrea	Toyota
Ludlow	Daryl	Ludlow Electrochemical Hardware
Lundberg	Wayne	KeyLogic Systems
Ly	Vy	Naval Surface Warfare Center Philadelphia Division (NSWCPD)
Lyubovsky	Maxim	U.S. Department of Energy
Ma	Liang	West Virginia University
Ma	Zhiwen	National Renewable Energy Laboratory
Mackay	Jocelyn	National Energy Technology Laboratory
Madden	Diane	National Energy Technology Laboratory
Maes	Miguel	NASA, White Sands Test Facility
Makhloufi	Camel	ENGIE
Maloney	Daniel	National Energy Technology Laboratory
Mancuso	Jim	Westport Power, Inc.
Maness	Pin-Ching	National Renewable Energy Laboratory
Manusco	Jim	Westport Power, Inc.
Marcinkoski	Jason	U.S. Department of Energy
Mardle	Peter	University of Birmingham
Maric	Radenka	University of Connecticut
Marina	Olga	Pacific Northwest National Laboratory
Markovich	Steven	National Energy Technology Laboratory

Last Name	First Name	Organization
Martin	Josh	National Renewable Energy Laboratory
Martin	Thomas	Greenerity GmbH
Martinez	Andrew	California Air Resources Board
Maruta	Akiteru	Technova Inc.
Marxen	Sara	CSA Group
Maserumule	Rebecca	Department of Science and Technology (DST), South Africa
Mason	Chad	Advanced Ionics
Masten	David	General Motors
Mastropasqua	Luca	University of California, Irvine
Mathison	Steve	Honda R&D Americas, Inc.
Mathuraiveeran	Thangaraj	Cummins Inc.
Matter	Paul	pH Matter, LLC
Matzger	Adam	University of Michigan
Mauger	Scott	National Renewable Energy Laboratory
May	Camille	Phillips 66
McClory	Matt	Toyota Motor North America
McCoy	Britney	U.S. Environmental Protection Agency
McDaniel	Anthony	Sandia National Laboratories
McDougle	Stephen	NASA, White Sands Test Facility
McIntosh	Steven	Lehigh University
McNamara	Joy	Savannah River National Laboratory
McQueen	Shawna	U.S. Department of Energy, Fuel Cell Technologies Office
McShane	William	U.S. Department of Energy, Water Power Technology Office
McWhorter	Scott	Savannah River National Laboratory
Medler	Kevin	Kentec Enviro Solutions
Meekins	Ben	University of South Carolina
Meeks	Noah	Southern Company Services, Inc.
Mehta	Darius	Garrett Advancing Motion
Melaina	Marc	Great Wall Motors
Mench	Matthew	University of Tennessee
Menon	Nalini	Sandia National Laboratories
Mermelstein	Joshua	Idaho National Laboratory
Mi	Zetian	University of Michigan, Ann Arbor

Last Name	First Name	Organization
Miftakhov	Valery	ZeroAvia, Inc.
Mikulin	John	U.S. Environmental Protection Agency
Miller	David	National Energy Technology Laboratory
Miller	Eric	U.S. Department of Energy
Miller	James	Argonne National Laboratory
Milliken	JoAnn	Rose Institute for Strategic Energy
Minh	Nguyen	University of California, San Diego
Minhas	Sunny	Intertek
Mittelsteadt	Cortney	Giner, Inc.
Miura	Shinichi	KOBELCO
Mizusaki	Kimiharu	Honda R&D Co., Ltd.
Mjwara	Phil	Department of Science and Technology (DST), South Africa
Modestino	Miguel	New York University
Moen	Christopher	Sandia National Laboratories
Molinaro	Dave	Hawaii Center for Advanced Transportation Technologies
Monroe	Mark	Microsoft
More	Karren	Oak Ridge National Laboratory
Moreland	Gregory	Oak Ridge National Laboratory (contract with CSRA)
Morgan	Brad	Tetramer Technologies, LLC
Morris	William	NuMat Technologies
Mosleh	Mohsen	Howard University
Mount	Robert	Power Innovations
Muhich	Christopher	Arizona State University
Mukerjee	Sanjeev	Northeastern University
Mukundan	Rangachary	Los Alamos National Laboratory
Muna	Alice	Sandia National Laboratories
Mundhwa	Mayur	Colorado School of Mines
Munnings	Christopher	Commonwealth Scientific and Industrial Research Organisation (CSIRO)
Munster	Jason	Shell New Fuels
Muromoto	Nobuyoshi	Honda Engineering Co., Ltd.
Murphy	Brian	Strategic Analysis, Inc.
Murthi	Vivek	Nikola Motor Company

Last Name	First Name	Organization
Musgrave	Charles	University of Colorado
Mustain	William	University of South Carolina
Myers	Charles	CSRA Inc.
Myers	Debbie	Argonne National Laboratory
Na	Beom-Tak	National Energy Technology Laboratory
Nagai	Tomoyuki	Toyota Motor North America
Naganuma	Yoshiaki	Toyota Motor North America, Research and Development (R&D)
Nagasawa	Kazunori	National Renewable Energy Laboratory
Nakamura	Hiroshi	Fuji Seiki Co., Ltd.
Natelson	Robert	U.S. Department of Energy, Bioenergy Technologies Office (Allegheny Science & Technology contractor)
Nawoj	Kristen	U.S. Department of Energy
Nealer	Rachael	U.S. Department of Energy
Nelson	Amy	AVL Fuel Cell Canada
Neyerlin	Kenneth	National Renewable Energy Laboratory
Nguyen	Nha	U.S. Department of Transportation
Nguyen	Tien	None
Nicholas	Jason	Michigan State University
Nicollet	Clement	Massachusetts Institute of Technology
Nielander	Adam	Stanford University
Nielsen	Ryan	Automated Dynamics, Trelleborg
Nishimura	Shin	Kyushu University
Novachek	Frank	Xcel Energy
Numata	Koichi	Toyota Motor Corporation
O'Brien	Christopher	Ivys Energy Solutions
OBrien	James	Idaho National Laboratory
Ocampo	Minette	pH Matter LLC
Odgaard	Madeleine	EWII Group
Oesterreich	Robert	Air Liquide
Ogitsu	Tadashi	Lawrence Livermore National Laboratory
O'Hayre	Ryan	Colorado School of Mines
Ohnuma	Akira	Toyota Boshoku Corporation
Okamoto	Mineharu	Iwatani Corporation of America
Olson	Gregory	CSRA Inc.

Last Name	First Name	Organization
O'Neil	Gregory	U.S. Department of Energy, National Energy Technology Laboratory
Onorato	Shaun	National Renewable Energy Laboratory
Osada	Norikazu	Toshiba Energy Systems & Solutions Corporation
Osbourne	Mitchell	Shell New Fuels
O'Shaughnessy	W. Shannan	GVD Corporation
Osserman	Stan	Hawaii Center for Advanced Transportation Technologies
Otgonbaatar	Uuganbayar	Exelon
Ott	Kevin	Los Alamos National Laboratory (Retired)
Paczkowski	Ben	U.S. Army Ground Vehicle Systems Center
Padgett	Elliot	Cornell University
Pal	Uday	Boston University
Palmqvist	Anders	Chalmers University of Technology
Pan	Keji	Redox Power Systems
Pant	Lalit	Lawrence Berkeley National Laboratory
Panwar	Mayank	Idaho National Laboratory
Parilla	Philip	National Renewable Energy Laboratory
Park	Andrew	The Chemours Company
Park	Gu-Gon	Korea Institute of Energy Research
Park	Hyun Seo	Korea Institute of Science and Technology
Park	Jaehyung	Argonne National Laboratory
Park	James	Sandia National Laboratories
Park	Jun-Young	Sejong University
Park	MinGee	Ilsung Machinery Co., Ltd.
Park	Seokhee	Korea Institute of Energy Research
Park	Youngchul	Hyundai Mobis
Parkan	John Michael	Providence Entertainment
Parker	Eric	U.S. Department of Energy (Contractor)
Parks	George	FuelScience LLC
Parvathikar	Sameer	RTI International
Parysek	Karen	Linde, PLC
Patel	Pinakin	T2M Global
Patel	Tapan	U.S. Army Corps of Engineers Construction Engineering Research Laboratory
Patil	Kailash	Giner, Inc.

Last Name	First Name	Organization
Patterson	Mark	Southern Research Institute
Penev	Michael	National Renewable Energy Laboratory
Peng	Jiayu	Massachusetts Institute of Technology
Peng	Suping	China University of Mining and Technology, Beijing
Peng	Zhenmeng	The University of Akron
Perry	Mike	United Technologies Research Center
Peters	Michael	National Renewable Energy Laboratory
Peterson	David	U.S. Department of Energy, Fuel Cell Technologies Office
Petitpas	Guillaume	Air Liquide
Petri	Aaron	U.S. Army Engineer Research and Development Center
Pez	Guido	Air Products (Retired)
Pietras	John	Saint-Gobain
Pietraß	Tanja	Los Alamos National Laboratory
Pintauro	Peter	Vanderbilt University
Pitts	Lawrence	Plug Power Inc.
Pivovar	Bryan	National Renewable Energy Laboratory
Polevaya	Olga	Nuvera Fuel Cells
Pomerantz	Michael	Bennett Pump Company
Popovich	Neil	National Renewable Energy Laboratory
Post	Matthew	National Renewable Energy Laboratory
Potyrailo	Radislav	GE Global Research
Prabhakaran	Venkateshkumar	Pacific Northwest National Laboratory
Prendergast	David	Lawrence Berkeley National Laboratory
Qiu	Yun	Enviro & Production Solutions
Quackenbush	Karen	Fuel Cell & Hydrogen Energy Association
Quong	Spencer	Quality Assurance International
Ramani	Vijay	Washington University in St. Louis
Rambach	Glenn	Third Orbit Power Systems, Inc.
Ramsden	Todd	National Renewable Energy Laboratory
Randolph	Katie	U.S. Department of Energy
Reddi	Krishna	Argonne National Laboratory
Reed	Jeffrey G.	University of California, Irvine
Reeve	Alison	National Hydrogen Strategy Taskforce
Regmi	Yagya	Lawrence Berkeley National Laboratory

