Hydrogen Storage System Modeling:

Public Access, Maintenance, and Enhancements

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DOE Hydrogen Program
2024 Annual Merit Review and Peer Evaluation Meeting
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Project ID: ST008
DOE WBS #: NREL – 4.2.0.502
PNNL – 4.2.0.702

NREL/PR-5700-89517

Project Goal

The overall vision of this project is to provide ownership and support for **maintaining existing material-based hydrogen storage systems models**. This includes making models accessible to the research community through a public web page and updating and enhancing storage systems models to support material developers in assessing their materials relative to DOE vehicle-level targets. Key elements for FY24:

- Continue to update and enhance existing models for broader application and user-friendliness.
- Develop tools to evaluate the performance of hydrogen storage materials developed under HyMARC activities or other fundamental hydrogen storage materials discovery research.
- Expand the application of current hydrogen storage models beyond light-duty vehicles to include medium-, heavy-duty, and mining vehicles and stationary application(s).
- Develop models for alternatives, such as LOHCs, to material-based systems (liquefied & gaseous H_2) and compare for various mobile and stationary use cases.

HyMARC
Hydrogen Materials Advanced Research Consortium

Overview

Timeline

- **Start: October 1, 2015**
- **End: September 30, 2024***

Budget

- **Total DOE Funds Received to Date**: $2,907,000**
    - **FY16 DOE Funding: $336,000**
    - **FY17 DOE Funding: $389,000**
    - **FY18 DOE Funding: $375,000**
    - **FY19 DOE Funding: $275,000**
    - **FY20 DOE Funding: $255,000**
    - **FY21 DOE Funding: $497,000**
    - **FY22 DOE Funding: $260,000**
    - **FY23 DOE Funding: $235,000**
    - **FY24 DOE Funding: $285,000**

Partners

- **National Renewable Energy Laboratory (NREL)**
- **Pacific Northwest National Laboratory (PNNL)**
- **Hydrogen Materials Advanced Research Consortium (HyMARC)**

*Project continuation and direction determined annually by DOE
**Since the project started

Potential Impact – Addressing Barriers with Models

Barriers	Model Addressing Barrier
A. System Weight and Volume	Sizing Tools
B. System Cost	Tank Volume/Cost Model
C. Efficiency	Framework Model - Onboard Efficiency - Fuel Economy
E. Charging/Discharging Rates	Framework Model Refueling Model
I. Dispensing Technology	Framework Model - Initial and Final System Conditions Refueling Model
K. System Life-Cycle Assessment	All Models

Approach

A collaborative effort to manage and enhance existing hydrogen storage system models and develop new models to support material developers in assessing their materials relative to DOE vehicle-level targets

- Transfer knowledge from vehicle-level system engineering studies to future materials research.
- Manage the hydrogen storage system model dissemination within the HyMARC web page.
- Manage, update, enhance, and validate the modeling framework and the specific storage system models developed for metal hydrides, adsorbents, and chemical hydrogen storage materials.
- Develop models that will accept direct materials property inputs and can be measured by materials researchers.
- **Ultimate Goal**: Provide validated modeling tools that researchers will use to evaluate the performance of their new materials in mobile and stationary applications relative to the available DOE Technical Targets.

Approach – Improving Model Utilities for Materials Researchers

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Isotherm Fitting Tool

Dubinin-Astakhov Parameters

Stand-Alone System Design Tools

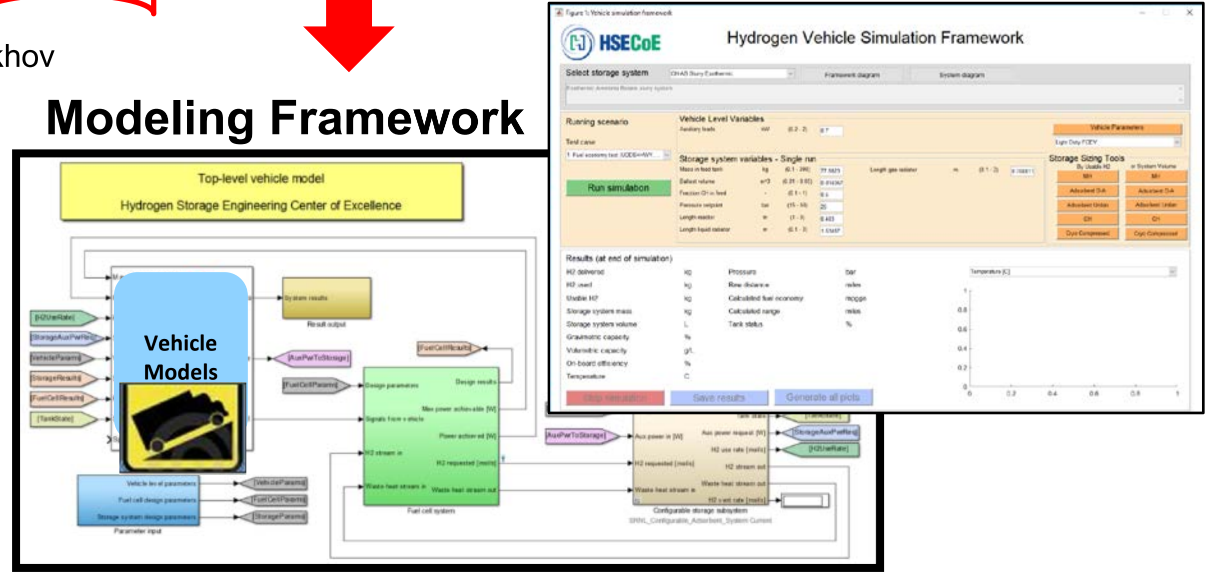
Component and System Mass and Volume

Stand-Alone Values

Estimated Gravimetric and Volumetric Capacity

Available at
https://www.hymarc.org/models.html

Modeling Framework



Vehicle Models

Light-Duty Vehicle
Medium-Duty Vehicle
(Class 4/6)
Heavy-Duty Vehicle
(Class 8)

DOE Technical Targets

Gravimetric and Volumetric Capacity
Durability and Operability
  Operating Temperature and Pressure
  Onboard Efficiency
Charging/Discharging Rates
  Start-up
  Refueling

Approach – Modeling Tools Available or In Progress

Note: Updates in blue text

Framework Model with:

Physical Storage	UTRC/NREL
Compressed/Cryo-Compressed H_2	SRNL/NREL
Chemical Hydrogen (CH)	PNNL/NREL
Adsorbent (AD)	SRNL/NREL
Metal Hydride (MH)	PNNL/NREL
Liquid Hydrogen (LH)	PNNL/NREL

FY23-24: Incorporate the CH-LOHC model into the framework model
FY24: Inclusion of passenger train and a stationary application.

Stand-Alone System Design Tools:

Adsorbent (AD)	SRNL
Chemical Hydrogen (CH)	PNNL
Metal Hydride (MH)	PNNL
Compressed/Cryo-Compressed H_2	SRNL
Liquid Hydrogen (LH)	PNNL/NREL

FY23-24: Expand CH model to catalyzed LOHC
FY24: plan to release CH-LOHC model

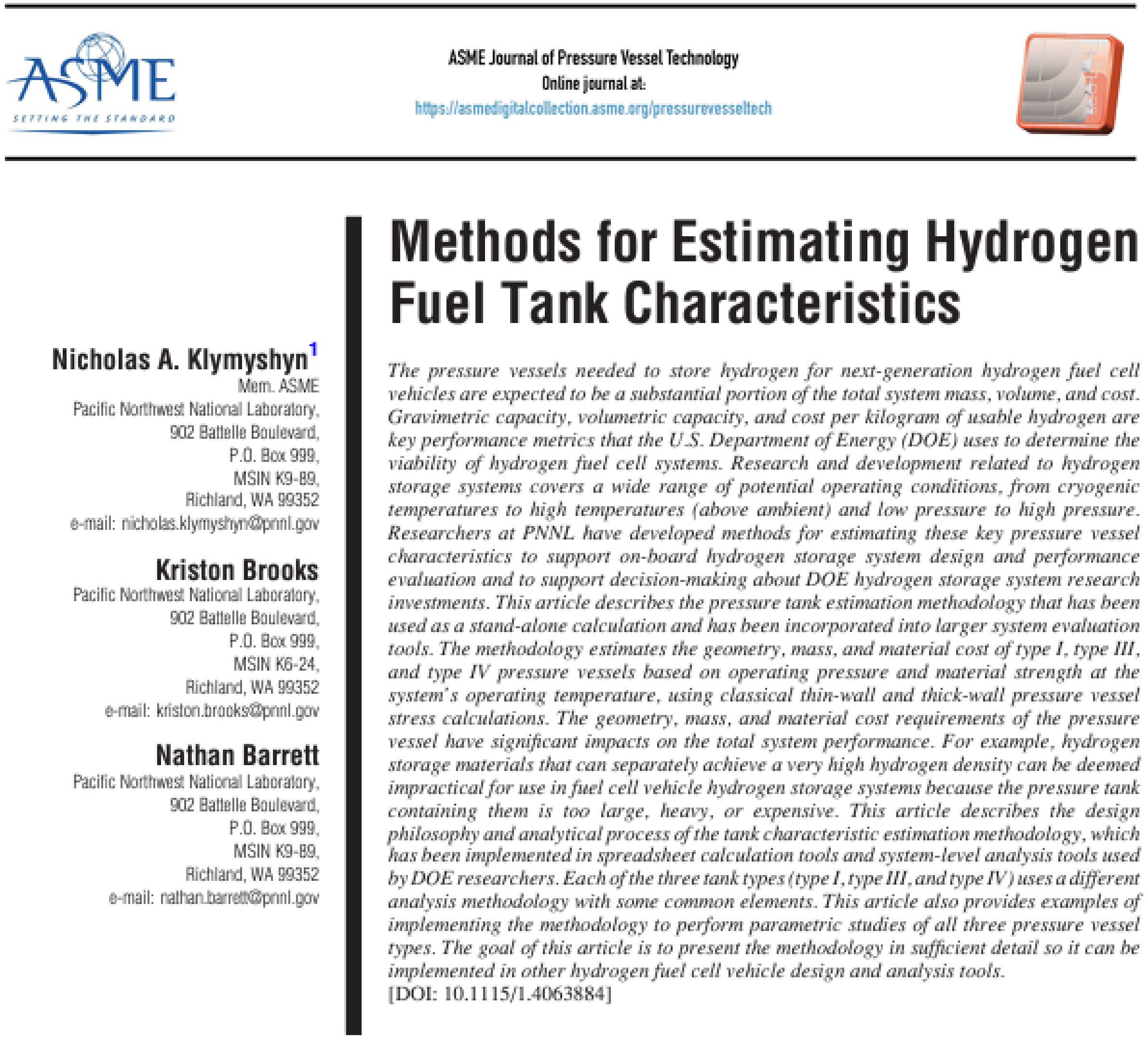
Additional Tools/Models:

