



Hydrogen from
Next-generation
Electrolyzers of Water

U.S. DEPARTMENT OF ENERGY

H2NEW: Hydrogen (H₂) from Next-Generation Electrolyzers of Water LTE Task 3c: System and Technoeconomic Analysis

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DOE Hydrogen Program

2021 Annual Merit Review and Peer Evaluation Meeting

Project ID # P196D



Task Team Members



Mark Ruth (NREL):
Subtask lead



Rajesh Ahluwalia (ANL):
Performance modeling lead



Alex Badgett (NREL):
Technoeconomic and
manufacturing analysis

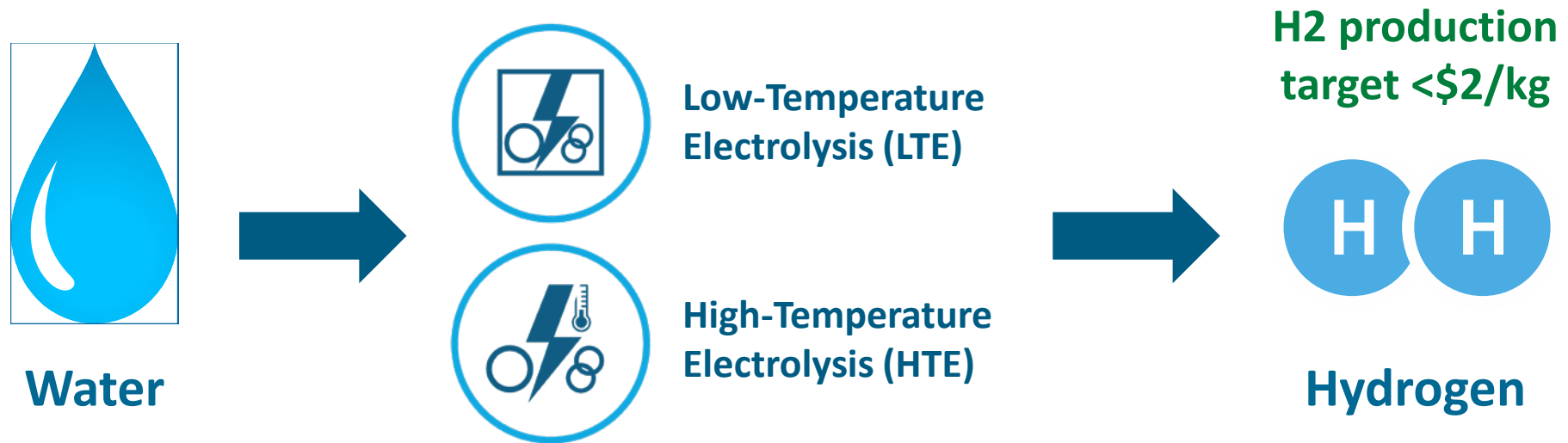


Andrew Star (ANL):
Performance model
development and use



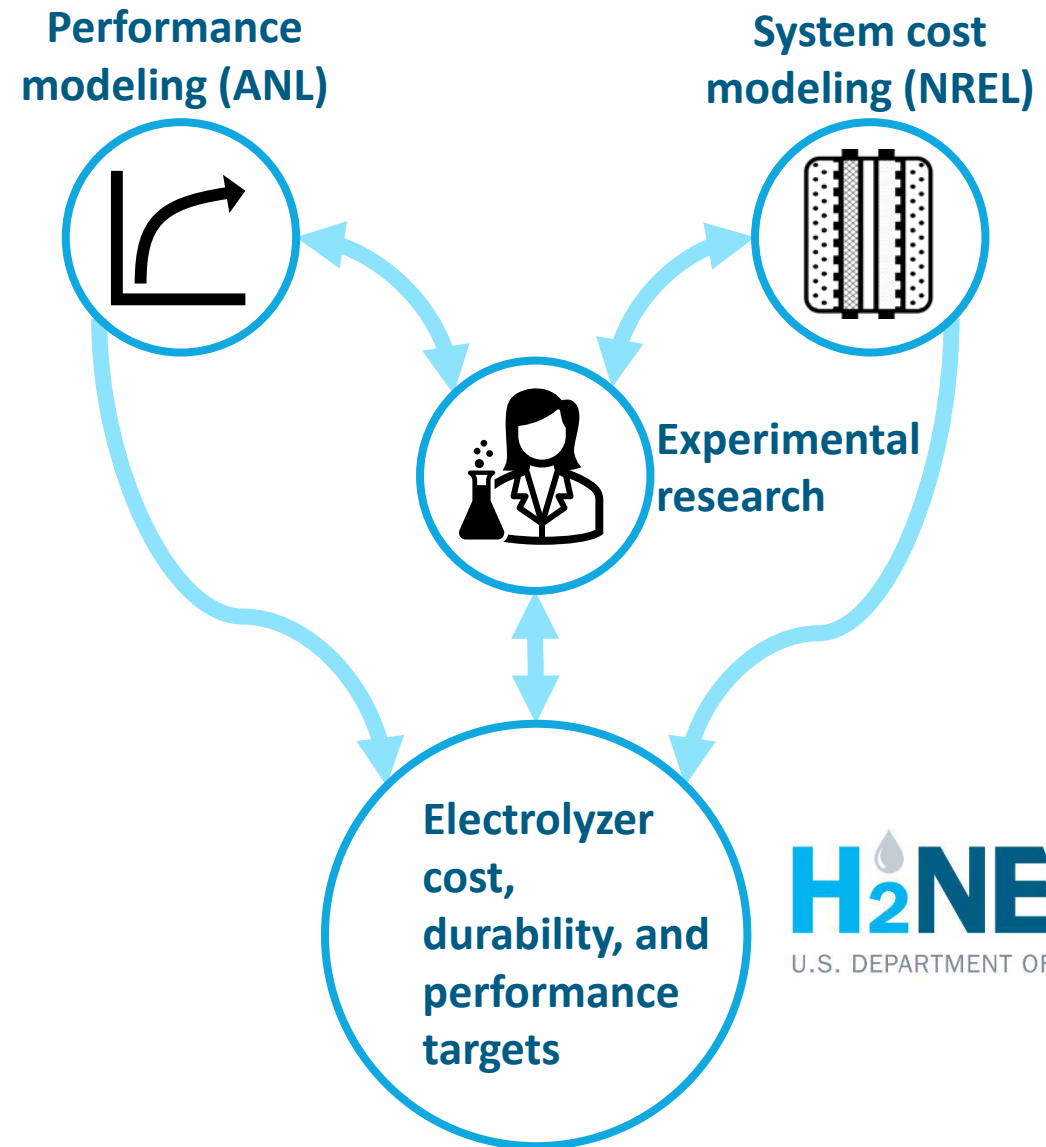
Rachel Rubin (NREL):
PyFast tool
development

Goal: H2NEW will address components, materials integration, and manufacturing R&D to enable manufacturable electrolyzers that meet required cost, durability, and performance targets, simultaneously, in order to enable \$2/kg hydrogen.