Last Name	First Name	Organization
Reshetenko	Tatyana	Hawaii Natural Energy Institute
Reznicek	Evan	Colorado School of Mines
Rice	Brian	University of Dayton Research Institute
Ricketson	Sean	U.S. Department of Transportation/Federal Transit Administration
Rinebold	Joel	Connecticut Center for Advanced Technology Inc.
Rittgers	Andrew	U.S. Department of Energy
Rivkin	Carl	National Renewable Energy Laboratory
Rizzo	Denise	U.S. Army Futures Command Combat Capabilities Development Command Ground Vehicle Systems Center
Roberts	Daniel	Commonwealth Scientific and Industrial Research Organisation
Robertson	Denzel	Air Liquide
Robinson	Ian	University of Maryland
Rockward	Tommy	Los Alamos National Laboratory
Rohatgi	Aashish	Pacific Northwest National Laboratory
Rojas-Carbonell	Santiago	University of Delaware
Ronevich	Joseph	Sandia National Laboratories
Ross	Kenneth	Pacific Northwest National Laboratory
Roy	Robin	Next Energy US
Roychoudhury	Subir	Precision Combustion, Inc.
Ruddock	Michael	Chevron Downstream Strategy
Rufael	Tecle	Chevron Energy Technology Company
Ruiz	Antonio	Nikola Motor Company
Rupnowski	Peter	National Renewable Energy Laboratory
Rustagi	Neha	U.S. Department of Energy
Ruth	Mark	National Renewable Energy Laboratory
Ryu	Heejune	Korea Institute of Science and Technology
Saito	Nobuhiro	Honda R&D Co., Ltd.
Saitoh	Kenichiro	JX Nippon Research Institute, Ltd.
Sakurahara	Kazuo	Honda R&D Co., Ltd./5G
Salvador	Paul	Carnegie Mellon University
San Marchi	Chris	Sandia National Laboratories
Sanborn	Scott	Sandia National Laboratories
Sanders	Michael	Colorado School of Mines

Last Name	First Name	Organization
Sasakura	Masaharu	The Institute of Applied Energy
Satjaritanun	Pongsarun	University of South Carolina
Satomi	Tomohide	Fuel Cell Commercialization Conference of Japan
Sattler	Christian	German Aerospace Center
Saur	Genevieve	National Renewable Energy Laboratory
Scarpino	Michael	U.S. Department of Transportation, Volpe Center
Schlueter	Debbie	IRD Fuel Cells, LLC
Schneider	Jesse	Nikola Motor Company
Schneider	Robert	Chiyoda International Corporation
Schoentgen	Raphael	Hydrogen Advisors
Schultz	Paul	Los Angeles Department of Water and Power
Schulz	Robert	Hydro-Quebec
Schumacher	Christian	U.S. Navy
Schuster	Darlene	American Institute of Chemical Engineers
Schwenzer	Birgit	National Science Foundation
Sedoglavich	Nemanya	Shell New Fuels
Selman	Nancy	Skyre, Inc.
Senior	Constance	National Institute of Clean and Low-Carbon Energy (NICE) America Research Inc.
Serov	Alexey	Pajarito Powder, LLC
Serre-Combe	Pierre	Commissariat à l’énergie atomique et aux énergies alternatives (CEA, French Atomic Energy Commission)
Setzler	Brian	University of Delaware
Severa	Godwin	Hawaii Natural Energy Institute, University of Hawaii
Shade	Norm	ACI Services Inc.
Shah	Yatish	Retired
Shao	Yuyan	Pacific Northwest National Laboratory
Sharman	Jonathan	Johnson Matthey
Shi	Lin	University of Delaware
Shibutani	Tomohide	Honda Engineering North America, Inc.
Shimpalee	Sirivatch	University of South Carolina
Shinde	Subhash L.	University of Notre Dame
Shindo	Atsushi	Fuji Seiki Co., Ltd.
Shreffler	Eric	Michigan Economic Development Corporation
Shrestha	Sanjay	Plug Power Inc.

Last Name	First Name	Organization
Shulda	Sarah	National Renewable Energy Laboratory
Shurland	Melissa	U.S. Department of Transportation/Federal Railroad Administration
Shutty	John	BorgWarner Inc.
Siegel	Donald	University of Michigan
Siegel	Kay Kimberly	H2Safe, LLC
Sikirica	Stephen	U.S. Department of Energy
Sim	Michelle	Southern California Gas Company
Simmons	Kevin	Pacific Northwest National Laboratory
Singh	Prabhakar	University of Connecticut
Singh	Vikalp	Air Liquide
Siriwardane	Ranjani	U.S. Department of Energy, National Energy Technology Laboratory
Smeltz	Andrew	De Nora
Smirnov	Sergei	New Mexico State University
Smith	David	Oak Ridge National Laboratory
Smith	Richard	Hydrogen Energy Center
Smith	William	Infinity Fuel Cell
Snyder	Joshua	Drexel University
Snyder	Seth	Idaho National Laboratory
Soloveichik	Grigorii	Advanced Research Projects Agency–Energy
Song	Kah Young	Kolon Industry
Song	Liang	Brookhaven National Laboratory
Song	Xueyan	West Virginia University
Sookhoo	Ryan	Hydrogenics Corporation
Sorensen	Paul	Shell New Fuels
Soto	Herie	Shell
Spendelow	Jacob	Los Alamos National Laboratory
Spinetta	Magali	Giner, Inc.
Spitzer	Kevin	U.S. Air Force
Sprik	Sam	National Renewable Energy Laboratory
Stamenkovic	Vojislav	Argonne National Laboratory
Stavila	Vitalie	Sandia National Laboratories
Stechel	Ellen	Arizona State University, LightWorks
Steinbach	Andrew	3M Company
Steiner	Myles	National Renewable Energy Laboratory

Last Name	First Name	Organization
Steiner	Nadia	University of Franche-Comté, FCLAB
Stephan	Markus	Maximator
Stetson	Ned	U.S. Department of Energy
Stevenson	Jeff	Pacific Northwest National Laboratory
Stewart	Sarah	Robert Bosch LLC
Stoffa	Joseph	U.S. Department of Energy, National Energy Technology Laboratory
Stottler	Gary	Stottler Development LLC
Straley	William	Fuji Seiki Co., Ltd.
Strange	Nicholas	National Renewable Energy Laboratory/SLAC National Accelerator Laboratory
Stringer	Steve	Los Alamos National Laboratory
Stuckey	Philip	United States Patent and Trademark Office
Sun	Pingping	Argonne National laboratory
Sun	Xiao-Guang	Oak Ridge National Laboratory
Sunderrajan	Suresh	Argonne National Laboratory
Sutherland	Ian	General Motors
Swamy	Priya	U.S. Department of Energy, Fuel Cell Technologies Office
Swanborn	Rombout	High yield Energy Technologies (HyET) Hydrogen USA
Swartz	Scott	Nexceris
Swider-Lyons	Karen	U.S. Navy, Naval Research Laboratory
Szymanski	Stephen	Nel Hydrogen
Taie	Zac	Oregon State University
Tajiri	Kazuya	Michigan Technological University
Takaishi	Hideyuki	Takaishi Industry Co., Ltd.
Tamburello	David	Savannah River National Laboratory
Tan	Li	University of Nebraska-Lincoln
Tanimura	Hiroshi	JRMA
Tao	Greg	Chemtronergy
Tavakoli Mehrabadi	Bahareh Alsadat	Carnegie Mellon University
Tchouvelev	Andrei	AVT Research Inc.
Tesfaye	Meron	University of California, Berkeley
Tessier	Pascal	Air Liquide
Tew	David	Advanced Research Projects Agency–Energy

Last Name	First Name	Organization
Thakare	Jivan	University of North Dakota, Energy & Environmental Research Center
Thompson	Christopher	GVD Corporation
Thompson	Simon	U.S. Department of Energy, Fuel Cell Technologies Office
Thornton	Matthew	National Renewable Energy Laboratory
Tian	Hanchen	West Virginia University
Toney	Michael	SLAC National Accelerator Laboratory
Tong	Jianhua "Joshua"	Clemson University
Torun	Secil	ENGIE
Tous	Ignacio	University of Maryland, Center for Advanced Transportation Technology Laboratory
Tran	Ba	Pacific Northwest National Laboratory
Trocciola	John	CSRA Inc.
Tsuchiya	Hiroshi	New Energy and Industrial Technology Development Organization, Japan
Tucker	Michael	Lawrence Berkeley National Laboratory
Tumas	William	National Renewable Energy Laboratory
Udovic	Terrence	National Institute of Standards and Technology
Ulsh	Michael	National Renewable Energy Laboratory
Ulyakhin	Sergey	Great Wall Motor
Umeda	Takami	Toyota Motor North America Research & Development (R&D)
Usuda	Hiroyuki	New Energy and Industrial Technology Development Organization, Japan
Usui	Osamu	Mitsubishi Heavy Industries America
Veenstra	Mike	Ford Motor Company
Vega	Edwin	West Virginia University
Veith	Gabriel	Oak Ridge National Laboratory
Veltman	Pieter	High yield Energy Technologies (HyET) Hydrogen BV
Venkataraman	Venkat	U.S. Department of Energy, National Energy Technology Laboratory
Venkatesh	T	Stony Brook University
Verma	Sumit	Shell International Exploration & Production Inc.
Vesely	Charles	Cummins Inc.
Vetrano	John	U.S. Department of Energy, Office of Basic Energy Sciences