MH Acceptability Envelope (MHAE)	SRNL
Tank Volume/Cost Model (Tankinator)	PNNL
AD Isotherm Fitting Tool	SRNL
MH Refueling Model	PNNL
Round-Trip Efficiency Estimator	PNNL

FY23-24: Release Tankinator 4.0

Accomplishments and Progress – Tankinator Published

- **Tankinator 4.0 was released in FY23**
- **“Methods for Estimating Hydrogen Fuel Tank Characteristics” published**
  - Describes the design philosophy and analytical process of the tank characteristic estimation methodology (spreadsheet calculation tools and system-level analysis tools)
  - Each of the three tank types (type I, type III, and type IV) uses a different analysis methodology with some common elements.
  - Provides examples of implementing the methodology to perform parametric studies of all three pressure vessel types.



ASME Journal of Pressure Vessel Technology
Online journal at:
https://asmedigitalcollection.asme.org/pressurevesseltech

Methods for Estimating Hydrogen Fuel Tank Characteristics

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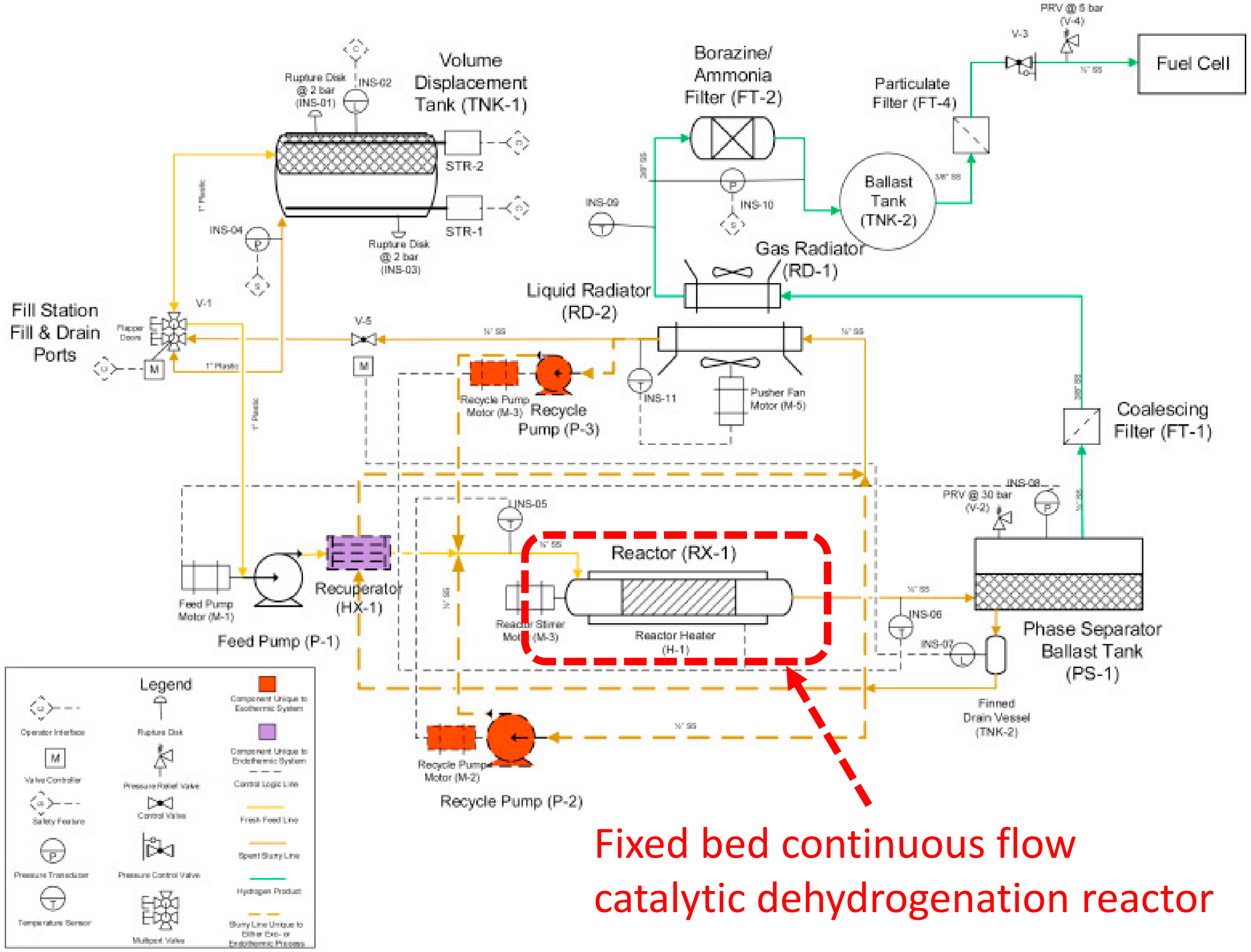
The pressure vessels needed to store hydrogen for next-generation hydrogen fuel cell vehicles are expected to be a substantial portion of the total system mass, volume, and cost. Gravimetric capacity, volumetric capacity, and cost per kilogram of usable hydrogen are key performance metrics that the U.S. Department of Energy (DOE) uses to determine the viability of hydrogen fuel cell systems. Research and development related to hydrogen storage systems covers a wide range of potential operating conditions, from cryogenic temperatures to high temperatures (above ambient) and low pressure to high pressure. Researchers at PNNL have developed methods for estimating these key pressure vessel characteristics to support on-board hydrogen storage system design and performance evaluation and to support decision-making about DOE hydrogen storage system research investments. This article describes the pressure tank estimation methodology that has been used as a stand-alone calculation and has been incorporated into larger system evaluation tools. The methodology estimates the geometry, mass, and material cost of type I, type III, and type IV pressure vessels based on operating pressure and material strength at the system's operating temperature, using classical thin-wall and thick-wall pressure vessel stress calculations. The geometry, mass, and material cost requirements of the pressure vessel have significant impacts on the total system performance. For example, hydrogen storage materials that can separately achieve a very high hydrogen density can be deemed impractical for use in fuel cell vehicle hydrogen storage systems because the pressure tank containing them is too large, heavy, or expensive. This article describes the design philosophy and analytical process of the tank characteristic estimation methodology, which has been implemented in spreadsheet calculation tools and system-level analysis tools used by DOE researchers. Each of the three tank types (type I, type III, and type IV) uses a different analysis methodology with some common elements. This article also provides examples of implementing the methodology to perform parametric studies of all three pressure vessel types. The goal of this article is to present the methodology in sufficient detail so it can be implemented in other hydrogen fuel cell vehicle design and analysis tools.