H2NEW has a clear target of establishing and utilizing experimental, analytical, and modeling tools needed to provide the scientific understanding of electrolysis cell performance, cost, and durability tradeoffs of electrolysis systems under predicted future operating modes

- This task leverages expertise in system cost and performance modeling from NREL and ANL to benchmark H2NEW cost, durability, and performance targets
- Experimental and analysis capabilities form a crucial feedback loop for validating progress towards H2NEW targets



Timeline and Budget

- Project start date: 10/1/2021
- FY21 DOE funding (if applicable): \$400K - \$275K NREL and \$125K ANL
- FY22 planned DOE funding: \$400K - \$275K NREL and \$125K ANL
- FY23 planned DOE funding: \$400K - \$275K NREL and \$125K ANL

Barriers

- \$2/kg green hydrogen production
- Developing affordable, reliable, and efficient electrolyzers

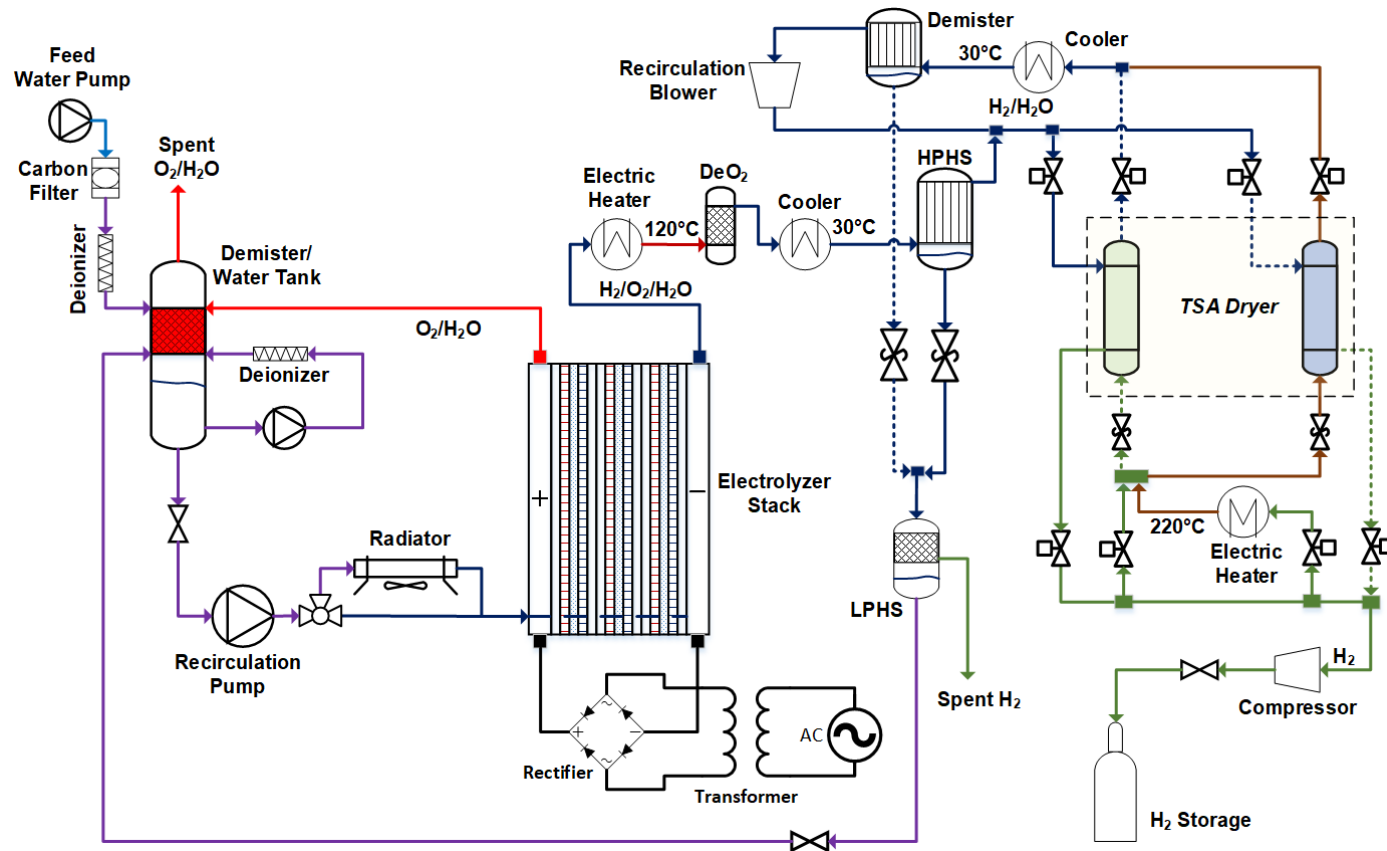
Partners

- Project lead: Bryan Pivovar (NREL)
- Task Leads: Rajesh Ahluwalia (ANL) and Mark Ruth (NREL)

- Enabling the H2NEW project to develop appropriate LTE stack cost, performance, and durability targets by
 - Linking R&D measurements and objectives to performance and economic impacts
 - Providing operating conditions and cycles for consideration and testing
 - Highlighting operating requirements and manufacturability
- Evaluating cost, performance, and durability tradeoffs to determine optimum LTE deployment to achieve \$2/kg production cost in renewable energy integration scenarios
- Involves optimization across multiple capabilities
 - System performance and durability assessment
 - Bottom-up manufacturing cost assessment
 - Systems analysis including interactions with the electricity grid

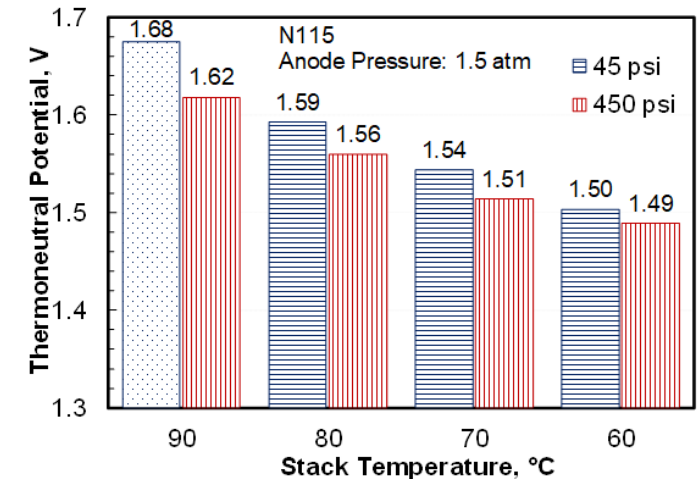
Approach: Developing a Reference PEM Electrolysis System by Building upon ANL-Developed Design

- GCTool model for accurate representation of the system layout, and BOP components and flows
- Model based losses for H₂ losses because of H₂/O₂ crossover, H₂ purge (LPHS), and O₂ removal (DeO₂)
- Parasitic loads: rectifier/transformer, chiller, TSA dryer (regeneration and blower)