Last Name	First Name	Organization
Viano	David	Commonwealth Scientific and Industrial Research Organisation (CSIRO)
Vickers	James	U.S. Department of Energy, Fuel Cell Technologies Office
Vijayagopal	Ram	Argonne National Laboratory
Vlassiouk	Ivan	General Graphene
Vora	Shailesh	National Energy Technology Laboratory
Vukmirovic	Miomir	Brookhaven National Laboratory
Wachsman	Eric	University of Maryland
Wagener	Earl H	Tetramer Technologies, LLC
Wagner	Andrew	Mainstream Engineering Corporation
Wakabayashi	Makoto	Nissan Chemical America Corporation
Waldecker	James	Ford Motor Company
Wang	Conghua	TreadStone Technologies, Inc.
Wang	Dunwei	Boston College
Wang	Guofeng	University of Pittsburgh
Wang	Huanhuan	University at Buffalo
Wang	Jia	Brookhaven National Laboratory
Wang	Lan	University of Delaware
Wang	Michael	Argonne National Laboratory
Wang	Rainey	Hydrogenics Corporation
Wang	Teng	University of Delaware
Wang	Xiaohua	Argonne National Laboratory
Wang	Yi	West Virginia University
Ward	Patrick	Savannah River National Laboratory
Watanabe	Masahiro	University of Yamanashi/Fuel Cell Nanomaterials Center
Watanabe	Shuto	Daiwa Institute of Research Ltd.
Weaver	Matthew	Giner ELX
Weber	Adam	Lawrence Berkeley National Laboratory
Weber	Robert	Pacific Northwest National Laboratory
Weeda	Marcel	Netherlands Organisation for Applied Scientific Research
Weeks	Brian	Gas Technology Institute
Wegeng	Robert	STARS Technology Corporation
Weisenberger	Matthew	University of Kentucky Center for Applied Energy Research

Last Name	First Name	Organization
Weng	Dacong	Honeywell Aerospace
Westover	Tyler	Idaho National Laboratory
Wheeler	Douglas	DJW Technology, LLC
Williams	Mark	KeyLogic Systems
Wilthaner	Markus	McKinsey & Company, Inc. Austria
Wipke	Keith	National Renewable Energy Laboratory
Wocken	Chad	University of North Dakota, Energy & Environmental Research Center
Wolden	Colin	National Renewable Energy Laboratory/Colorado School of Mines
Wolverton	Christopher	Northwestern University
Wood	Brandon	Lawrence Livermore National Laboratory
Wood	David	Oak Ridge National Laboratory
Woods	Stephen	NASA, White Sands Test Facility
Wu	Gang	University at Buffalo
Wu	Song	Mitsubishi Hitachi Power Systems Americas
Wycisk	Ryszard	Vanderbilt University
Xie	Crystal	Crystallogy Consulting
Xie	Jian	Indiana University Purdue University
Xie	Xiaohong	Pacific Northwest National Laboratory
Xie	Zhiqiang	University of Tennessee
Xu	Hui	Giner, Inc.
Xu	Hui	Argonne National Laboratory
Xu	Yunjie	Illinois Institute of Technology
Yan	Litao	Pacific Northwestern National Laboratory
Yandrasits	Michael	3M Corporate Research Materials Lab
Yang	Fan	Giner, Inc.
Yang	Fuming	State Power Investment Corporation Institute, China
Yang	Gaoqiang	University of Tennessee Space Institute
Yang	Tae-Hyun	Korea Institute of Energy Research
Yang	Xia	National Institute of Clean and Low-Carbon Energy (NICE) America Research Inc.
Yang	Xin	University of South Carolina
Yang	Yang	University of Central Florida
Yang	Zhiwei	United Technologies Research Center
Yasumatsu	Hisato	Toyota Technological Institute

Last Name	First Name	Organization
Yellamilli	Sai Nitin	Xergy Inc
Yildrim	Mustafa	IRD Fuel Cells A/S
Yokomoto	Katsumi	New Energy and Industrial Technology Development Organization (NEDO), Japan
Yomori	Hiroyuki	Japan Electric Power Information Center
You	Eunyoung	Hyundai Mobis
Youn	Edward	National Institute of Clean and Low-Carbon Energy (NICE) America Research Inc.
Young	James	National Renewable Energy Laboratory
Zafeiratou	Eleni	Fuel Cells and Hydrogen Joint Undertaking (FCH JU)
Zakutayev	Andriy	National Renewable Energy Laboratory
Zelenay	Piotr	Los Alamos National Laboratory
Zenyuk	Iryna	University of California, Irvine
Zhang	Hanguang	University at Buffalo
Zhang	Kun	Shell International Exploration and Production
Zhang	Xu	University of Miami
Zhao	Zipeng	University of California, Los Angeles
Zheng	Jinyang	Zhejiang University
Zhong	Yu	Worcester Polytechnic Institute
Zhou	Joe	Sunstone
Zhou	Lingfeng	West Virginia University
Zhou	Xiao-Dong	University of Louisiana at Lafayette
Zhou	Yucun	Georgia Institute of Technology
Zhu	Jiahong	Tennessee Technological University
Zhu	Tianli	United Technologies Research Center
Zimmerman	Jonathan	Sandia National Laboratories
Zou	Shouzhong	American University
Zulevi	Barr	Pajarito Powder LLC

General Project Evaluation Form

This evaluation form is for use with the following Hydrogen and Fuel Cells subprogram and project category review panels/projects: Hydrogen Fuel R&D (Hydrogen Production R&D and Hydrogen Storage); Fuel Cell R&D; Infrastructure and Systems R&D (Hydrogen Infrastructure R&D, Technology Acceleration, and Systems Analysis; and Safety, Codes and Standards.

Evaluation Criteria: U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review

Please provide specific, concise comments to support your evaluation. It is important that you write in full sentences and clearly convey your meaning to prevent incorrect interpretation.

1. Approach

To performing the work – the degree to which project objectives and critical barriers have been clearly identified and are being addressed, and the extent to which the project is well-designed, feasible, and integrated with other relevant efforts. **(Weight = 20%)**

4.0 - Outstanding. Sharply focused on overcoming critical barriers; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers.
3.0 - Good. Generally effective but could be improved; contributes to overcoming some barriers.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers.
2.0 - Fair. Has significant weaknesses; may have some impact on overcoming barriers.
1.5 - Poor. Minimally responsive to project objectives; unlikely to contribute to overcoming the barriers.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

☐ 4.0 - Outstanding

☐ 3.5 - Excellent

☐ 3.0 - Good

☐ 2.5 - Satisfactory

☐ 2.0 - Fair

☐ 1.5 - Poor

☐ 1.0 - Unsatisfactory

Comments on Approach to performing the work:

2. Accomplishments and Progress

Toward overall project and DOE goals – the degree to which progress towards project objectives has been made and measured against well-defined performance indicators, and the degree to which the project has demonstrated progress toward addressing critical barriers to achieving DOE goals. **(Weight = 45%)**

4.0 - Outstanding. Outstanding progress towards project objectives is demonstrated through clear and measurable performance indicators; results have directly led to overcoming one or more critical barriers.
3.5 - Excellent. Excellent progress towards project objectives is demonstrated through clear and measurable performance indicators; results suggest that one or more critical barriers will be overcome.
3.0 - Good. Significant progress has been made, but there are weaknesses that need to be addressed to improve the rate of progress or improve the clarity of the project's objectives and performance indicators; contributes to overcoming some barriers.
2.5 - Satisfactory. Moderate progress has been made, but there are weaknesses that need to be addressed to improve the rate of progress or improve the clarity of the project's objectives and performance indicators; contributes to overcoming some barriers.
2.0 - Fair. Modest progress -- rate of progress has been slow; may have some impact on overcoming barriers.
1.5 - Poor. Minimal progress towards project objectives and poorly defined performance indicators; unlikely to contribute to overcoming the barriers.
1.0 - Unsatisfactory. Little to no demonstrated progress toward project objectives; unlikely to contribute to overcoming the barriers.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Accomplishments and Progress toward overall project and DOE goals:

3. Collaboration and Coordination with Other Institutions

The degree to which the project effectively engages and coordinates project partners and interacts with other entities and projects to accelerate project progress and improve the likelihood of the project's success and impact. **(Weight = 10%)**

4.0 - Outstanding. Close, appropriate collaboration with other institutions; partners are full participants and well-coordinated.
3.5 - Excellent. Good collaboration; partners participate and are well-coordinated.
3.0 - Good. Collaboration exists; partners are fairly well-coordinated.
2.5 - Satisfactory. Some collaboration exists; coordination between partners could be significantly improved.
2.0 - Fair. A little collaboration exists; coordination between partners could be significantly improved.
1.5 - Poor. Most work is done at the sponsoring organization with little outside collaboration; little or no apparent coordination with partners.
1.0 - Unsatisfactory. No apparent coordination with partners.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Collaboration and Coordination with other institutions:

4. Relevance/Potential Impact

The degree to which the project supports and advances progress toward the Hydrogen and Fuel Cells Program goals and objectives, as delineated in the Multi-Year RD&D plan and/or the Program and sub-program overview presentations from the 2019 AMR. **(Weight = 15%)**

4.0 - Outstanding. Project is critical to the Hydrogen and Fuel Cells Program and has potential to significantly advance progress toward DOE RD&D goals and objectives.
3.5 - Excellent. The project aligns well with the Hydrogen and Fuel Cells Program and DOE RD&D objectives and has the potential to advance progress toward DOE RD&D goals and objectives.
3.0 - Good. Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
2.5 - Satisfactory. Project aspects align with some of the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
2.0 - Fair. Project partially supports the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
1.5 - Poor. Project has little potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives.
1.0 - Unsatisfactory. Project has little to no potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Relevance/Potential Impact:

5. Proposed Future Work

The degree to which the project has effectively planned its future in a logical manner by incorporating appropriate decision points, considering barriers to its goals and, when sensible, mitigating risk by providing alternate pathways. **Note:** if a project has ended, please select "Not Applicable." **(Weight = 10%)**

4.0 - Outstanding. Plans clearly build on past progress and are sharply focused on critical barriers to project goals; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers.
3.0 - Good. Plans generally build on past progress and should contribute to overcoming some barriers.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers.
2.0 - Fair. Plans may lead to improvements, but need better focus on addressing project weaknesses; may have some impact on overcoming barriers.
1.5 - Poor. Minimally responsive to project objectives; unlikely to resolve project weaknesses and contribute to overcoming barriers.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming barriers.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Proposed Future Work:

SUMMARY OF REVIEWER COMMENTS

Project Strengths:

Project Weaknesses:

Recommendations for Additions/Deletions to Project Scope:

HydroGEN Seedling Project Evaluation Form

This evaluation form is for use with HydroGEN seedling projects.