[DOI: 10.1115/1.4063884]

Accomplishments and Progress – Expanding Chemical Hydrogen Model to LOHCs

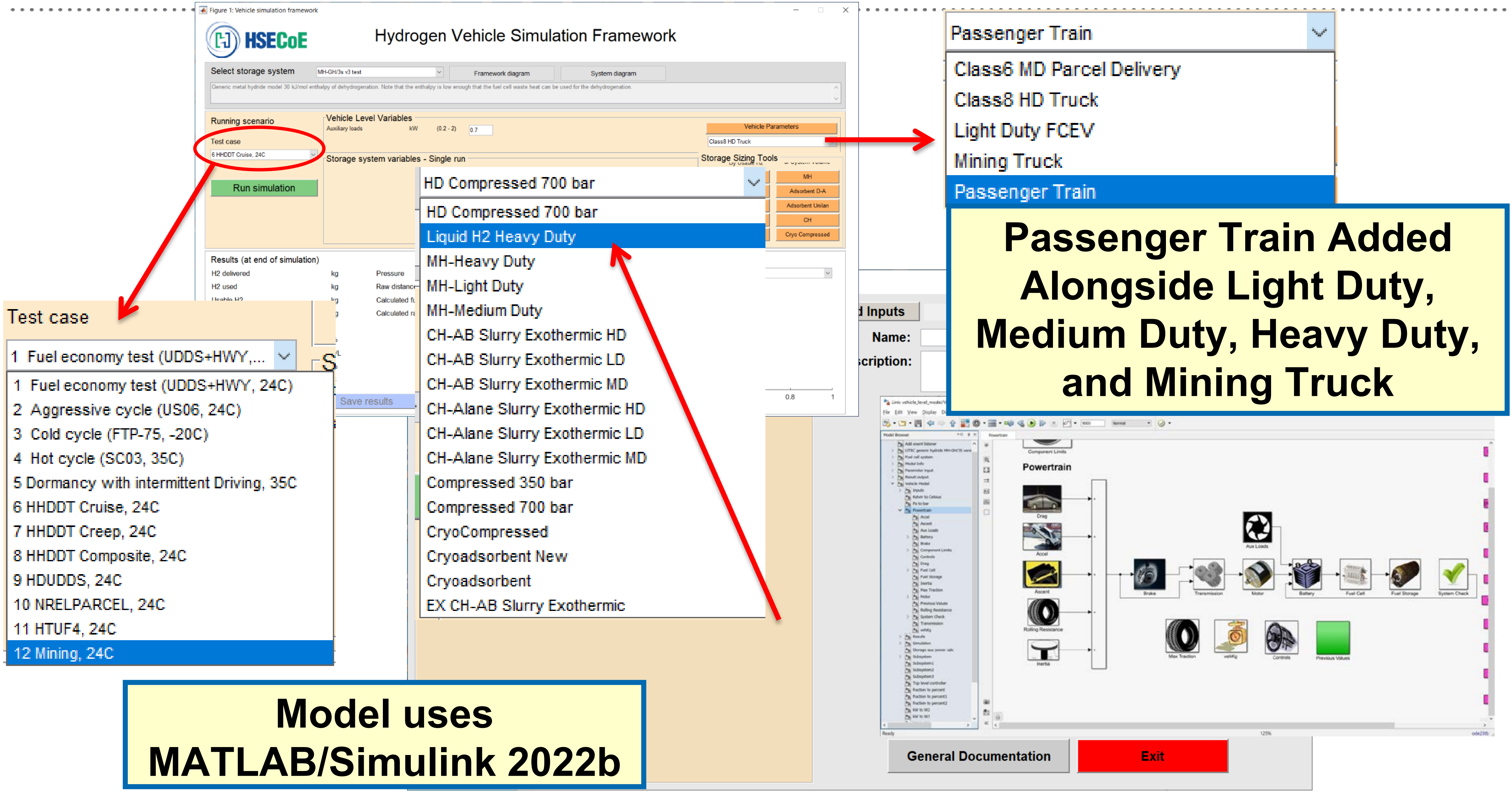
- **Expanded the CH Stand-Alone System Design Tools to include the capability of using Liquid Organic Hydrogen Carriers (LOHCs)**
  - Tested for various LOHCs and corresponding catalysts, including methylcyclohexane, H18-dibenzyl-toluene, ethylene glycol, and ethanol.
  - Supported SNL/SoCalGas team for the initial fuel selection for a hydrogen-powered train application
  - Incorporated with the Vehicle Framework for LD/MD/HD vehicles
  - Identified challenges and needs for further improvement

- **Plan to release a CH-LOHCs model in FY24**



Fixed bed continuous flow catalytic dehydrogenation reactor

Accomplishments and Progress – Vehicle Framework Graphical User Interface



Select storage system: MH-GH/3s v3 test

Generic metal hydride model 30 kJ/mol enthalpy of dehydrogenation. Note that the enthalpy is low enough that the fuel cell waste heat can be used for the dehydrogenation.

Test case: 6 HHDDT Cruise, 24C

Auxiliary loads kW (0.2 - 2) 0.7

Class8 HD Truck

H2 delivered kg

H2 used kg

Usable H2 kg

Pressure

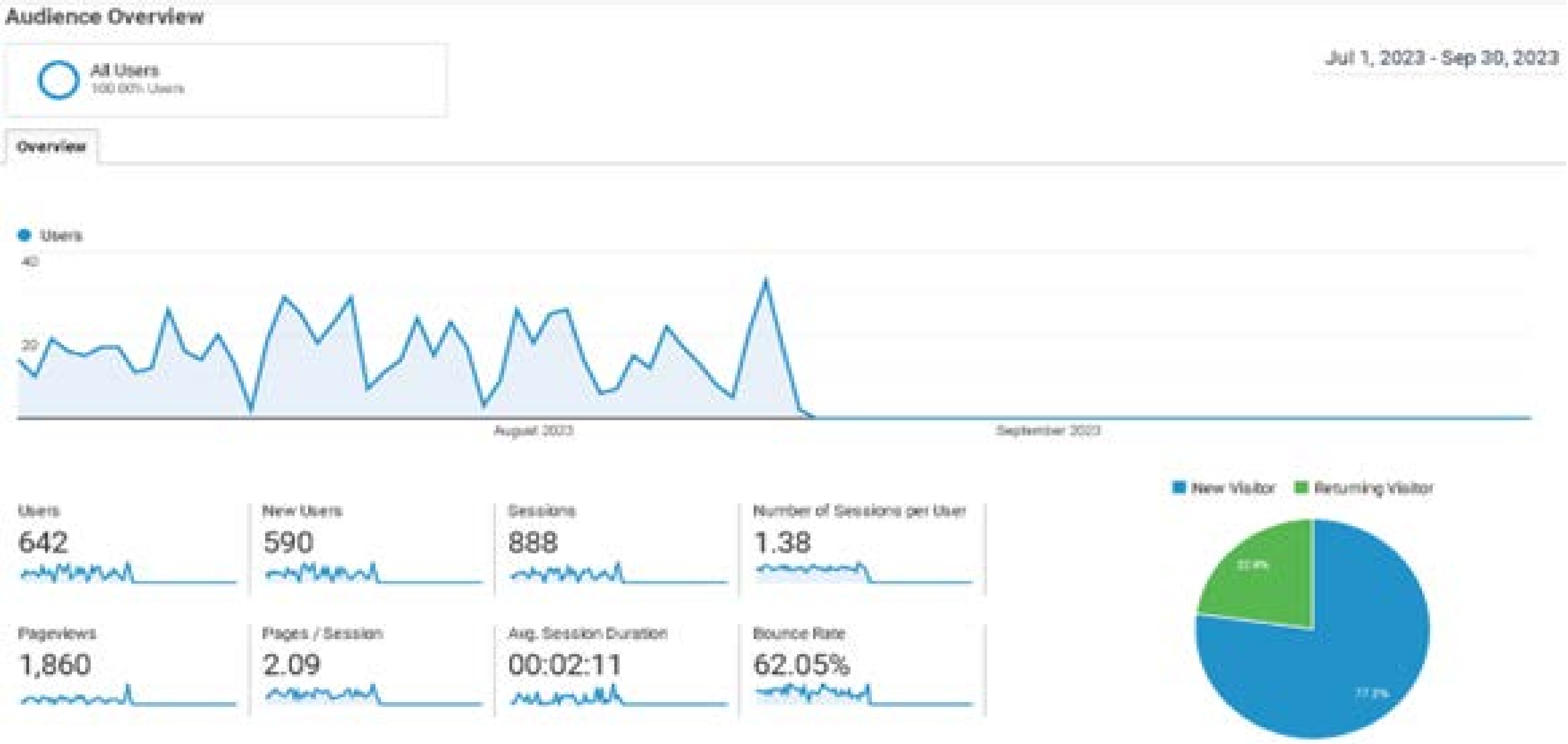
Raw distance

Passenger Train Added Alongside Light Duty, Medium Duty, Heavy Duty, and Mining Truck

Model uses MATLAB/Simulink 2022b

MD: medium-duty, HD: heavy-duty

Accomplishments and Progress – Model Website Analytics: Activity (July 1, 2023–September 30, 2023)