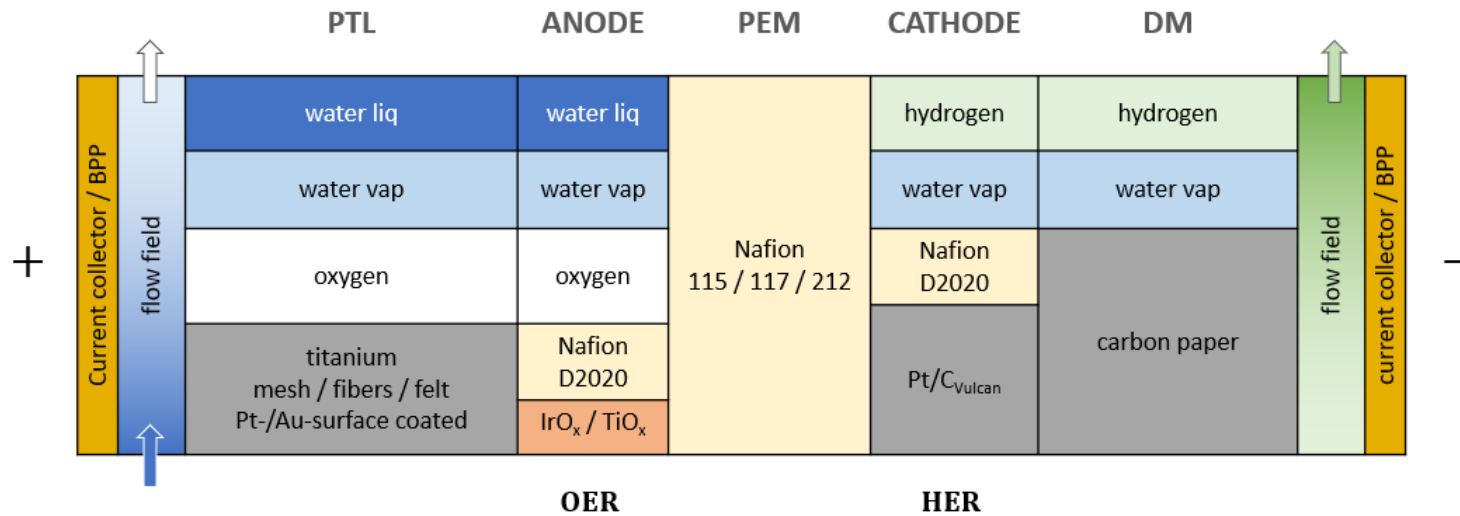
Sample Parasitic Loads

Mechanical BOP	kWh/kg-H ₂
Water Pumps	0.10
Radiator Fan	0.71
Cooling Tower	0.02
TSA Dryer System	
DeO ₂ Electrical Heater	0.14
Regen Electrical Heater	0.19
Tail Gas H ₂ Blower	0.00
Electrical BOP	
Rectifier/Transformer	3.69
Hydrogen Loss	
DeH ₂	0.22
Crossover H ₂ and O ₂	0.43
Total	5.51



Approach: System Performance and Durability Models

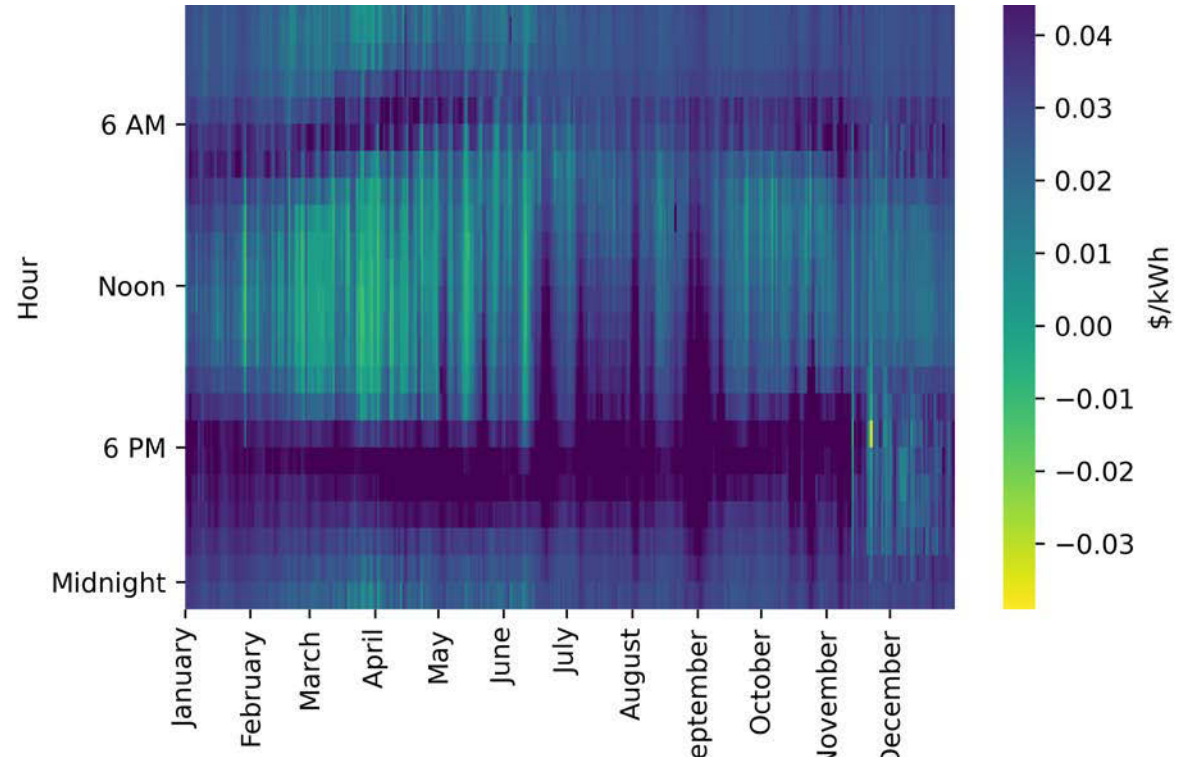
- Multi-physics model synthesizes porous electrode, concentrated solution, and effective medium theories
- Steady-state electrolyzer operation, valid for slowly fluctuating load
- One spatial dimension (through-plane) explicitly resolved
- Conserved variables: material, momentum, charge, energy
- Species: $H_{2,g}$, $O_{2,g}$, $O_{2,d}$, water (liquid), water (vapor), protons, electrons
- Crossover fluxes of H_2 and O_2
- OER reaction kinetic sub-model
- Outputs: iV , current efficiency, voltage efficiency, temperature and heat rejection



Approach: Optimal Operations Strategy for a Variety of Electricity Sources and Prices

- Electricity prices are going down and becoming more volatile as wind and photovoltaic (PV) solar generation increases.
- Intermittent operation at wholesale LMPs provides opportunities to decrease cost
- Task involves identifying operating strategy necessary to achieve low prices and potential impacts on durability
- Task also involves analyzing LTE electrolyzers directly connected to wind and photovoltaic solar electricity generation