Evaluation Criteria: U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review

Please provide specific, concise comments to support your evaluation. It is important that you write in full sentences and clearly convey your meaning to prevent incorrect interpretation.

1. Approach

To performing the work – the degree to which barriers have been clearly identified, and are being addressed through project innovation; and the extent to which the project is well-designed, feasible, and integrated with the HydroGEN Consortium network. A strong emphasis should be placed on the appropriateness of the budget period 1 scope of work toward validation of the project's technology innovation. **(Weight = 20%)**

4.0 - Outstanding. Sharply focused on critical barriers and validating technology innovation; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers and validating technology innovation.
3.0 - Good. Generally effective but could be improved; contributes to overcoming some barriers and validating technology innovation.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers and validating technology innovation.
2.0 - Fair. Has significant weaknesses; may have some impact on overcoming barriers and/or validating technology innovation.
1.5 - Poor. Minimally responsive to project objectives; unlikely to contribute to overcoming the barriers or validating technology innovation.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming the barriers or validating technology innovation.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Approach to performing the work:

2. Relevance/Potential Impact

The degree to which the project supports and advances progress toward the DOE Hydrogen and Fuel Cells Program goals and objectives, and also supports the HydroGEN Consortium mission. A strong emphasis should be placed on the project's potential to advance the discovery and development of novel, advanced water splitting materials systems which will enable meeting the DOE ultimate hydrogen production goal of $2/kg H2. An additional factor to consider is how well the project fits into, leverages, and potentially enhances the framework and resources of the HydroGEN Consortium. **(Weight = 15%)**

4.0 - Outstanding. Project is critical to the Hydrogen and Fuel Cells Program and has potential to significantly advance progress toward DOE RD&D goals and objectives and is significantly leveraging and contributing to the resources and framework of the HydroGEN consortium.
3.5 - Excellent. The project aligns well with the Hydrogen and Fuel Cells Program and DOE RD&D objectives and has the potential to advance progress toward DOE RD&D goals and objectives and is aptly leveraging and contributing to the resources and framework of the HydroGEN consortium.
3.0 - Good. Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives and the project is adequately leveraging and contributing to the resources and framework of the HydroGEN consortium.
2.5 - Satisfactory. Project aspects align with some of the Hydrogen and Fuel Cells Program and DOE RD&D objectives and the project is leveraging and contributing to the resources and framework of the HydroGEN consortium to some extent.
2.0 - Fair. Project partially supports the Hydrogen and Fuel Cells Program and DOE RD&D objectives and the project is not adequately leveraging and contributing to the resources and framework of the HydroGEN consortium.
1.5 - Poor. Project has little potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives and the project has minimal interaction with HydroGEN to leverage and contribute to the resources and framework of the HydroGEN consortium.
1.0 - Unsatisfactory. Project has little to no potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives and the project is not leveraging and contributing to the resources and framework of the HydroGEN consortium.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Relevance/Potential Impact:

3. Accomplishments and Progress

Toward overall project and DOE goals – the degree to which progress has been made and measured against performance indicators, and the degree to which the project has demonstrated progress toward DOE goals as well as the HydroGEN Consortium mission. A particular emphasis should be placed on the strength of the data presented by the accomplishments (including data from the HydroGEN nodes leveraged by the project) in terms of supporting accomplishments. An additional emphasis should be placed on the strength of the project's budget period 1 Go/No-Go Criteria and on project progress toward meeting this criteria. **(Weight = 30%)**

4.0 - Outstanding. Sharply focused on critical barriers with significant and convincing data to support the accomplishments towards ambitious Go/No-Go Criteria; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers and provides data that considerably supports the accomplishments towards impactful Go/No-Go Criteria.
3.0 - Good. Generally effective but could be improved; contributes to overcoming some barriers and provides adequate data to support accomplishments towards meaningful Go/No-Go Criteria.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers and provides some data to support accomplishments towards adequate Go/No-Go Criteria.
2.0 - Fair. Has significant weaknesses; may have some impact on overcoming barriers and has limited data and accomplishments to support the Go/No-Go Criteria; Go/No-Go Criteria may be weak.
1.5 - Poor. Minimally responsive to project objectives; unlikely to contribute to overcoming the barriers and meet the Go/No-Go Criteria; Go/No-Go criteria is not adequate or missing.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming the barriers and meet the Go/No-Go Criteria; Go/No-Go criteria is not adequate or missing.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Accomplishments and Progress toward overall project and DOE goals:

4. Collaboration Effectiveness

With HydroGEN and, if applicable, other research entities – the degree to which the project has engaged with the HydroGEN EMN and has effectively used nodes to accelerate materials development and improve the likelihood of the project's success and impact. This also includes the effectiveness of project engagement with the broader materials research community, including work with HydroGEN's cross-cutting benchmarking/protocols (2b) project team, the HydroGEN Data Team, pathway-specific Working Groups, and others. An additional factor is the broader value and impact of the project's data sharing through the HydroGEN data hub. **(Weight = 25%)**

4.0 - Outstanding. Close, appropriate collaboration with other institutions, specifically the HydroGEN Consortium with appropriate use of nodes, contributions to the benchmarking/protocols (2b) project and the HydroGEN Data Hub; partners are full participants and well-coordinated.
3.5 - Excellent. Good collaboration, specifically the HydroGEN Consortium with appropriate use of nodes, contributions to the benchmarking/protocols (2b) project and the HydroGEN Data Hub; partners participate and are well-coordinated.
3.0 - Good. Collaboration exists with the HydroGEN Consortium and includes node utilization and engagement with the benchmarking/protocols (2b) project and the HydroGEN Data Hub; partners are fairly well-coordinated.
2.5 - Satisfactory. Some collaboration exists; coordination between partners could be significantly improved, specifically with respect to the HydroGEN Consortium node utilization activities, and engagement with the benchmarking/protocols (2b) project and the HydroGEN Data Hub.
2.0 - Fair. A little collaboration exists; coordination between partners could be significantly improved, specifically with respect to the HydroGEN Consortium node utilization activities, and engagement with the benchmarking/protocols (2b) project and the HydroGEN Data Hub.
1.5 - Poor. Most work is done at the sponsoring organization with little outside collaboration; little or no apparent coordination with partners and HydroGEN Consortium.
1.0 - Unsatisfactory. No apparent coordination with partners and HydroGEN Consortium.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Collaboration and Coordination with other institutions:

5. Proposed Future Work

The degree to which the project has effectively planned its potential future work (contingent on the project's continuation past budget period 1) in a logical manner and leverages progress in budget period 1 toward meeting end-of-project goals and advancing the materials research mission of the HydroGEN Consortium. **(Weight = 10%)**

4.0 - Outstanding. Sharply focused on critical barriers, meeting end-of-project goals and advancing the materials research mission of the HydroGEN Consortium; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers, meeting most end-of-project goals and advancing the materials research mission of the HydroGEN Consortium.
3.0 - Good. Generally effective but could be improved; contributes to overcoming some barriers, meeting some end-of-project goals and has potential to advance the materials research mission of the HydroGEN Consortium.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers, meeting some end-of-project goals and may contribute to advancing the materials research mission of the HydroGEN Consortium.
2.0 - Fair. Has significant weaknesses; may have some impact on overcoming barriers, make minimal progress towards end-of project goals and insignificantly contributes to advancing the materials research mission of the HydroGEN Consortium.

1.5 - Poor. Minimally responsive to project objectives; unlikely to contribute to overcoming the barriers or meet end-of-project goals and will most likely not contribute to advancing the materials research mission of the HydroGEN Consortium.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming the barriers or meet end-of-project goals and is unlikely to contribute to advancing the materials research mission of the HydroGEN Consortium.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Proposed Future Work:

Project Strengths:

Project Weaknesses:

Recommendations for Additions/Deletions to Project Scope:

New Project Evaluation Form

This evaluation form is for use with newly awarded R&D projects presented at the 2019 AMR.

Evaluation Criteria: U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review

Please provide specific, concise comments to support your evaluation. It is important that you write in full sentences and clearly convey your meaning to prevent incorrect interpretation.

1. Approach

To performing the work – the degree to which project objectives and critical barriers have been clearly identified and are being addressed, and the extent to which the project is well-designed, feasible, and integrated with other relevant efforts. **(Weight = 40%)**

4.0 - Outstanding. Sharply focused on overcoming critical barriers; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers.
3.0 - Good. Generally effective but could be improved; contributes to overcoming some barriers.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers.
2.0 - Fair. Has significant weaknesses; may have some impact on overcoming barriers.
1.5 - Poor. Minimally responsive to project objectives; unlikely to contribute to overcoming the barriers.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Approach to performing the work:

2. Accomplishments and Progress

Toward overall project and DOE goals – the degree to which progress towards achieving project objectives has been made and measured against well-defined performance indicators, and the degree to which the project has demonstrated progress toward addressing critical barriers to achieving DOE goals. ***Note:*** *Please evaluate accomplishments/progress made considering the amount of time the project has been underway; if a project has not been underway long enough to have made any progress, you may select "Not Applicable."* **(Weight = 10%)**

4.0 - Outstanding. Outstanding progress towards project objectives is demonstrated through clear and measurable performance indicators; results have directly led to overcoming one or more critical barriers.