Users 642

New Users 590

Sessions 888

Number of Sessions per User 1.38

Pageviews 1,860

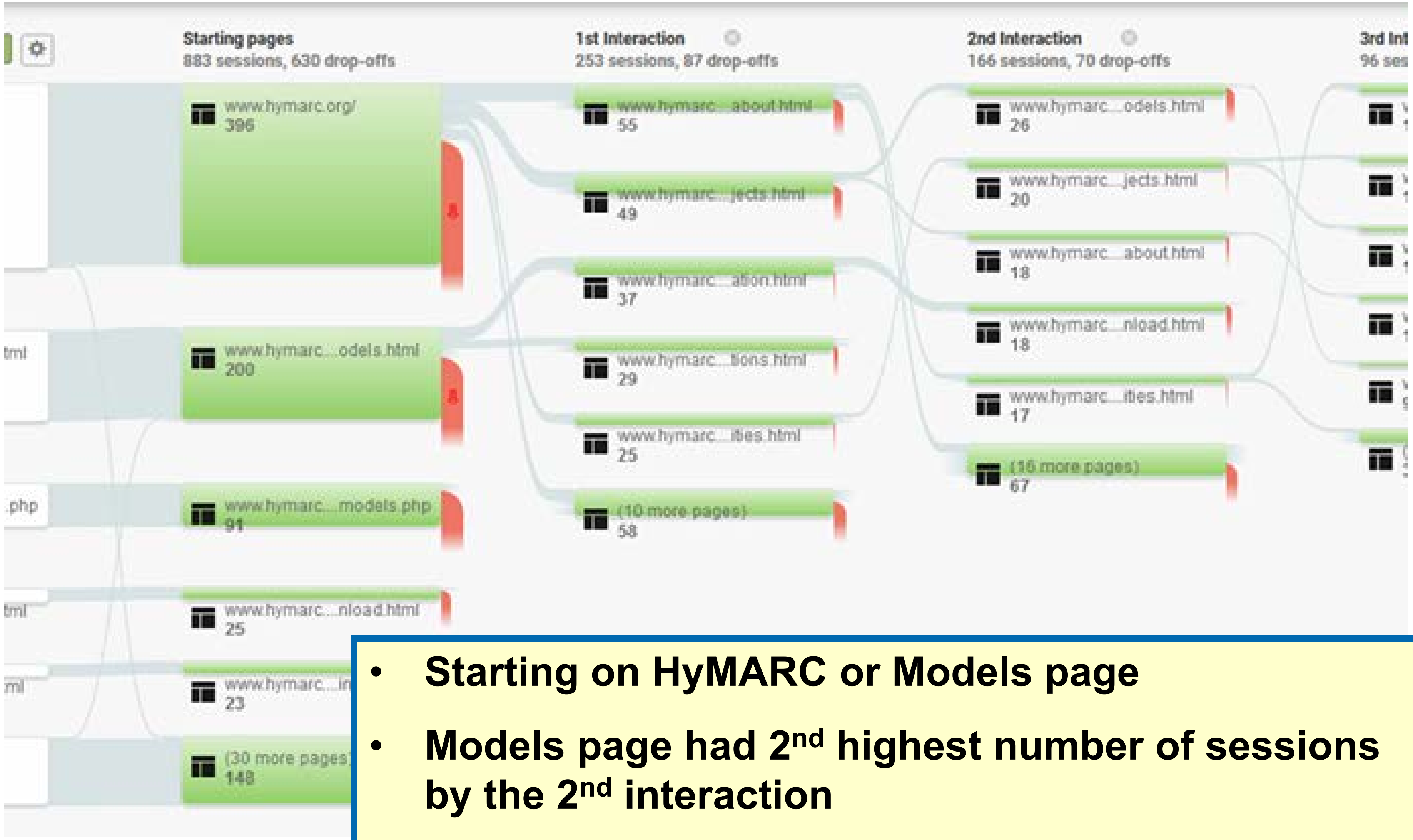
Pages / Session 2.09

Avg. Session Duration 00:02:11

Bounce Rate 62.05%

Activity every week; 77% of sessions were by new visitors
(New web configuration analytics stopped tracking in late August)

Accomplishments and Progress – Model Website Analytics: Web Flow (July 1, 2023–September 30, 2023)



- **Starting on HyMARC or Models page**
- **Models page had 2nd highest number of sessions by the 2nd interaction**

Accomplishments and Progress – Model Website Analytics: Locations (October 1, 2023 – March 15, 2024)

Event count by Country

COUNTRY	EVENT COUNT
United States	85
India	66
South Korea	52
Morocco	51
China	47
Italy	43
United Kingdom	30

Model download registration by country shows global interest from India, South Korea, Morocco, China, Italy, UK and others

Accomplishments and Progress – Model Downloads (through March 15, 2024)

MODEL	Total	Totals AMR2023	Additional through FY24 Q2
H_2 Storage Tank Mass and Cost Model	**825**	675	150
MHAE Model	**356**	285	71
MHFE Model	**426**	350	76
Vehicle Simulator Framework Model	**625**	502	123
CH System Design Stand-Alone	**430**	332	98
Adsorbent System Design Stand-Alone	**397**	315	82
MH System Design by Usable H_2	**346**	263	83
MH System Design by System Volume	**315**	225	90

Most downloads are for *Tank Mass and Cost Model* and *Vehicle Simulator Model*

Collaboration and Coordination

Organization	Relationship	Type	Responsibility
NREL	Team Member	National Lab	Update website and framework
PNNL	Team Member	National Lab	Chemical hydrogen and catalytic LOHC modeling
SNL-SoCalGas	Material Research	National Lab/ Collaboration	LOHC data
HyMARC—PNNL	Material Research	National Lab/ Collaboration	LOHC data

DEIA/Community Benefits Plans and Activities

- **This project did not have a Diversity, Equity, Inclusion, and Accessibility (DEIA) plan or Community Benefits Plan (CBP)**

Proposed Future Work – FY24 Milestones and Next Steps

Deliverable		Due
FY24-Q1	Improve LOHC models in the Vehicle Framework for LD/MD/HD vehicles.	**Complete**
FY24-Q2	Provide update on web portal activity—web site hits and time on site, web site use location and model downloads.	**Complete**
FY24-Q3	Develop reactor model for chemical hydrogen storage materials based on catalytic liquid organic hydrogen carriers (LOHCs).	**6/30/2024**
FY24-Q4	Storage System Modeling: Develop and integrate at least 2 mobile and/or stationary applications into the Vehicle Framework and demonstrate its use with adsorbents, MH, chemical hydrogen and liquid H_2 storage	**9/30/2024**

Any proposed future work is subject to change based on funding levels

Summary

Relevance	• Provide materials-based hydrogen storage researchers with models and materials requirements to assess their material's performance over a range of applications.
Approach	• Improve stand-alone model and framework utility by bridging the gap between the information generated by the materials researcher and the DOE Technical Targets.
Technical Accomplishments and Progress	• Tankinator 4.0 and methods published in the ASME Journal of Pressure Vessel Technology • Stand-alone tools and framework are being expanded beyond light, medium- and heavy-duty vehicles to mining vehicles and passenger train • Modeling and adding CH-LOHC into the framework model • Stand-alone tools and framework have been used to evaluate materials for HyMARC to help better understand the potential benefits of new materials.
Collaborations	• Project team includes NREL and PNNL • Maintained communications with material developers from HyMARC and other academic institutions regarding new hydrogen storage materials.
Proposed Future Research	• Expand the use of models by demonstrating their utility with other storage materials, such as LOHCs, and vehicle class options, and compare to storage using liquid H_2 and gaseous H_2.

Any proposed future work is subject to change based on funding levels

Technical Backup and Additional Information

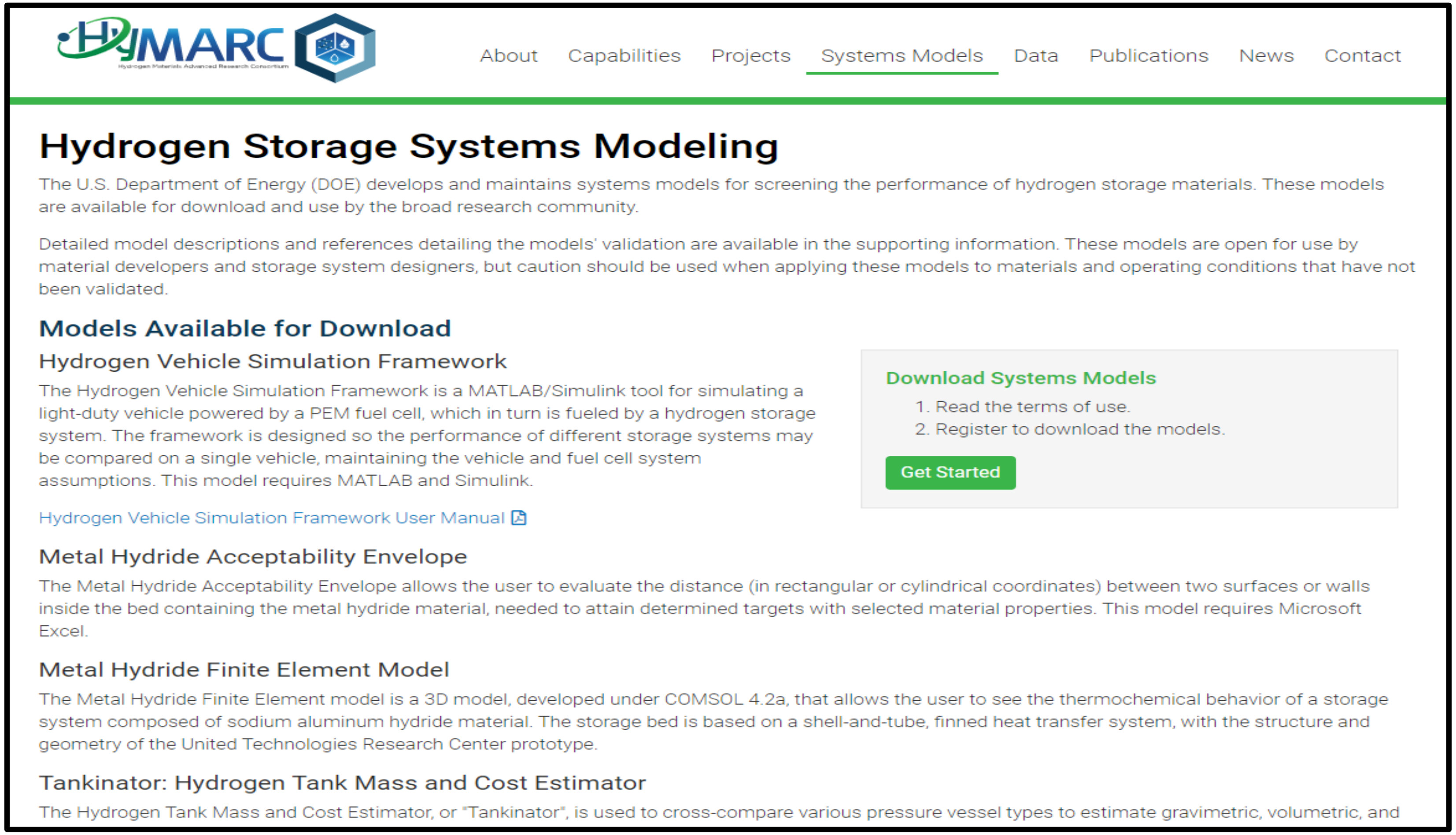
Technology Transfer Activities

- Maintaining model web portal on HyMARC site.
- Continued collaboration and outreach with industry and university partners to expand the application of the models.