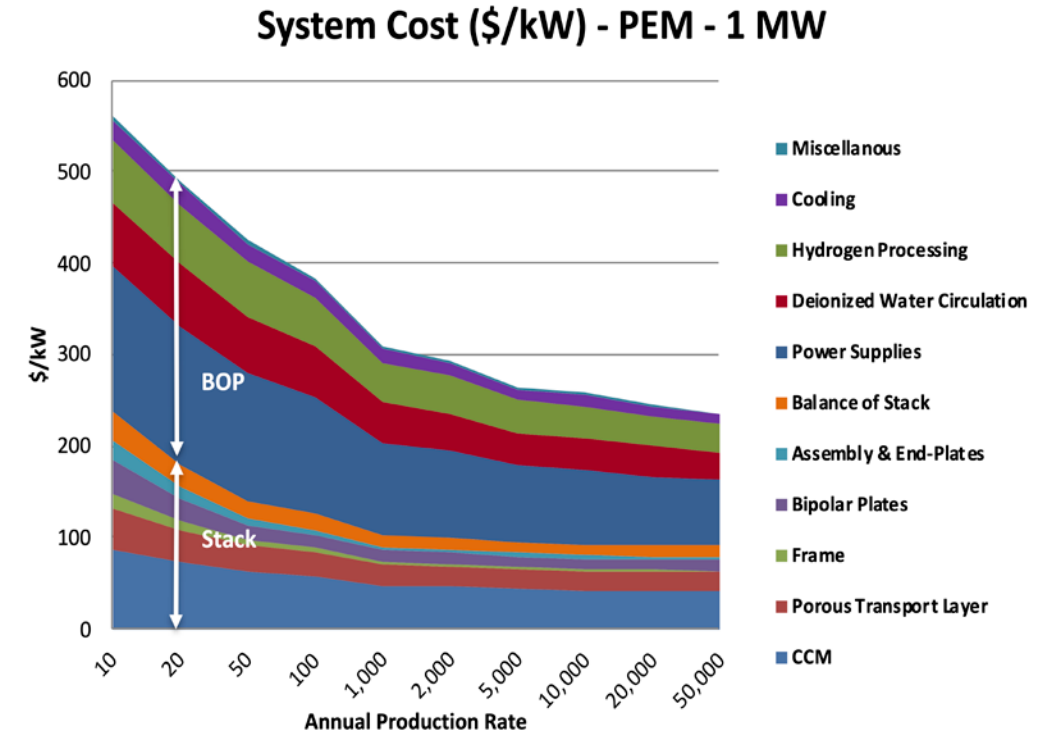
Locational Marginal Electricity Prices (LMPs) for California ISO Palo Verde Node in 2017



Approach: Bottom-Up Manufacturing Cost Assessment Building Upon Previous Analysis

- Developing a bottom-up manufacturing cost model for the updated reference PEM system
- Adding manufacturing cost assessments of balance of plant (BOP) components – previous work involved only quotes for them
- Updating manufacturing processes and assumptions based on project team input

System Cost Estimate from Previous Analysis

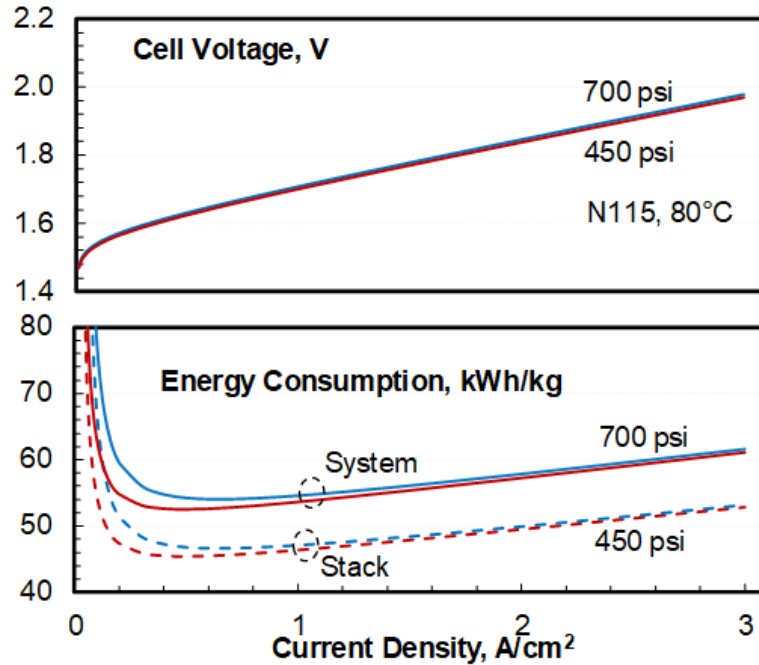


Source: Mayyas, A., Ruth, M., Pivovar, B., Bender, G. & Wipke, K. Manufacturing Cost Analysis for Proton Exchange Membrane Water Electrolyzers. (2019).

Accomplishment: Preliminary Electrolysis System Models Predict Performance, Recommend Optimal Cell Design and Operation Strategy

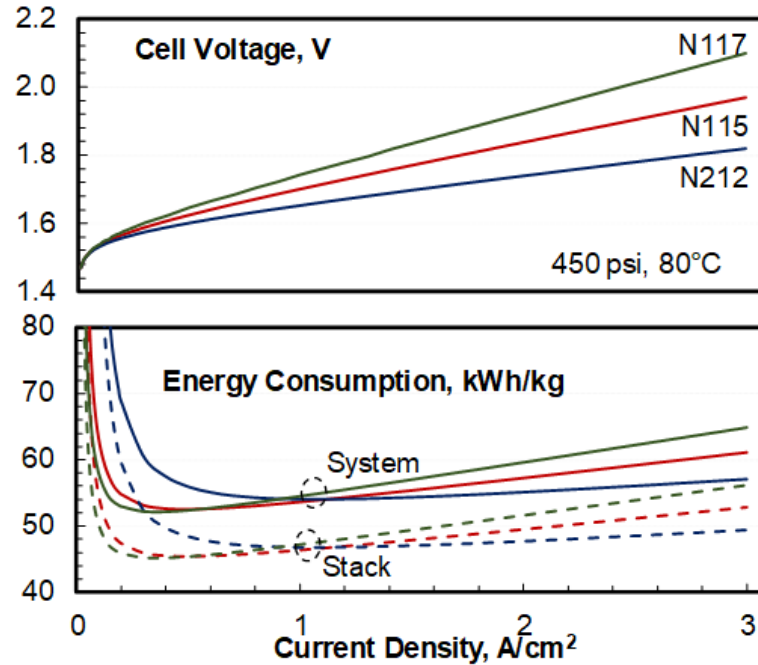
Operating Pressure

- Mainly affects H₂ crossover and energy consumption at low current density
- Stack turndown set by energy consumption, thermoneutral voltage and operating temperature



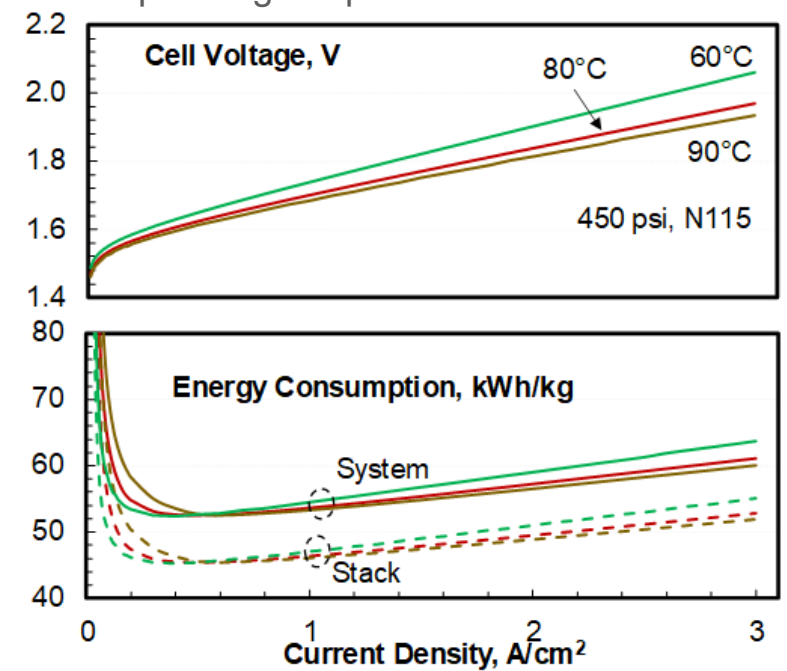
Membrane Resistance and H₂/O₂ Crossover

- Cross-over current density below which energy consumption can be smaller for thicker membranes
- Optimal membrane thickness depends on the duty cycle and operating pressure