3.5 - Excellent. Excellent progress towards project objectives is demonstrated through clear and measurable performance indicators; results suggest that one or more critical barriers will be overcome.
3.0 - Good. Significant progress has been made, but there are weaknesses that need to be addressed to improve the rate of progress or improve the clarity of the project's objectives and performance indicators; contributes to overcoming some barriers.
2.5 - Satisfactory. Moderate progress has been made, but there are weaknesses that need to be addressed to improve the rate of progress or improve the clarity of the project's objectives and performance indicators; contributes to overcoming some barriers.
2.0 - Fair. Modest progress -- rate of progress has been slow; may have some impact on overcoming barriers.
1.5 - Poor. Minimal progress towards project objectives and poorly defined performance indicators; unlikely to contribute to overcoming the barriers.
1.0 - Unsatisfactory. Little to no demonstrated progress toward project objectives; unlikely to contribute to overcoming the barriers.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Accomplishments and Progress toward overall project and DOE goals:

3. Collaboration and Coordination with Other Institutions

The degree to which the project effectively engages and coordinates project partners and interacts with other entities and projects to accelerate project progress and improve the likelihood of the project's success and impact. **(Weight = 15%)**

4.0 - Outstanding. Close, appropriate collaboration with other institutions; partners are full participants and well-coordinated.
3.5 - Excellent. Good collaboration; partners participate and are well-coordinated.
3.0 - Good. Collaboration exists; partners are fairly well-coordinated.
2.5 - Satisfactory. Some collaboration exists; coordination between partners could be significantly improved.
2.0 - Fair. A little collaboration exists; coordination between partners could be significantly improved.
1.5 - Poor. Most work is done at the sponsoring organization with little outside collaboration; little or no apparent coordination with partners.
1.0 - Unsatisfactory. No apparent coordination with partners.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good

- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Collaboration and Coordination with other institutions:

4. Relevance/Potential Impact

The degree to which the project supports and advances progress toward the Hydrogen and Fuel Cells Program goals and objectives, as delineated in the Multi-Year RD&D plan and/or the Program and sub-program overview presentations from the 2019 AMR. **(Weight = 15%)**

4.0 - Outstanding. Project is critical to the Hydrogen and Fuel Cells Program and has potential to significantly advance progress toward DOE RD&D goals and objectives.
3.5 - Excellent. The project aligns well with the Hydrogen and Fuel Cells Program and DOE RD&D objectives and has the potential to advance progress toward DOE RD&D goals and objectives.
3.0 - Good. Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
2.5 - Satisfactory. Project aspects align with some of the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
2.0 - Fair. Project partially supports the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
1.5 - Poor. Project has little potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives.
1.0 - Unsatisfactory. Project has little to no potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D goals and objectives.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Relevance/Potential Impact:

5. Proposed Future Work

The degree to which the project has effectively planned its future in a logical manner by incorporating appropriate decision points, considering barriers to its goals and, when sensible, mitigating risk by providing alternate pathways. **(Weight = 20%)**

4.0 - Outstanding. Plans clearly build on past progress and are sharply focused on critical barriers to project goals; difficult to improve significantly.
3.5 - Excellent. Effective; contributes to overcoming most barriers.
3.0 - Good. Plans generally build on past progress and should contribute to overcoming some barriers.
2.5 - Satisfactory. Has some weaknesses; contributes to overcoming some barriers.
2.0 - Fair. Plans may lead to improvements, but need better focus on addressing project weaknesses; may have some impact on overcoming barriers.
1.5 - Poor. Minimally responsive to project objectives; unlikely to resolve project weaknesses and contribute to overcoming barriers.
1.0 - Unsatisfactory. Not responsive to project objectives; unlikely to contribute to overcoming barriers.

- ☐ 4.0 - Outstanding
- ☐ 3.5 - Excellent
- ☐ 3.0 - Good
- ☐ 2.5 - Satisfactory
- ☐ 2.0 - Fair
- ☐ 1.5 - Poor
- ☐ 1.0 - Unsatisfactory

Comments on Proposed Future Work:

SUMMARY OF REVIEWER COMMENTS

Project Strengths:

Project Weaknesses:

Recommendations for Additions/Deletions to Project Scope:

2019 AMR Hydrogen and Fuel Cells Program Review Questions

Program Reviewer Fuel Cell Expertise Selection: Are you a reviewer with general Hydrogen and Fuel Cell Program expertise, Solid Oxide Fuel Cell (SOFC) specific expertise or expertise in both program areas? (Your response to this question will change the set of questions that you are asked to evaluate below. You will have the option to skip any questions you do not feel qualified to answer).

○ General Hydrogen and Fuel Cell Program Expertise (Limited or no Solid Oxide Fuel Cell Experience)
○ Solid Oxide Fuel Cell Program Expertise Only
○ Both Solid Oxide and General Hydrogen and Fuel Cell Program Expertise

The Hydrogen and Fuel Cells Program has a mission and strategy that are clearly articulated and has appropriate goals and milestones as well as quantitative metrics that are SMART (Specific, Measurable, Actionable, Relevant, and Timely).

Please comment on the overall Hydrogen and Fuel Cells Program (including activities in the DOE Fuel Cell Technologies Office, Office of Fossil Energy, Office of Science, Office of Nuclear Energy, and ARPA-E) as well as each subprogram/activity area, as appropriate. (Note: Hydrogen delivery is now included under the Hydrogen Infrastructure R&D area. Technology Acceleration includes the prior-year subprograms Technology Validation, Manufacturing R&D, and Market Transformation).

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

	Strongly Disagree				Neutral			Strongly Agree			
	1	2	3	4	5	6	7	8	9	10	NA
Hydrogen and Fuel Cells Program Overall	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Production R&D	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Storage R&D	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Infrastructure R&D	○	○	○	○	○	○	○	○	○	○	○

Fuel Cell R&D	○	○	○	○	○	○	○	○	○	○	○
Technology Acceleration	○	○	○	○	○	○	○	○	○	○	○
Safety, Codes and Standards	○	○	○	○	○	○	○	○	○	○	○
Systems Analysis	○	○	○	○	○	○	○	○	○	○	○

Comments:

The Hydrogen and Fuel Cells Program is well focused and managed, and is effectively fostering research and development (R&D) to enable innovation and advance the state of technology for hydrogen and fuel cell technologies to be competitive and achieve widespread commercialization and deployment by industry.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

Strongly Disagree				**Neutral**			**Strongly Agree**			
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**NA**
○	○	○	○	○	○	○	○	○	○	○

Comments:

The Hydrogen and Fuel Cells Program's portfolio of projects is appropriately balanced across research areas to help achieve the Program's mission and goals.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

Strongly Disagree				Neutral				Strongly Agree		
1	2	3	4	5	6	7	8	9	10	NA
○	○	○	○	○	○	○	○	○	○	○

Comments:

The Hydrogen and Fuel Cells Program's R&D aligns well with industry and stakeholder needs, and is appropriate given complementary private sector, state and other non-DOE investments.

Please comment on the overall Hydrogen and Fuel Cells Program as well as each subprogram/activity area, as appropriate.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

	Strongly Disagree				Neutral				Strongly Agree		
	1	2	3	4	5	6	7	8	9	10	NA
Hydrogen and Fuel Cells Program Overall	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Production R&D	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Storage R&D	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Infrastructure R&D	○	○	○	○	○	○	○	○	○	○	○
Fuel Cell R&D	○	○	○	○	○	○	○	○	○	○	○

Technology Acceleration	○	○	○	○	○	○	○	○	○	○	○
Safety, Codes and Standards	○	○	○	○	○	○	○	○	○	○	○
Systems Analysis	○	○	○	○	○	○	○	○	○	○	○

Comments:

The Hydrogen and Fuel Cells Program is funding high-impact projects that have the potential to significantly advance the state of technology for the hydrogen and fuel cells industry.

Please comment on the overall Hydrogen and Fuel Cells Program as well as each subprogram/activity area, as appropriate.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

	Strongly Disagree				**Neutral**			**Strongly Agree**			
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**NA**
Hydrogen and Fuel Cells Program Overall	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Production R&D	○	○	○	○	○	○	○	○	○	○	○
Hydrogen Storage R&D	○	○	○	○	○	○	○	○	○	○	○

Hydrogen Infrastructure R&D	○	○	○	○	○	○	○	○	○	○	○
Fuel Cell R&D	○	○	○	○	○	○	○	○	○	○	○
Technology Acceleration	○	○	○	○	○	○	○	○	○	○	○
Safety, Codes and Standards	○	○	○	○	○	○	○	○	○	○	○
Systems Analysis	○	○	○	○	○	○	○	○	○	○	○

Comments:

In your opinion, what were the most significant accomplishments within the Hydrogen and Fuel Cells Program during the past year? Please consider the entire AMR content and entire DOE portfolio, including poster sessions, rather than the plenary talks alone.

Please respond for any subprogram/activity area as appropriate (e.g., hydrogen production, hydrogen storage, hydrogen infrastructure, fuel cells, technology acceleration, safety, codes and standards, solid oxide, ARPA-E, Basic Science, etc.).

Please state areas requiring more attention or improvement. If you do not have a response, please select ‘Not Applicable’.

☐ Not Applicable

Early-Stage Research and Development: The Hydrogen and Fuel Cells Program is focused on early-stage R&D as aligned with Administration objectives for federal research funding. Please provide suggestions for early stage R&D that the Hydrogen and Fuel Cells Program should consider for promoting its goals and objectives.

If you do not have a response, please select 'Not Applicable'.

☐ Not Applicable

Energy Materials Network (EMN) Consortia: Do you have any comments or recommendations on the Hydrogen and Fuel Cell Program's EMN consortia approach? Please state what is working effectively and areas that may benefit from further improvement.