Technology Transfer Activities – Maintaining Model Web Portal

H2 Storage models are accessible through the HyMARC/System Models site.

https://www.hymarc.org/models.html



Hydrogen Storage Systems Modeling

The U.S. Department of Energy (DOE) develops and maintains systems models for screening the performance of hydrogen storage materials. These models are available for download and use by the broad research community.

Detailed model descriptions and references detailing the models' validation are available in the supporting information. These models are open for use by material developers and storage system designers, but caution should be used when applying these models to materials and operating conditions that have not been validated.

Models Available for Download

Hydrogen Vehicle Simulation Framework

The Hydrogen Vehicle Simulation Framework is a MATLAB/Simulink tool for simulating a light-duty vehicle powered by a PEM fuel cell, which in turn is fueled by a hydrogen storage system. The framework is designed so the performance of different storage systems may be compared on a single vehicle, maintaining the vehicle and fuel cell system assumptions. This model requires MATLAB and Simulink.

Hydrogen Vehicle Simulation Framework User Manual

Download Systems Models

1. Read the terms of use.
2. Register to download the models.

Metal Hydride Acceptability Envelope

The Metal Hydride Acceptability Envelope allows the user to evaluate the distance (in rectangular or cylindrical coordinates) between two surfaces or walls inside the bed containing the metal hydride material, needed to attain determined targets with selected material properties. This model requires Microsoft Excel.

Metal Hydride Finite Element Model

The Metal Hydride Finite Element model is a 3D model, developed under COMSOL 4.2a, that allows the user to see the thermochemical behavior of a storage system composed of sodium aluminum hydride material. The storage bed is based on a shell-and-tube, finned heat transfer system, with the structure and geometry of the United Technologies Research Center prototype.

Tankinator: Hydrogen Tank Mass and Cost Estimator

The Hydrogen Tank Mass and Cost Estimator, or "Tankinator", is used to cross-compare various pressure vessel types to estimate gravimetric, volumetric, and

Publications and Presentations

Nickolas Klymyshyn, Kriston Brooks, and Nathan Barrett, “**Methods for Estimating Hydrogen Fuel Tank Characteristics**,” J. Pressure Vessel Technol. 2024, 146, 11501. https://doi.org/10.1115/1.4063884.

Previous Accomplishments – Stand-Alone Sizing Routine for Mining Vehicle

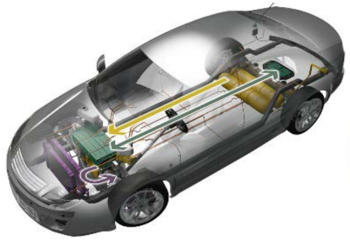
Property	Units	Metal Hydride	Chemical Hydrogen	Adsorbent
Material Studied	--	$NaAlH_4$	NH_3BH_3	MOF-5
System Mass	kg	4510	3239	3146
System Volume	L	4066	5645	5899
# Tanks		5	4	5
Active Material Mass	kg	2260	1939	497
Active Material Volume	L	2898	2179	4409
Single Tank Mass	kg	350	656	409
Single Tank Volume	L	580	553	1167
Tank Length	m	2.0	2.0	3.0
Tank Diameter	m	0.75	0.59	0.72
BOP Mass	kg	500	1170	252
BOP Volume	L	1167	3433	65.8

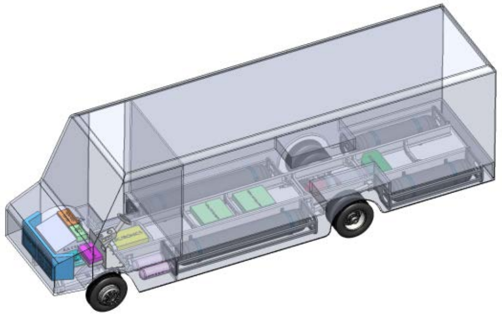
800 kW fuel cell 1.2 MWh battery: Assume 50% of full power 7 hours/day = 140 kg H_2

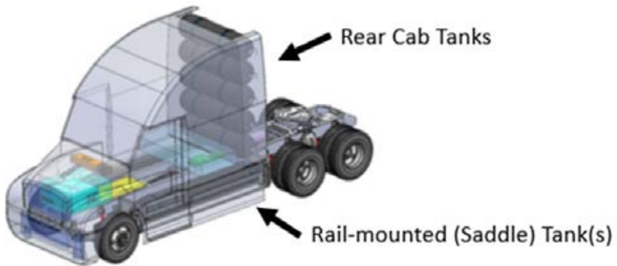
Previous Accomplishments – Liquid Hydrogen Sizing Routine

Property	Units	Light Duty	Medium Duty	Heavy Duty	Mining
H2 Storage	kg	5.6	20	60	140
Maximum Power	kW	80	150	300	800
Saddle Tanks		1	2	2	2
Rear Tanks		0	0	2	6
Single Tank Mass	kg	26	37	56.5	56.5
Single Tank Diameter	m	0.29	0.35	0.44	0.44
Single Tank Length	m	1.3	1.58	1.97	1.97
Total Mass	kg	86	181	397	890
Total Volume	m3	0.2	0.59	1.57	3.65

- **Inputs**
    - **Usable H2 or maximum volume**
    - **Initial Temperature or Pressure**
    - **System Power Rating**
- **Calculation**
    - **Sizes multiple tanks**
    - **Sizes vaporizer**
    - **Total Mass and Volume**