Operating Temperature

- Cross-over current density below which energy consumption can be smaller at lower operating temperature
- Trade-off between membrane durability and energy consumption as affected by operating temperature



Anode: 0.4 mg_{IrO₂}/cm² loading; Unsupported ~ 5-nm IrO₂ catalyst (Alfa Aesar); ~250-μm thick, Ti based PTL with protective Pt coating; D2020 ionomer
Membrane: N212 or N117 **Cathode:** 0.1 mg_{Pt}/cm² loading with Pt/C catalyst material (TKK); untreated carbon paper PTL; D2020 ionomer

Accomplishment: Models Contextualize Advances in Cell Components and Quantify Remaining Progress Needed To Achieve DOE Targets

Stack Performance Targets

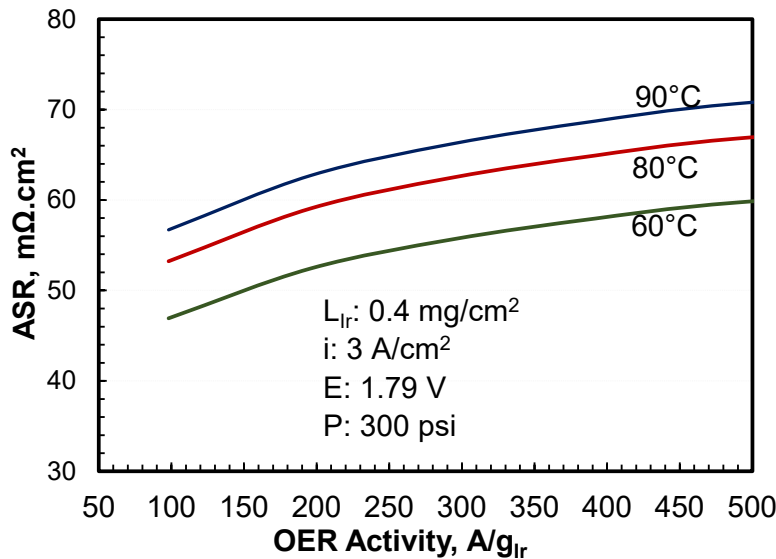
70% voltage efficiency

97.5% current efficiency

V/I target: 1.79 V at 3 A/cm², 300 psi, 0.4 mg_{Ir}/cm² anode catalyst loading

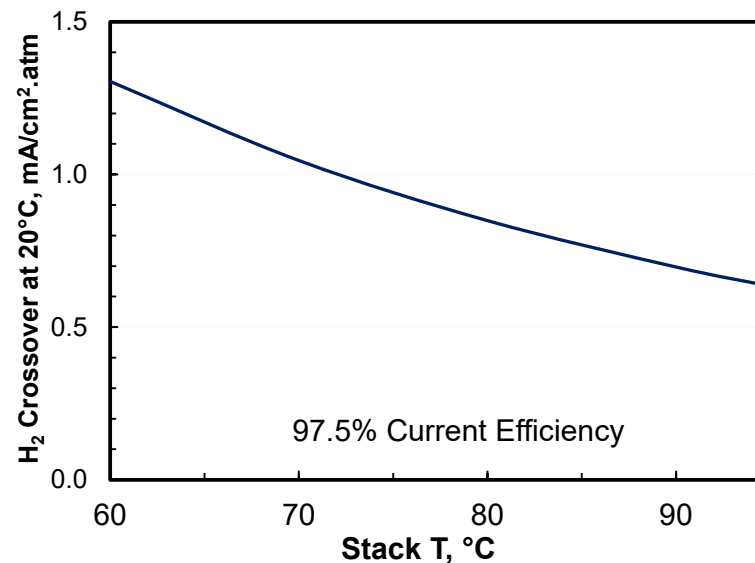
Target ASR and OER Activity

- OER Activity: Shorting-corrected current density at iR-corrected 1.45 V, 80°C, 1 atm; Reference value: ~100 A/g_{Ir} for 0.4 mg_{Ir}/cm², 60 mV/dec Tafel slope
- Reference Values of ASR N211 membrane: 20 mΩ.cm² at 100% RH, 80°C, 0.1 S/cm conductivity
Example contact resistance: 12 mΩ.cm²
- Possible to meet V/I target at 80°C with N212 membrane and status OER activity



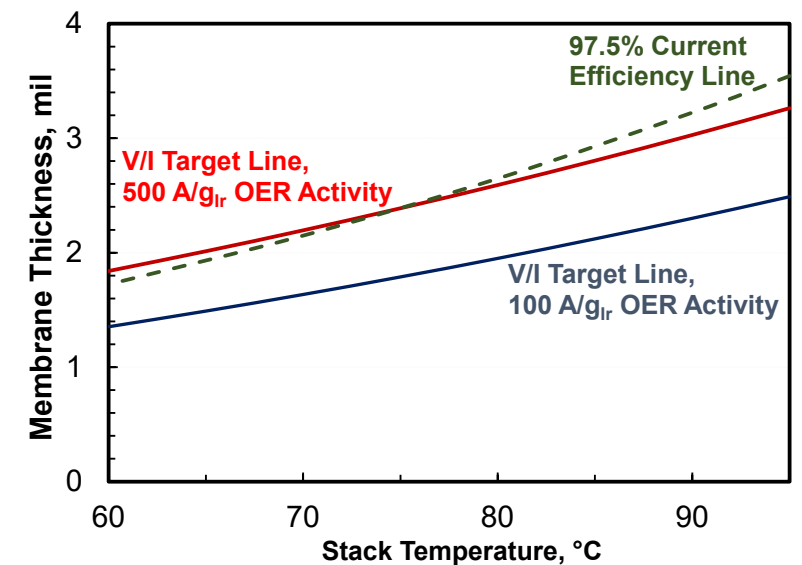
Target H₂ Crossover at 20°C

- Stack efficiency = Voltage efficiency (70%) x Current efficiency (97.5%)
- Reference H₂ crossover for N211 in fuel cells: 3 mA/cm².atm at 100% RH.
- Meeting current efficiency target at 80°C with N212 membrane requires 40% reduction in H₂ crossover