If you do not have a response, please select 'Not Applicable'.

☐ Not Applicable

H2@Scale: What are the strengths and weaknesses of the H2@Scale initiative? Do you have any recommendations for other H2@Scale research topics or recommendations to enable the scale up and value proposition of H2@Scale (e.g. a region with low electricity prices, excess curtailment, and hydrogen supply opportunity along with a co-located demand for hydrogen, etc.)? Please provide any other recommendations on H2@Scale.

If you do not have a response, please select 'Not Applicable'.

☐ Not Applicable

Collaboration: The Hydrogen and Fuel Cells Program is collaborating with appropriate groups of stakeholders. Please add any additional comments, particularly on which stakeholders (e.g. academia, companies, small businesses, types of industries, etc.) should be more engaged and in what manner.

Please rate your response on a scale of 1 through 10, with 1 indicating that you strongly disagree and 10 indicating that you strongly agree, or NA if you have no opinion. Please add any additional comments.

Please also provide recommendations for how the Hydrogen and Fuel Cells Program can better coordinate R&D with other offices in the Department of Energy (e.g., Office of Fossil Energy, Office of Nuclear Energy, Office of Science, ARPA-E, etc.), as well as with entities outside the Department of Energy (e.g. states, other agencies, industry, etc.).

Strongly Disagree				Neutral				Strongly Agree		
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**NA**
○	○	○	○	○	○	○	○	○	○	○

Recommendations:

International Collaboration: The Hydrogen and Fuel Cells Program collaborates through a number of international partnerships. For example, the International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE) is an international partnership to coordinate activities on hydrogen and fuel cells across 18 countries and the European Commission. The U.S. assumed the chair role for IPHE in 2018. Please comment on actions DOE in conjunction with IPHE can undertake or activities that are effective/need improvement to accelerate progress in hydrogen and fuel cell technologies.

If you do not have a response, please select 'Not Applicable'.

☐ Not Applicable

Prizes: Agencies have shown interest in implementing prizes and competitions as a mechanism to complement the conventional grant process. Examples include the H-Prize (H2Refuel) for a small-scale hydrogen fueling appliance that complements large retail stations. Please provide comments on the prize/competition approach and provide any suggestions for future prizes or competitions that would align with the goal of accelerating the widespread success of hydrogen and fuel cell technologies.

If you do not have a response, please select ‘Not Applicable’.

☐ Not Applicable

Please comment on the overall strengths and weaknesses of the Hydrogen and Fuel Cells Program and its portfolio of projects. Please provide strengths and weaknesses for each subprogram as appropriate. On which technology areas should the Hydrogen and Fuel Cells Program put more or less focus for future activities?

If you do not have a response, please select ‘Not Applicable’.

☐ Not Applicable

Do you have any other comments or suggestions to improve the overall effectiveness of the Hydrogen and Fuel Cells Program or any of its specific subprograms?

If you do not have a response, please select ‘Not Applicable’.

☐ Not Applicable

List of Projects Presented but Not Reviewed

Project ID	Project Title	Principal Investigator Name	Organization
ARPAE01	Advanced Solid Oxide Fuel Cell Stack for Hybrid Power Systems	Scott Swartz	Nexceris, LLC
ARPAE02	Low-Cost Intermediate-Temperature Fuel Flexible Protonic Ceramic Fuel Cell Stack	Chuancheng Duan	Colorado School of Mines
ARPAE03	Protonic Ceramics for Energy Storage and Electricity Generation with Ammonia	Chuancheng Duan	Colorado School of Mines
ARPAE04	Development of a Novel High-Efficiency, Low-Cost Hybrid Solid Oxide Fuel Cell/ Internal Combustion Engine Power Generator	Robert Braun	Colorado School of Mines
ARPAE05	2D Materials-Based Proton Conductive Membranes	Ivan Blassiouk and Sergei Smirnov	General Graphene/New Mexico State University
ARPAE06	High-Power Metal-Supported Solid Oxide Fuel Cells for Electric Vehicle Range Extenders	Emir Dogdibegovic	Lawrence Berkeley National Laboratory
ARPAE07	Dual-Mode Energy Conversion and Storage Flow Cell	Christopher Capuano	Nel Hydrogen
ARPAE08	Advanced Catalyst and Engineered Catalyst Supports for Fuel Cells, Electrolyzers, and Energy Storage	Barr Zulevi	Pajarito Powder LLC
ARPAE09	Channeling Engineering of Hydroxide Ion Exchange Polymers and Reinforced Membranes	Chulsung Bae	Rensselaer Polytechnic Institute
ARPAE10	Highly Conductive, Stable, and Robust Hydroxide Exchange Membranes Based on Poly(aryl Piperidinium)	Santiago Rojas-Carbonell	University of Delaware
ARPAE11	Direct Ammonia Fuel Cells for Transport Applications	Reza Abbasi	University of Delaware
ARPAE12	Advanced Alkaline Membrane Hydrogen/ Air Fuel Cell System with Novel Technique for Air CO_2 Removal	Brian Setzler	University of Delaware
ARPAE14	Adaptive Solid Oxide Fuel Cell for Ultrahigh-Efficiency Power Systems	Fred C. Jahnke	FuelCell Energy, Inc.

Project ID	Project Title	Principal Investigator Name	Organization
ARPAE15	Cost-Effective, Intermediate-Temperature Fuel Cells for Carbon-Free Power Generation	Greg Tao	Chemtronergy, LLC
FC105	Novel Structured Metal Bipolar Plates for Low-Cost Manufacturing	C.H. Wang	TreadStone Technologies, Inc.
FC117	Fiscal Year 2018 Small Business Innovation Research (SBIR) Phase IIB: Ionomer Dispersion Impact on Polymer Electrolyte Membrane Fuel Cell and Electrolyzer Durability	Hui Xu	Giner, Inc.
FC128	Facilitated Direct Liquid Fuel Cells with High-Temperature Membrane Electrode Assemblies	Emory DeCastro	Advent Technologies, Inc.
FC142	Extended Surface Electrocatalyst Development	Bryan Pivovar	National Renewable Energy Laboratory
FC143	Highly Active, Durable, and Ultralow-Platinum-Group-Metal Nanostructured Thin Film Oxygen Reduction Reaction Catalysts and Supports	Andrew Steinbach	3M Company
FC167	Fiscal Year 2018 Small Business Innovation Research (SBIR) Phase II Release 1: Multi-Functional Catalyst Support	Minette Ocampo	pH Matter, LLC
FC176	Fiscal Year 2017 Small Business Innovation Research (SBIR) Phase II Release 1: Novel Hydrocarbon Ionomers for Durable Polymer Electrolyte Membranes	William Harrison	Nanosonic, Inc.
FC301	Membrane Working Group	Bryan Pivovar and Yu Seung Kim	National Renewable Energy Laboratory and Los Alamos National Laboratory
FE1	Progress in Solid Oxide Fuel Cell Technology Development at FuelCell Energy	Hossein Ghezel-Ayagh	FuelCell Energy, Inc.
FE2	Progress of National Energy Technology Laboratory Solid Oxide Fuel Cell Research Portfolio	Gregory Hackett	National Energy Technology Laboratory
FE3	Solid Oxide Fuel Cell Developmemnt at Pacific Northwest National Laboratory: Overview	Jeff Stevenson and Brian Koeppel	Pacific Northwest National Laboratory
FE4	Durability and Reliability of Materials and Components for Solid Oxide Fuel Cells	Edgar Lara-Curzio	Oak Ridge National Laboratory

Project ID	Project Title	Principal Investigator Name	Organization
FE5	Evaluation of Cathode Evolution for Reliable Solid Oxide Fuel Cell Performance	Brian Ingram	Argonne National Laboratory
FE6	Durable, Cost-Effective, Energy-Efficient Tubular Solid Oxide Fuel Cells	Praveen Cheekatamarla	Atrex Energy, Inc.
FE7	Metal-Supported Ceria Electrolyte-Based Solid Oxide Fuel Cell Stack for Scalable, Low-Cost, High-Efficiency, and Robust Stationary Power Systems	Charles Vesely and Bal Dosanjh	Cummins Power Generation, Inc.
FE8	Advanced Solid Oxide Fuel Cell Development at Redox Power Systems	Bryan Blackburn and Sean Bishop	Redox Power Systems
FE9	Innovative, Versatile, and Cost-Effective Solid Oxide Fuel Cell Stack Concept	Nguyen Minh	University of California - San Diego
FE10	Processing of Solid Oxide Fuel Cell Anodes for Enhanced Intermediate Temperature Catalytic Activity at High Fuel Utilization	Soumendra N. Basu	Trustees of Boston University
FE11	On-Demand Designing of Internal Surface Architecture of Porous Electrodes for Dramatic Enhancement of Solid Oxide Fuel Cell Performance and Durability	Xueyan Song	West Virginia University Research Corporation
FE12	Improving Ni-Based Solid Oxide Fuel Cell Anode Resilience and Durability Through Secondary Phase Formation	Robert A. Walker	Montana State University
FE13	Modification of Solid Oxide Fuel Cell Anodes and Cathodes by ALD	Raymond J. Gorte	University of Pennsylvania
FE14	Development of Getters for the Co-capture of Airborne Trace Contaminants and Carbon Tolerant Anode for Application in Solid Oxide Fuel Cell Systems	Prabhakar Singh	University of Connecticut
FE15	A Transformational NG-Fueled Dynamic Solid Oxide Fuel Cell for Datacenter In-Rack Power	Kevin Huang	University of South Carolina
FE16	Development of High-Temperature Anode Gas Recycle Blowers for Solid Oxide Fuel Cells	Jose Luis Cordova	Mohawk Innovative Technology
FE17	New Silver-Based Alloys for Solid Oxide Fuel Cell Brazing and Circuit Patterning	Jason Nicholas	Michigan State University