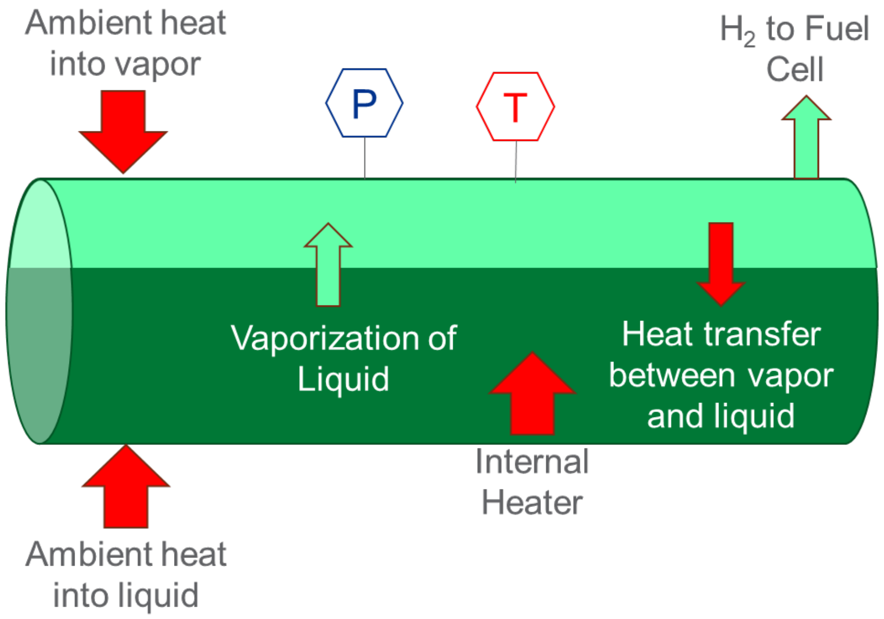


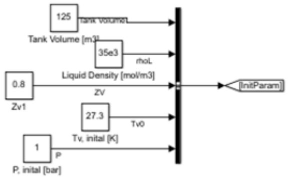


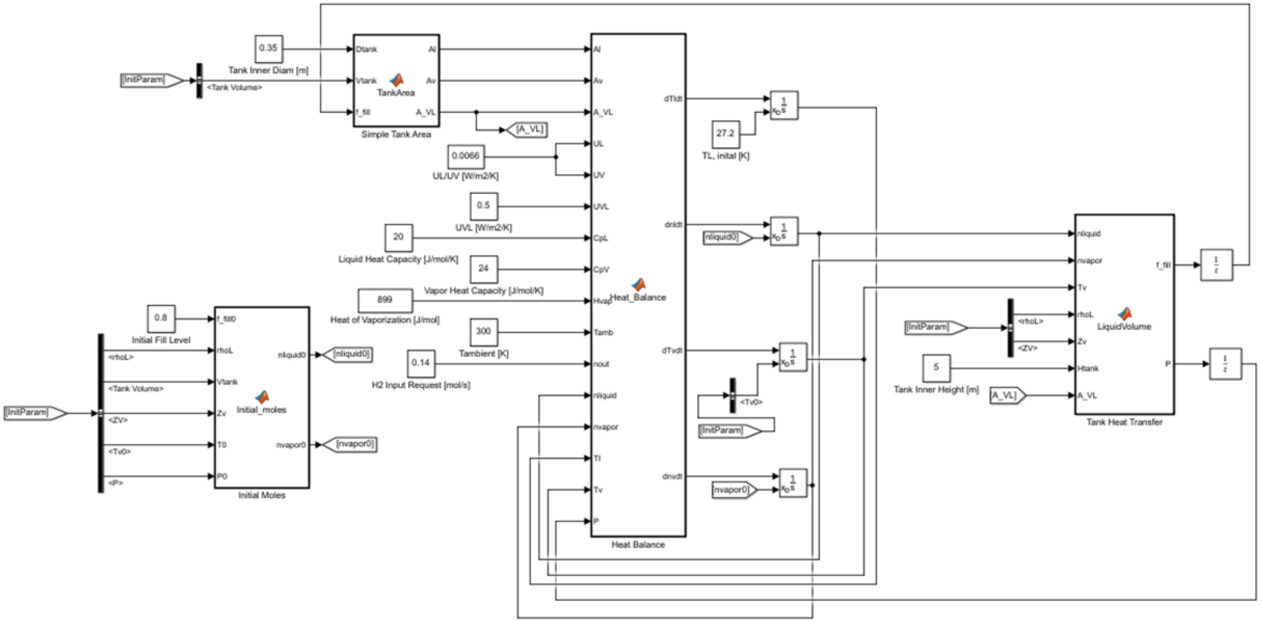
NREL image

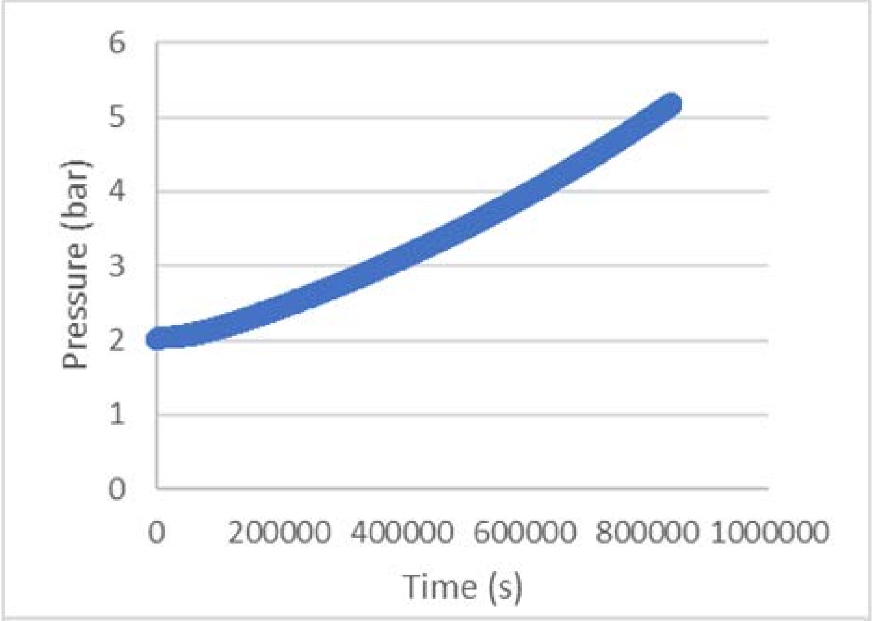
Previous Accomplishment – Liquid Hydrogen Framework Storage Module

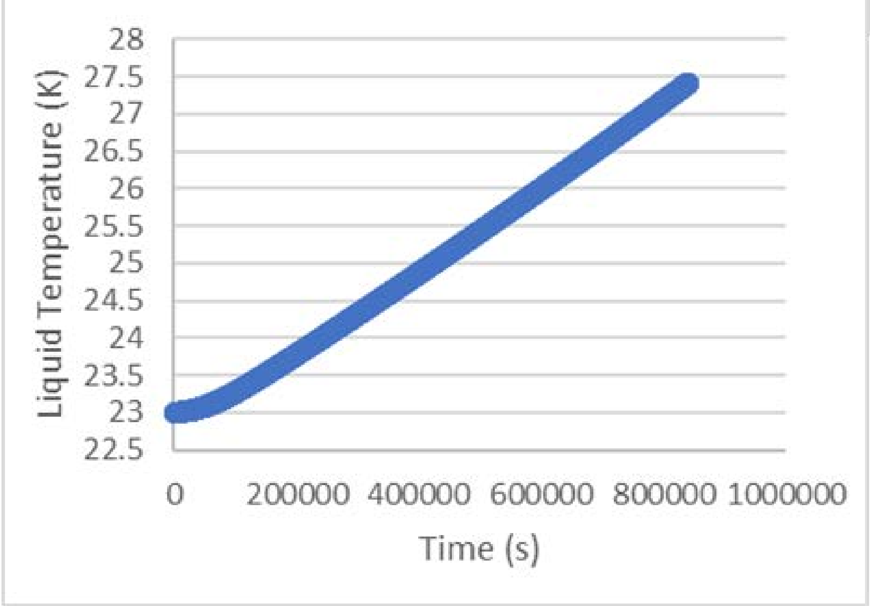
- Developing liquid H_2 boil-off model
- Use during dormancy and operations





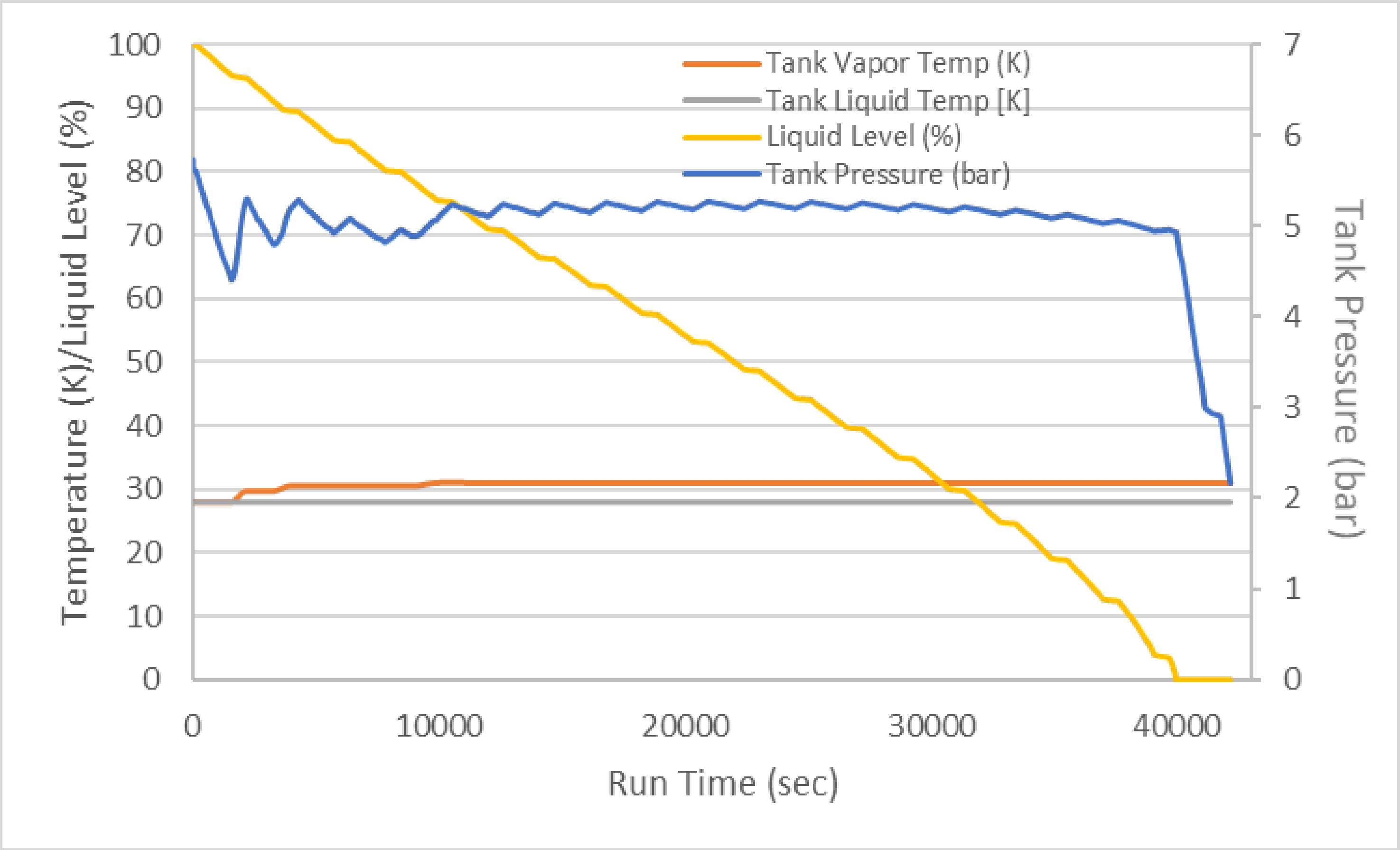






Previous Accomplishment – Liquid Hydrogen Framework Storage Module, Heavy Duty Vehicle