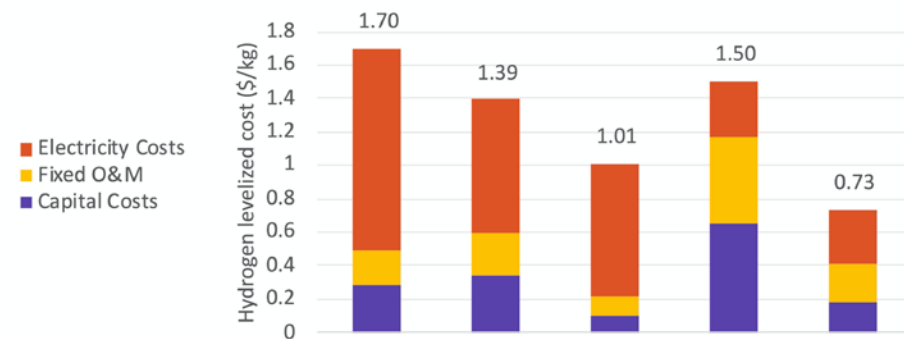
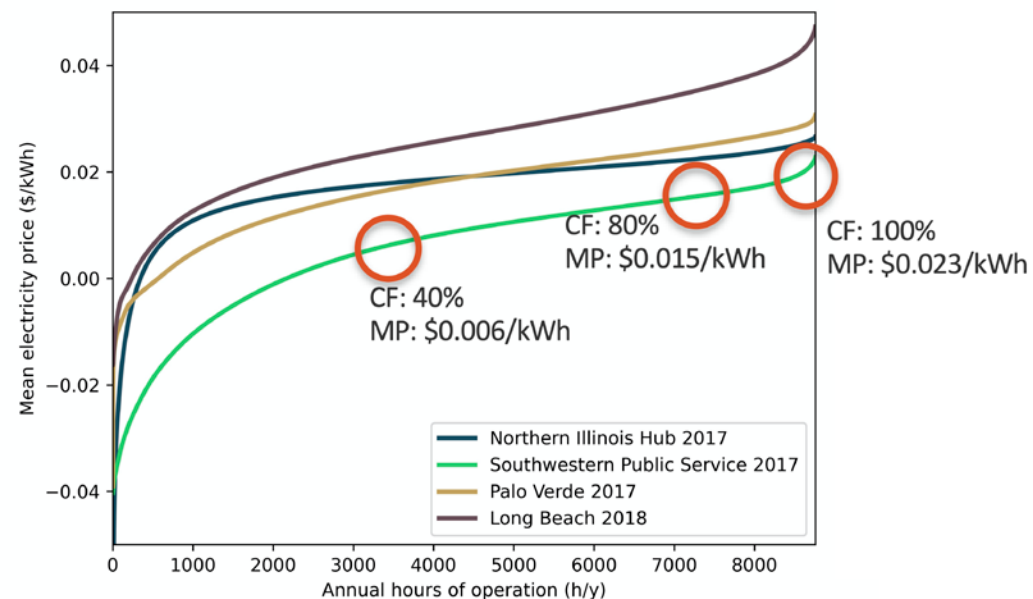
Example Target Application to PFSA Membrane

- With the status 100 A/g_{Ir} OER activity, it is more difficult to meet the current efficiency target than V/I target
- With 2 to 3.5 mil PFSA membranes and 5x OER activity, possible to meet both V/I and current efficiency targets



Accomplishment: Developed Levelized Cost Calculations Across a Variety of Electricity Sources and Prices

- Intermittent operation at wholesale LMPs provides opportunities to decrease average electricity cost
- Electricity prices like those in the Southwestern Public Service (SPS) Node in 2017 have low wholesale electricity prices
- Low-cost electrolyzers operating at those low-electricity prices can result in very low hydrogen levelized costs

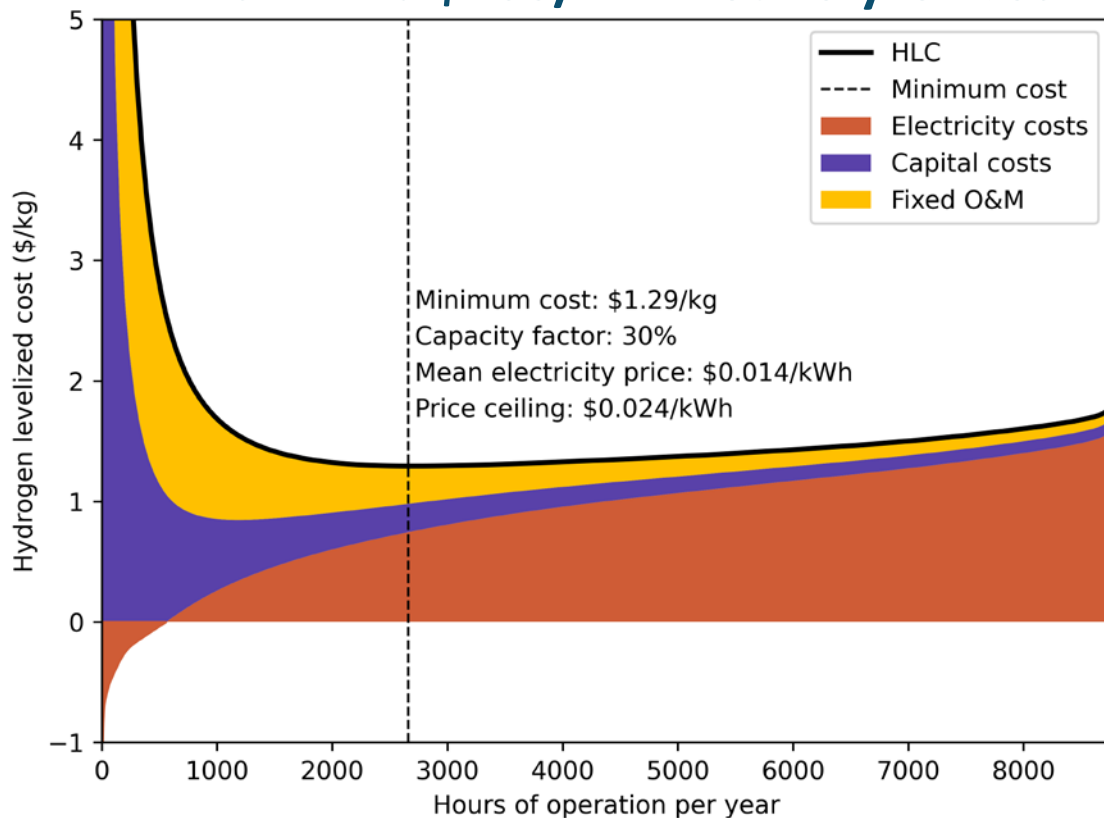


Electricity price	\$0.023/kWh	\$0.015/kWh	\$0.015/kWh	\$0.006/kWh	\$0.006/kWh
Capital cost	\$400/kW	\$400/kW	\$100/kW	\$400/kW	\$100/kW
Capacity factor	100%	80%	80%	40%	40%

Badgett, A., M. Ruth, B. Pivovar. "Economic Considerations for Hydrogen Production with a Focus on Polymer Electrolyte Membrane Electrolysis" Submitted as a chapter in Hydrogen Production by Water Electrolysis. Ed. Tom Smolinka. April 9, 2021.

Accomplishment: Quantified Tradeoffs Between Capacity Factor and Operating with Only Low-Cost Electricity

Composition of Costs Using All Possible Threshold Prices and Palo Verde 2017 LMPs with a \$100/kW Electrolyzer Cost