Project ID	Project Title	Principal Investigator Name	Organization
FE18	Mitigation of Chromia Poisoning in Solid Oxide Fuel Cell Cathodes	Fanglin (Frank) Chen	University of South Carolina
FE19	Development of Accelerated Test Protocols and High-Efficiency Cathodes for Solid Oxide Fuel Cells	Xiao-Dong Zhou	University of Louisiana at Lafayette
FE20	Cathode Cleaning for Chromium Poisoning Recovery	Uday Pal	Trustees of Boston University
FE21	Highly Active and Durable Cathodes for Solid Oxide Fuel Cells	Meilin Liu	Georgia Tech Research Corporation
FE22	Operating Stresses and Their Effects on Degradation of Lanthanum Strontium Manganite (LSM)-Based Solid Oxide Fuel Cell Cathodes	Mark DeGuire	Case Western Reserve University
FE23	Synthesis of Novel Cathode Hetero-Structures for Solid Oxide Fuel Cells	Srikanth Gopalan	Trustees of Boston University
FE24	Development and Validation of Low-Cost, Highly Durable, Spinel-Based Contact Materials for Solid Oxide Fuel Cell Cathode-Side Contact Application	Jiahong Zhu	Tennessee Technological University
FE25	Minimizing Cr Evaporation from Balance-of-Plant Components by Utilizing Cost-Effective Alumina-Forming Austenitic Steels	Xingbo Liu	West Virginia University Research Corporation
FE26	Probing Temperature Profiles in a Solid Oxide Fuel Cell During its Operation with 5 mm Spatial Resolution and its Implication for Optimization	Kevin Chen	University of Pittsburgh
FE27	Multi-Gas Sensors for Enhanced Reliability of Solid Oxide Fuel Cell Operation	Radislav Potyrailo	General Electric Company
FE28	Tuning Surface Stoichiometry of Solid Oxide Fuel Cell Electrodes at the Molecular and Nano Scales for Enhanced Performance and Durability	Eric Wachsman	University of Maryland
FE29	Influence of Surface Chemistry of Fluorite-Type Cathode Materials on Oxygen Reduction Reaction	Clement Nicolett	Massachusetts Institute of Technology
FE30	Computationally Guided Design of MULTIPLE Impurities Tolerant Electrode	Yu Zhong	Worcester Polytechnic Institute

Project ID	Project Title	Principal Investigator Name	Organization
FE050	Electrogenerative Reactors for Process Intensified Cogeneration of Power and Liquid Fuel from Shale Gas	Wenyuan Li	West Virginia University
FE051	Operating Stresses and Their Effects on Degradation of Lanthanum Strontium Manganite (LSM)-Based Solid Oxide Fuel Cell Cathodes	Chenxin Deng	Case Western Reserve University
FE052	Overview of Metal-Supported Solid Oxide Fuel Cells and Electrolyzers	Emir Dogdibegovic	Lawrence Berkeley National Laboratory
FE053	Enhancing Oxygen Exchange Activity by Tailoring Perovskite Surfaces	Raymond Gorte	University of Pennsylvania
FE054	Recent Sealing Developments for Solid Oxide Fuel Cells	Neil Kidner	Nexceris LLC
FE055	(M, Mn or Fe)$_3$O$_4$ Spinel for Advanced Electrical Conductive Layer for Solid Oxide Fuel Cell Stacks	Jung Pyung Choi	Pacific Northwest National Laboratory
FE056	Small-Scale Solid Oxide Fuel Cell Test Platform (SSTP)	Brent Kirby	Pacific Northwest National Laboratory
FE057	Composite Cathode Contact Material Development at Pacific Northwest National Laboratory: Validation in Stack Fixture Test and Effect of Strong Fibers	Yeong-Shyung Chou	Pacific Northwest National Laboratory
FE058	Cr Mitigation by Lanthanum Strontium Manganite (LSM)–Lanthanum Strontium Cobalt Ferrite (LSCF) Composite for Solid Oxide Fuel Cells	Yeong-Shyung Chou	Pacific Northwest National Laboratory
FE059	Effects of Cr Concentrations in Air on Lanthanum Strontium Manganite (LSM)/ Yttria-Stabilized Zirconia (YSZ) and Lanthanum Strontium Cobalt Ferrite (LSCF) Cathode Degradation	John Hardy	Pacific Northwest National Laboratory
FE060	Investigating Sr Vapor Phase Evolution from Lanthanum Strontium Manganite (LSM)/Yttria-Stabilized Zirconia (YSZ) and Lanthanum Strontium Cobalt Ferrite (LSCF) Cathodes During and After Sintering	John Hardy	Pacific Northwest National Laboratory
FE061	Use of Reduced Order Models (ROMs) to Predict Solid Oxide Fuel Cell Stack Performance	Jie Bao	Pacific Northwest National Laboratory

Project ID	Project Title	Principal Investigator Name	Organization
FE062	Influence of Anode Creep on the Structural Reliability of Solid Oxide Fuel Cells	Brian Koeppel	Pacific Northwest National Laboratory
FE063	Capture of Trace Airborne Impurities and Mitigation of Electrode Poisoning in Solid Oxide Fuel Cells	Junsung Hong	University of Connecticut
FE064	Carbon-Resistant High-Entropy Alloy Anode for Internal Reforming of Hydrocarbons in Solid Oxide Fuel Cells	Boxun Hu	University of Connecticut
FE065	Hydrogen-Assisted Corrosion of Stainless Steel in Dual Atmosphere Exposure Conditions	Michael Reisert and Ashish Aphale	University of Connecticut
FE066	Energetics of Carbon Deposition on Metallic Surfaces in Solid Oxide Fuel Cells	Rajesh Kumar and Boxun Hu	University of Connecticut
FE067	Progress in Electrode Engineering of Solid Oxide Fuel Cells at National Energy Technology Laboratory	Shiwoo Lee	National Energy Technology Laboratory
FE068	Quantifying the Nature and Impact of Mesoscale Heterogeneities in Solid Oxide Fuel Cell Electrodes	Paul Salvador	Carnegie Mellon University
FE069	Performance Degradation Modeling of Solid Oxide Fuel Cells using a Multiphysics Framework	Harry Abernathy	National Energy Technology Laboratory
FE070	Cation Diffusion in Bulk Tetragonal ZrO2 for Solid Oxide Fuel Cells: Effect of Hydrogen on Cation Transport	Yueh-Lin Lee	National Energy Technology Laboratory
FE071	Reduced-Order Model for Microstructure Evolution Simulation in Solid Oxide Fuel Cell with Dynamic Discrepancy Reduced Modeling	Yinkai Lei	National Energy Technology Laboratory
FE072	High Throughput, In-line Coating Metrology Development for Solid Oxide Fuel Cell Manufacturing	Sean Bishop	Redox Power Systems
FE073	Red-Ox Robust Ceramic Anode Supported Solid Oxide Fuel Cells	Keji Pan	Redox Power Systems
H2000	H2@Scale Overview	Bryan Pivovar	National Renewable Energy Laboratory

Project ID	Project Title	Principal Investigator Name	Organization
H2001	Scalable Electrolytic Systems for Renewable Hydrogen Production	Guido Bender	National Renewable Energy Laboratory
H2006	Membrane Electrode Assembly Manufacturing Automation Technology for the Electrochemical Compression of Hydrogen	Michael Ulsh	National Renewable Energy Laboratory
H2007	Megawatt-Scale Polymer-Electrolyte-Membrance-Based Electrolyzers for Renewable Energy System Applications	Kevin Harrison	National Renewable Energy Laboratory
H2011	Risk Analysis and Modeling to Improve Hydrogen Fuel Cell Vehicle Repair Garages	Brian Ehrhart	Sandia National Laboratories
H2013	Development, Validation, and Benchmarking of Quantitative Risk Assessment Tools for Hydrogen Refueling Stations	Alice Muna	Sandia National Laboratories
H2022	A Tool to Estimate the Benefits of Tube-Trailer Consolidation Scheme for Station Builders	Amgad Elgowainy	Argonne National Laboratory
H2026	Hybrid Electrical–Thermal Hydrogen Production Process Integrated with a Molten Salt Reactor Nuclear Power Plant	Donald Anton	Savannah River National Laboratory
H2030	Hydrogen Materials Compatibility of Low-Cost, High-Pressure, Polymer Hydrogen Dispensing Hoses	Kevin Simmons	Pacific Northwest National Laboratory
H2035	Region-Specific Merchant Hydrogen Market Assessment and Technoeconomic Assessment of Electrolytic Hydrogen Generation	Richard Boardman	Idaho National Laboratory
H2036	Validating an Electrolysis System with High Output Pressure	Sam Sprik	National Renewable Energy Laboratory
H2039	Turboexpander: Alternative Fueling Concept for Fuel Cell Electric Vehicle Fast Fill	Matthew Post	National Renewable Energy Laboratory
H2041	California Hydrogen Infrastructure Research Consortium	Jennifer Kurtz	National Renewable Energy Laboratory
H2045	Methane Pyrolysis for Base-Grown Carbon Nanotubes and CO_2-free Hydrogen over Transition Metal Catalysts	Robert Dagle	Pacific Northwest National Laboratory