- **HHDDT Cruise Drive Cycle**
- **Usable H2 = 57.91 kg**
- **On-Board Efficiency = 99.8%**
- **Distance Travelled = 467.4 miles**
- **Fuel Economy = 8.073 mpgge**
- **Very little internal heater usage—only in early operation**



LH2 achieves very high on-board efficiency

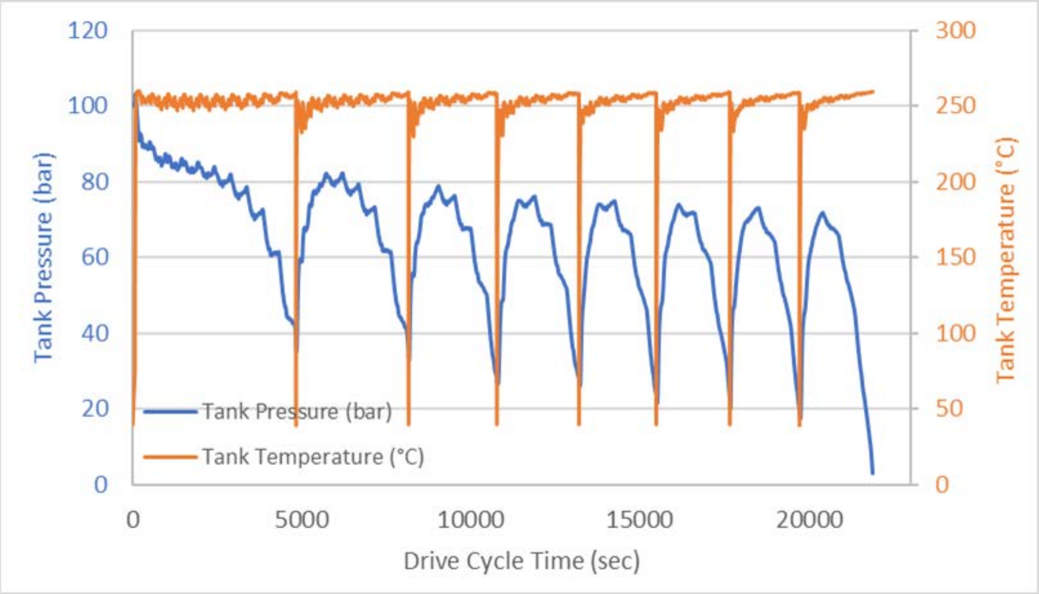
Previous Accomplishment – Evaluation of HyMARC Storage Materials

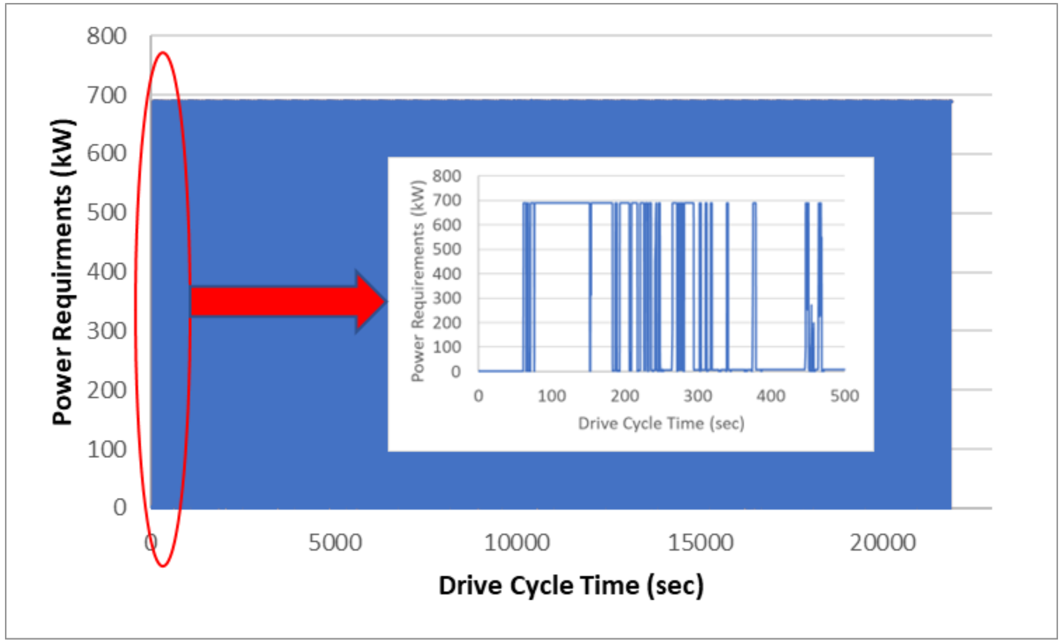
SNL Analysis of Materials: Bulk and Nano-Scaled $2LiH_2/Mg(NH_2)_2$

Property	Light-Duty Vehicle		Heavy-Duty Vehicle	
Metal Hydride	$2LiH_2/Mg(NH_2)_2$			
Tank Material	Al-MS-89			
Kinetics Augmentation	10X			
Initial Pressure (bar)	50		100	
Drive Cycle	UDDS		(HHDDT) Cruise	
Input Useable H_2 (kg)	5.6		60	
Material Inputs	**Bulk**	**Nano**	**Bulk**	**Nano**
H_2 Capacity (g/g)	0.049	0.023	0.049	0.023
Thermal Conductivity (W/m/K)	0.92	1.09	0.92	1.09
Density (kg/m^3)	1230	840	1230	840
Sizing Routine Design Results	**Bulk**	**Nano**	**Bulk**	**Nano**
Number of Tanks	1	1	3	7
Mass of Tanks	48	128	1236	3322
Hydride Mass (kg)	144	307	1546	3293
System Mass (kg)	274	536	3440	7490
System Volume (L)	261	668	2932	7753
Output Useable H_2 (kg)	5.3	5.3	58	63
Framework Drive Cycle Results	**Bulk**	**Nano**	**Bulk**	**Nano**
Fuel Economy (mpgge)	43.5	39.4	5.9	5.4
Onboard Efficiency (%)	72%	68%	74%	73%
Distance Traveled (miles)	443	423	463	461

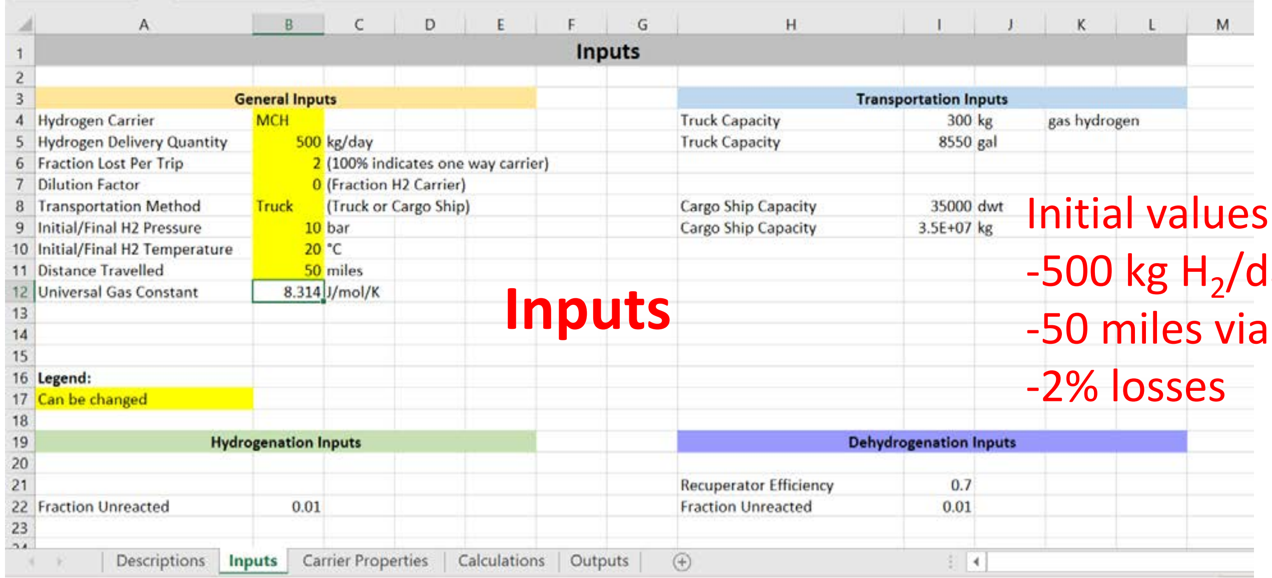
Previous Accomplishment – Mining Vehicle in Framework

- **Metal Hydride: Nano-Li3N (4.74 wt%)**
  - **6179 kg System Mass**
  - **5.4 m3 System Volume**
  - **Number Tanks = 8**
  - **Tank Length = 2 m**
  - **Tank Diameter = 0.7 m**
  - **Pmax = 100 bar**
  - **H2 Burned = 36.8 kg**
- **Mining Drive Cycle:**
  - **Average Speed = 10.4 mph**
  - **H2 Delivered = 175 kg**
  - **On-Board Efficiency = 95%**
  - **Distance = 63.5 miles**
  - **Fuel Economy = 0.34 mpgge**