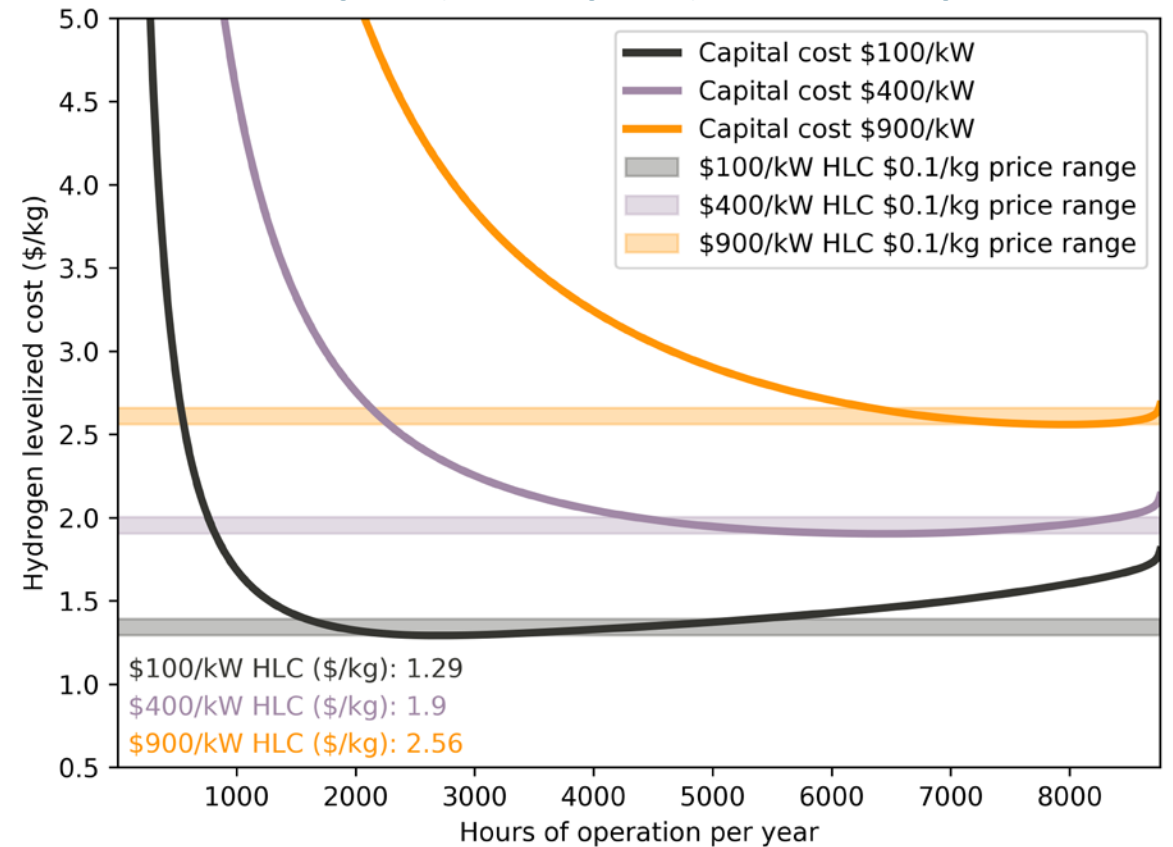
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- Levelized cost is a combination of capital costs, fixed operating costs (e.g., maintenance, labor), and electricity costs
- Increased capacity factors reduce capital and fixed operating costs per unit of hydrogen produced but the average electricity price increases increasing electricity cost per unit produced
- Operating only during hours with low-price electricity reduces electricity cost per unit produced but capital and operating cost increases
- Minimum hydrogen levelized cost is between each extreme

Accomplishment: Quantified Benefit of Electrolyzer Cost Reductions on Levelized Cost with Wholesale Electricity Prices

- Performed tradeoff analysis between capacity factor and electricity prices across three electrolyzer purchase costs (\$100/kW, \$400/kW, \$900/kW)
- Capital costs impact hydrogen levelized costs – Lower capital costs result in lower levelized costs especially when capacity factor is reduced to minimize levelized cost
- With the 2017 Palo Verde wholesale electricity prices, the minimum levelized cost drops from \$2.56/kg with a \$900/kW electrolyzer cost to \$1.29/kg with a \$100/kW electrolyzer cost

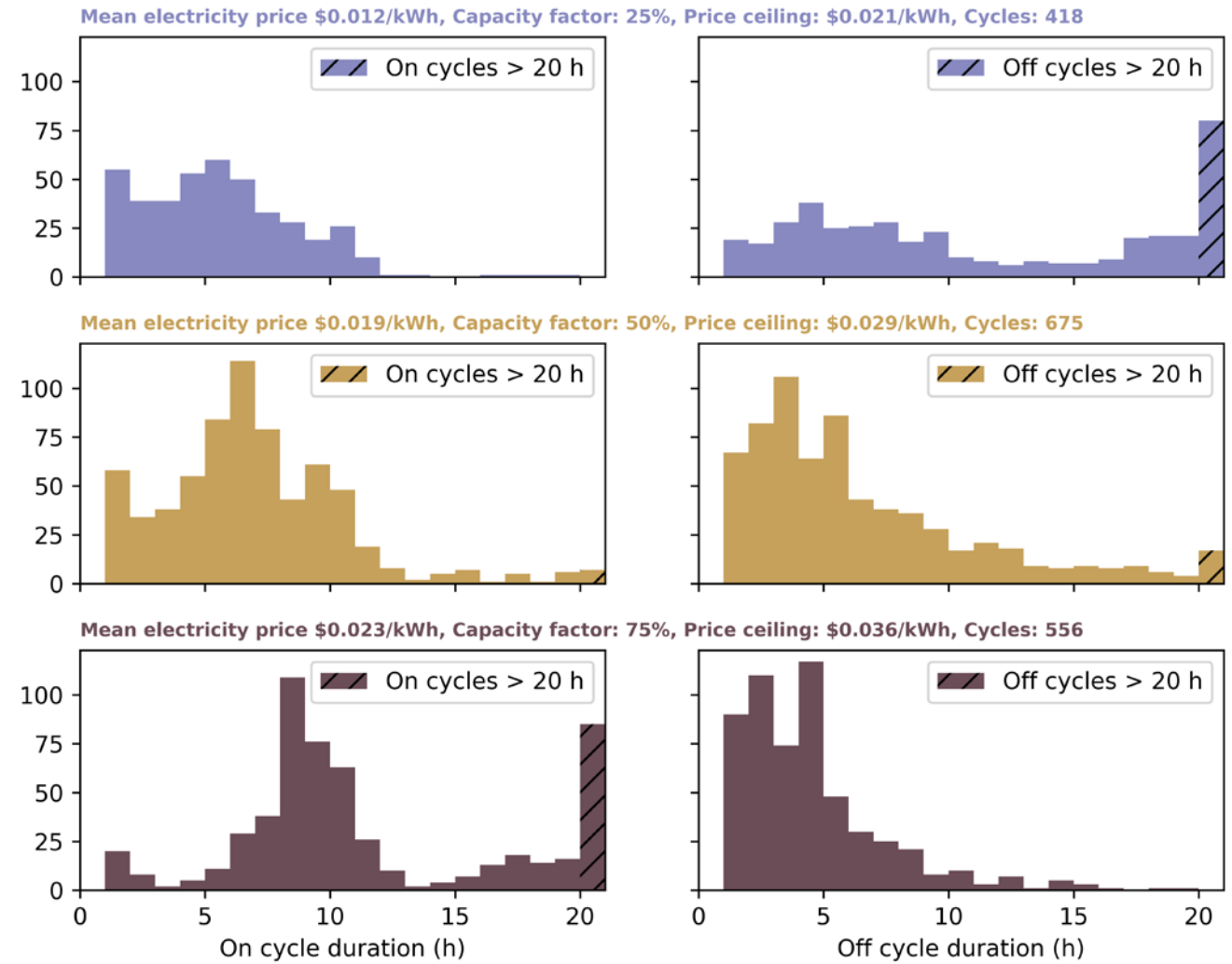
Hydrogen Levelized Costs with Palo Verde 2017 LMPs and Electrolyzer Costs of \$100/kW, \$400/kW, and \$900/kW



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Accomplishment: Developed Operating Cycles for Use in Durability Considerations and Experimental Design

- Regular cycling is needed to minimize hydrogen levelized costs by operating during times of low wholesale electricity prices
- Optimal on/off cycling is likely at least once per day and may be twice per day
- Cycling will likely impact electrolyzer durability (especially with lower-cost electrolyzers).
- Operating cycle strategies will inform H2NEW Task 1 strategies and experimental results will impact hydrogen levelized costs



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Accomplishments: Responses to Previous Year Reviewers' Comments

- This is a new project and has not been reviewed before.