Project ID	Project Title	Principal Investigator Name	Organization
H2050	Holistic Fuel Cell Electric Vehicle/ Hydrogen Station Optimization Model	Michael Peters	National Renewable Energy Laboratory
H2052	Merchant Hydrogen at Scale: A Technical–Economic Case Study of the Potential for Nuclear Hydrogen Production	Richard Boardman	Idaho National Laboratory
H2053	Hydrogen Safety Panel Evaluation of Hydrogen Facilities	Nick Barilo	Pacific Northwest National Laboratory
H2056	Hydrogen Safety Outreach to Expedite Hydrogen Fueling and Energy Project Deployment and Promote Public Acceptance for Zero-Emission Vehicles and Reliable Distributed Power Generation	Nick Barilo	Pacific Northwest National Laboratory
IA003	Overview of Hydrogen and Fuel Cells Research and Development for Navy Undersea Applications	Christian Schumacher	Naval Undersea Warfare Center
IA004	Fuel Cells for Long Endurance Unmanned Aerial Systems	Thomas Howell	Air Force Research Laboratory
IA005	Aluminum Hydride Title III Project	Shailesh Shah	U.S. Army Communications, Electronics Research, Development and Engineering Center
IA006	Army Ground Vehicle Systems Center Fuel Cell Update	Kevin Centeck	U.S. Army Combat Capabilities Development Command
IA007	Transit Research and Hydrogen Fuel Cells	Sean Ricketson	U.S. Department of Transportation
IA008	Federal Railroad Administration Hydrogen and Fuel Cell Research	Melissa Shurland	U.S. Department of Transportation
IA010	Heavy-Duty Technology Advancement: Interagency Collaboration for Public Health	John Mikulin	U.S. Environmental Protection Agency
IA011	NASA Fuel Cell and Hydrogen Activities	Ian Jakupca	NASA Glenn Research Center
IA012	Interagency Collaboration: FAST Act Section 1413 – Alternative Fuels Corridor Designations	Michael Scarpino	U.S. Department of Transportation, Volpe Center

Project ID	Project Title	Principal Investigator Name	Organization
IA015	Distributed Low-Energy Wastewater Treatment (D-LEWT) for Fuel Generation and Water Reuse	Aaron Petri and Tapan Patel	U.S. Army Corps of Engineers, Engineer Research and Development Center, Construction Engineering Research Laboratory
IA016	Neutron Imaging Study of the Water Transport in Operating Fuel Cells	David Jacobson	National Institute of Standards and Technology
IA017	Fuel Cell Boats in Marine Sanctuaries	Dana Wilkes	U.S. Department of Commerce, National Oceanic and Atmospheric Administration
IA018	Fundamental Science Underpinning Hydrogen and Fuel Cells	John Vetrano	U.S. Department of Energy, Office of Basic Energy Sciences
IA019	Catalytic Conversion of Natural Gas to Form Hydrogen and Solid Carbon	Ranjani Siriwardane and Christopher Matranga	National Energy Technology Laboratory
IA020	HydroGEN/National Science Foundation Designing Materials to Revolutionize and Engineer our Future (DMREF) Program: Blueprint for Photocatalytic Water Splitting – Mapping Multidimensional Compositional Space to Simultaneously Optimize Thermodynamics and Kinetics	L Piper	Binghamton University
IA021	HydroGEN/National Science Foundation Designing Materials to Revolutionize and Engineer our Future (DMREF) Program: High-Temperature Defects: Linking Solar Thermochemical and Thermoelectric Materials	Eric Toberer	Colorado School of Mines
IA022	HydroGEN/National Science Foundation Designing Materials to Revolutionize and Engineer our Future (DMREF) Program: Membrane Databases – New Schema and Dissemination	Michael Hickner	Pennsylvania State University
IA023	HydroGEN/National Science Foundation Designing Materials to Revolutionize and Engineer our Future (DMREF) Program: Experimental Validation of Designed Photocatalysts for Solar Water Splitting	Ismaila Dabo	Pennsylvania State University
IA024	U.S. Department of Energy, Office of Nuclear Energy – Hydrogen and Fuel Cell Activities	Richard Boardman	Idaho National Laboratory/ U.S. Department of Energy, Office of Nuclear Energy

Project ID	Project Title	Principal Investigator Name	Organization
IA025	Hydrogen and Fuel Cell Activities in Hawaii	Dave Molinaro	Hawaii Center for Advanced Transportation Technologies
IA026	The Fuel Cell Corridor – Global Center of the Fuel Cell Industry	Pat Valente	Ohio Fuel Cell Coalition
IA027	Hydrogen and Fuel Cell Activities in California	Andrew Martinez and Leslie Goodbody	California Air Resources Board
IA028	Hydrogen and Fuel Cell Activities in Colorado	Mahesh Albuquerque	Colorado Division of Oil & Public Safety
IA029	Northeast Hydrogen Fuel Cell Activity Review 2019	Charlie Myers	Massachusetts Hydrogen Coalition
IN003	Hydrogen Compression Application of the Linear Motor Reciprocating Compressor (LMRC)	Eugene Broerman	Southwest Research Institute
IN013	Dispenser Reliability Research and Development: Materials Compatibility	Nalini Menon	Sandia National Laboratories
P038	Biomass to Hydrogen (B2H2)	Pin-Ching Maness	National Renewable Energy Laboratory
P129	Novel Hybrid Microbial Electrochemical System for Efficient Hydrogen Generation from Biomass	Hong Liu	Oregon State University
P148A	HydroGEN: Low-Temperature Electrolysis	Guido Bender	National Renewable Energy Laboratory
P148B	HydroGEN: High-Temperature Electrolysis	Richard Boardman	Idaho National Laboratory
P148C	HydroGEN: Photoelectrochemical Hydrogen Production	Adam Weber	Lawrence Berkeley National Laboratory
P148D	HydroGEN: Solar Thermochemical Hydrogen Production	Anthony McDaniel	Sandia National Laboratories

Project ID	Project Title	Principal Investigator Name	Organization
P148E	Low- and High-Temperature Electrolysis, Photoelectrochemical and Solar Thermochemical Water-Splitting Materials Characterization and Development at Lawrence Berkeley National Laboratory under the HydroGEN Consortium	Nemanja Danilovic	Lawrence Berkeley National Laboratory
P148F	$CuGa_3Se_5/Zn_{1-x}Mg_xO$ Photocathodes for Photoelectrochemical Water Splitting	Imran Khan	Lawrence Berkeley National Laboratory
P148G	Linking Low-Temperature Electrolysis/ Hybrid Materials to Electrode Properties to Performance	Guido Bender	National Renewable Energy Laboratory
P148H	HydroGEN Photoelectrochemical Supernode—Emergent Degradation Mechanisms with Integration and Scale-Up of Photoelectrochemical Devices	James Young	National Renewable Energy Laboratory
P148I	Chalcopyrite Alloy Materials for Photoelectrochemical Hydrogen Production—Development of Theoretical Synthesis Support System for HydroGEN	Tadashi Ogitsu	Lawrence Livermore National Laboratory
P148J	Photoelectrochemical and Low-Temperature Water-Splitting Materials Research at Lawrence Livermore National Laboratory Under HydroGEN Consortium	Tadashi Ogitsu	Lawrence Livermore National Laboratory
P148K	Design, Synthesis, and Characterization of High-Quality Solar Thermochemical for Hydrogen Production Materials	Robert Bell	National Renewable Energy Laboratory
P148L	Developing an Atomistic Understanding of the Layered Perovskite $Ba_4CeMn_3O_{12}$ and its Polytypes for Thermochemical Water Splitting – A HydroGEN Supernode	Anthony McDaniel	Sandia National Laboratories
P148M	High-Temperature Electrolysis Capabilities at Pacific Northwest National Laboratory: Materials Development, Cell/Stack Manufacturing, Testing, Characterization, and Modeling	Olga Marina	Pacific Northwest National Laboratory
P148N	Advancements in High-Temperature Proton-Conducting Electrolyzer Materials	Dong Ding	Idaho National Laboratory
P151	New Approaches to Improved Polymer Electrolyte Membrane Electrolyzer Ion Exchange Membranes	Earl Wagener	Tetramer Technologies LLC
P179	BioHydrogen ($BioH_2$) Consortium to Advance Fermentative Hydrogen Production	Pin-Ching Maness	National Renewable Energy Laboratory

Project ID	Project Title	Principal Investigator Name	Organization
P180	Viability Study for Bipolar Membrane Electrode Assembly (BPMEA) Water Splitting	Hoon Chung	Los Alamos National Laboratory
P181	Active and Stable Electrocatalyst Supports and Microporous Layers for Anode Applications in Polymer Electrolyte Membrane Electrolyzers	Nem Danilovic	Lawrence Berkeley National Laboratory
ST008	Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements	Matt Thornton	National Renewable Energy Laboratory
ST128a	Hydrogen Materials—Advanced Research Consortium (HyMARC) Research Efforts on Nanoscale Metal Hydrides at Sandia National Laboratories	Vitalie Stavila	Sandia National Laboratories
ST129a	Multiscale Modeling of Interface Kinetics within the Hydrogen Materials—Advanced Research Consortium (HyMARC)	Tae Wook Heo	Lawrence Livermore National Laboratory
ST135	Hydrogen Materials—Advanced Research Consortium (HyMARC): Technical Activities at the National Institute of Standards and Technology	Thomas Gennett	National Renewable Energy Laboratory
ST138	Hydrogen Materials—Advanced Research Consortium (HyMARC) Seedling: Development of Magnesium Boride Etherates as Hydrogen Storage Materials	Godwin Severa	University of Hawaii
ST140	Emergency Hydrogen Refueler for Individual Consumer Fuel Cell Vehicles	Michael Kimble	Skyhaven Systems
ST200	Materials for Cryogenic Hydrogen Storage Technologies	Kevin Simmons	Pacific Northwest National Laboratory
ST201	Hydrogen Materials—Advanced Research Consortium (HyMARC): Technical Activities at SLAC	Nick Strange	National Renewable Energy Laboratory
TA004	Continuous Fiber Composite Electrofusion Coupler	Brett Kimball	Automated Dynamics
TA025	Laser Three-Dimensional Printing of Highly Compacted Protonic Ceramic Electrolyzer Stack	Jianhua "Joshua" Tong	Clemson University
TA026	Low-Cost, High-Performance Catalyst Coated Membranes for Polymer Electrolyte Membrane Water Electrolyzers	Andrew Steinbach	3M Company

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TA027	Catalyst Layer Design, Manufacturing, and In-Line Quality Control	Radenka Maric	University of Connecticut