- This task is being performed by two laboratories: NREL and ANL
- This task interacts with the rest of the H2NEW consortium which includes seven additional laboratories. Interactions include getting design and operating input and data from consortium partners and informing R&D staff of operating cycles and other considerations.
- Designs and assumptions are reviewed by industrial and academic partners on the consortium's advisory committee.
- Designs and manufacturing assessments involve interactions with Strategic Analysis, Inc.

- Baseline performance has not been finalized
- Impacts of degradation on technoeconomics have not been quantified
- Manufacturing costs are preliminary especially for key balance of plant components (e.g., power electronics)
- New designs, experimental results, and opportunities are being developed but their potential impact on overall performance and economics are unknown
- Electrolyzer end-of-life and recyclability and material circularity is unknown
- Potential benefits of direct coupling to renewables (e.g., PV-electrolyzer coupling without conversion to AC power) are hypothesized but unknown
- Impacts of adding a large number of electrolyzers to the grid on electricity prices are unknown

- Planned work during FY22
 - Finalizing a reference PEM electrolyzer system design and implementing it in the performance, manufacturing, and system models
 - Improve manufacturing cost model to capture current knowledge and improve estimates for key components (e.g., power electronics)
 - Add durability factors to performance models and economic models and quantify impacts of degradation on economics
- Planned work during outyears
 - Work with researchers to identify options and implement them in the models for use in comparisons and providing feedback to researchers
 - Adapt models to identify component reductions and potential benefits of direct coupling to renewables
 - Develop and perform price-maker analyses to quantify potential impacts of increased loads on electricity generation and prices

Proposed future work is subject to change based on funding levels.

- Performance, manufacturing, and system analysis is underway and tools are being developed and implemented
- Results will be used to evaluate cost, performance, and durability tradeoffs to determine optimum LTE deployment to achieve \$2/kg production cost in renewable energy integration scenarios
- Operating pressure, temperature, and membrane properties are key considerations
- Tradeoffs between using low-price electricity and cycling are a key consideration while developing operating strategies and durability objectives
- Interactions with others in H2NEW lead to improved analysis and provide opportunities for analysis results to guide research and target setting

Thank You!

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Supporting Slides

- This analysis provides context for technology transfer across H2NEW
- No additional specific technology transfer is occurring in this task

- This task is quantifying progress of H2NEW toward DOE's \$2/kg production target.

- Badgett, A., M. Ruth, B. Pivovar. “Economic Considerations for Hydrogen Production with a Focus on Polymer Electrolyte Membrane Electrolysis” Submitted as a chapter in Hydrogen Production by Water Electrolysis. Ed. Tom Smolinka. April 9, 2021.
- Badgett, A., M. Ruth, B. James, B. Pivovar “Techno-economic Analysis (TEA) Methods Identifying Cost Reduction Potential for Water Electrolysis Systems” Submitted to *Current Opinion in Chemical Engineering*. February 4, 2021.

Key Assumptions and Knowledge Gaps for Technoeconomic Calculations in this Presentation

Assumption	Notes
Wholesale electricity market access	In the electricity price analyses shown here, we have assumed that electrolyzers will have access to wholesale electricity priced at hourly intervals. This access enables lower hydrogen costs through operation as a dispatchable load, however electrolyzers do not currently operate in this manner and those electricity markets are not regularly available to them at this time. We have discussed this with regard to the benefits that electrolysis that can offer as a dispatchable, scalable resource providing benefits in capacity and economic return. Areas of opportunity include connecting the electricity market more strongly to transportation and industrial sectors, offering capacity and seasonal storage options beyond other traditional storage pathways, accessing markets beyond grid to grid, and allowing for one way storage removing energy from the electricity sector that doesn't need to be returned to the grid. However, regulations that allow access to wholesale markets or having electrolyzers deployed behind the meter will likely be critical for economically competitive HLC.
Electrolyzer durability, performance, and cost	Most of the H2A analysis inputs explored in this work either assumed that the efficiency of the device was constant over its operation or achieved a high net average efficiency of operation (66% efficiency). This assumption was made regardless of the cost of the electrolysis system or the manner in which it was operated. The only caveat to this is that each electrolysis system modeled had the same number of calendar hours of operation, basically assuming that dispatchable operation has the same impact as a different number of operating hours, or any impacts of operating dynamically. The research community has demonstrated that operating strategy impacts the durability of electrolysis systems, and the exact tradeoff between operating strategy and degradation has emerged as a critical research area. Based on past durability of PEM electrolyzers and the performance of PEM fuel cells systems, it has been proposed that operating strategies can be developed that meet combined cost, performance and durability targets for PEM electrolyzers, but meeting durability requirements or achieving cost reductions while maintaining required performance levels remains an area of scientific uncertainty and is being actively investigated.
Fixed O&M costs	Fixed annual O&M costs within this Chapter were estimated using H2A default assumptions (a fixed percentage of installed capital costs) and did not vary with the number of hours the system was assumed to be operated annually or the manner in which it was operated. O&M costs are unlikely to be a fixed percentage of capital costs. Rather, they are likely to depend significantly on how systems are operated. Testing and operational strategy development are needed to better estimate O&M costs and under what circumstances they become critical to HLC.
Evolution of electricity markets including impact of electrolyzers	In a number of the analyses presented, historical LMPs were used to illustrate how HLC could be optimized with different electrolyzer deployment strategies. In general, the costs for wholesale electricity have been decreasing and becoming more variable. That combination increases the value proposition of flexible loads like electrolyzers because they can support balancing electricity generation and load. Costs of balancing generation and load are likely to increase as variable renewable energy penetration further increases. These trends do not guarantee what the future electricity markets will be and none of the analysis performed in this Chapter attempted to capture the potential impact that large scale electrolysis (or other energy storage options) might have on wholesale electricity markets. These are complicated interactions that are likely to evolve considerably in the coming years.
Renewables deployment	Many of the emerging challenges to the electric sector are being driven by the improving economics and increased deployment of renewable energy. Renewable energy is increasing in deployment through a combination of economic factors and other policy or legislative actions. As renewable penetration increases, technologies like electrolysis can provide benefits by enabling large scale energy storage over seasonal durations creating opportunities for increased value of wind and solar resources. There is a synergy between electrolysis and renewable energy deployment that allows each to make the other more economical, but often deployment of renewable energy is not done solely on an economic basis, and electrolyzers can benefit from increasing renewable deployment.
Policy drivers/ legislative actions	Policy is a powerful tool that can either support or discourage further development of electrolysis. It can incentivize electrolysis deployment directly by applying to the electrolyzer itself or indirectly by applying to other factors that influence electrolysis. Those other factors could include increasing variable renewable electricity generation, enabling access to wholesale electricity rates, and through other economic drivers such as costs on different emissions. While the analyses conducted here do not consider the effects of any future policy mechanisms, we acknowledge the importance of such mechanisms to influence deployment of electrolysis.
Hydrogen storage and transmission	None of the work presented in this Chapter focused on the significant challenges of hydrogen storage and transmission and the costs associated with these challenges. In order to advance electrolysis technology and ensure that low HLC availability has broad impact, both hydrogen storage and transmission need advances in parallel. In addition, hydrogen distribution for smaller-scale demand nodes (e.g., fueling stations) need advances for those markets to grow.