Previous Accomplishment – Round Trip Efficiency Estimator

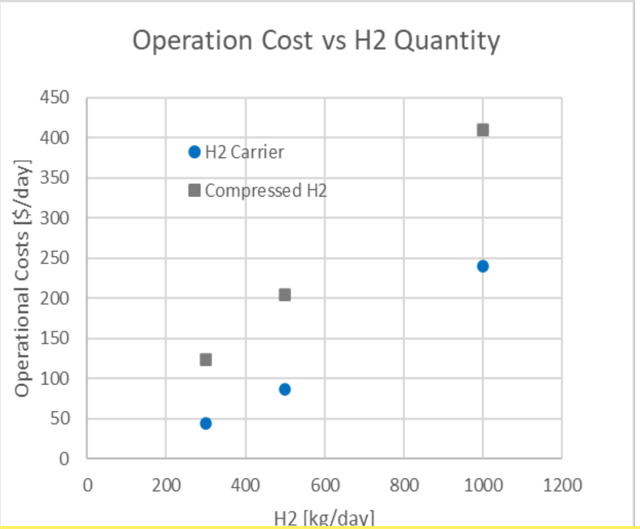


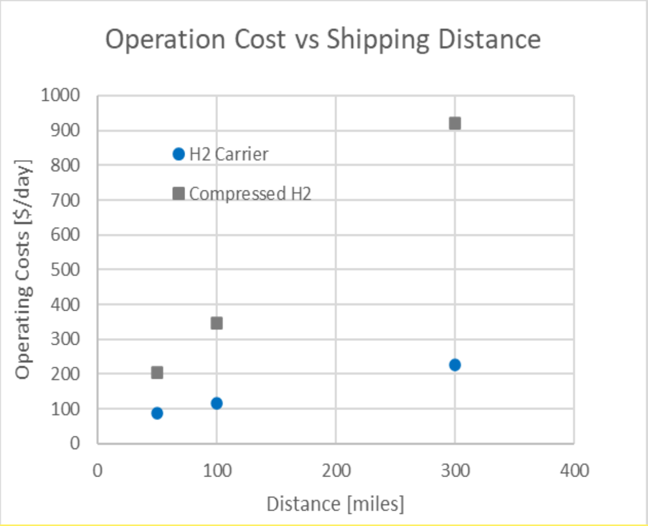
	A	B	C	H	I	J	K
1	**Inputs**						
2							
3	**General Inputs**			**Transportation Inputs**			
4	Hydrogen Carrier	MCH		Truck Capacity	300	kg	gas hydrogen
5	Hydrogen Delivery Quantity	500	kg/day	Truck Capacity	8550	gal	
6	Fraction Lost Per Trip	2	(100% indicates one way carrier)				
7	Dilution Factor	0	(Fraction H2 Carrier)				
8	Transportation Method	Truck	(Truck or Cargo Ship)	Cargo Ship Capacity	35000	dwt	
9	Initial/Final H2 Pressure	10	bar	Cargo Ship Capacity	3.5E+07	kg	
10	Initial/Final H2 Temperature	20	°C				
11	Distance Travelled	50	miles				
12	Universal Gas Constant	8.314	J/mol/K				
13							
14							
15							
16	**Legend:**						
17	Can be changed						
18							
19	**Hydrogenation Inputs**			**Dehydrogenation Inputs**			
20							
21				Recuperator Efficiency	0.7		
22	Fraction Unreacted	0.01		Fraction Unreacted	0.01		
23							

Inputs

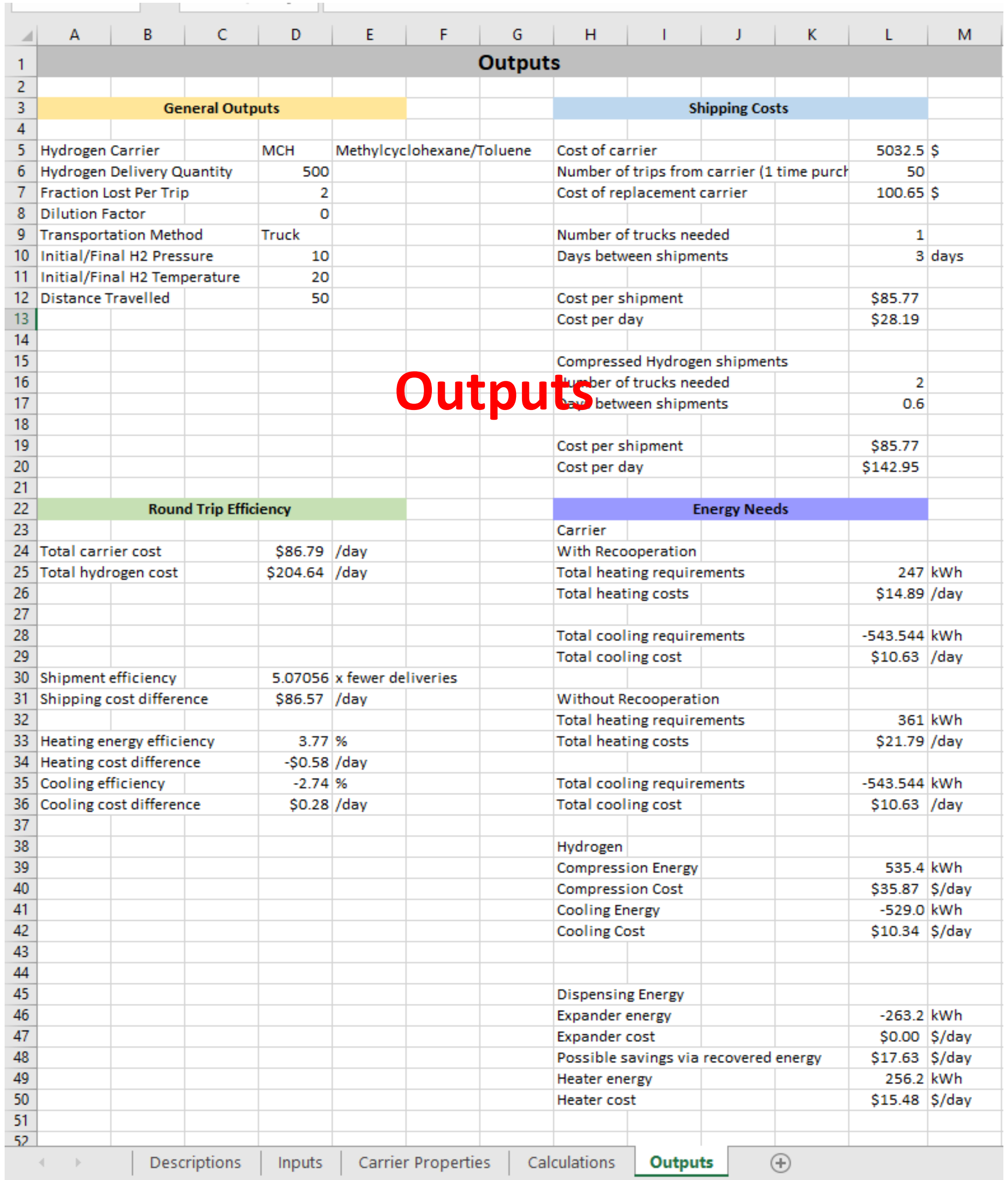
Initial values:
- 500 kg H_2/day
- 50 miles via truck
- 2% losses

Sample Results





H_2 carrier had lower daily operating cost due to savings in shipping



	A	D	E	H	L	M
1	**Outputs**					
2						
3	**General Outputs**			**Shipping Costs**		
4						
5	Hydrogen Carrier	MCH	Methylcyclohexane/Toluene	Cost of carrier	5032.5	$
6	Hydrogen Delivery Quantity	500		Number of trips from carrier (1 time purch	50	
7	Fraction Lost Per Trip	2		Cost of replacement carrier	100.65	$
8	Dilution Factor	0				
9	Transportation Method	Truck		Number of trucks needed	1	
10	Initial/Final H2 Pressure	10		Days between shipments	3	days
11	Initial/Final H2 Temperature	20				
12	Distance Travelled	50		Cost per shipment	$85.77	
13				Cost per day	$28.19	
14						
15				Compressed Hydrogen shipments		
16				Number of trucks needed	2	
17				Days between shipments	0.6	
18						
19				Cost per shipment	$85.77	
20				Cost per day	$142.95	
21						
22	**Round Trip Efficiency**			**Energy Needs**		
23				Carrier		
24	Total carrier cost	$86.79	/day	With Recooperation		
25	Total hydrogen cost	$204.64	/day	Total heating requirements	247	kWh
26				Total heating costs	$14.89	/day
27						
28				Total cooling requirements	-543.544	kWh
29				Total cooling cost	$10.63	/day
30	Shipment efficiency	5.07056	x fewer deliveries			
31	Shipping cost difference	$86.57	/day	Without Recooperation		
32				Total heating requirements	361	kWh
33	Heating energy efficiency	3.77	%	Total heating costs	$21.79	/day
34	Heating cost difference	-$0.58	/day			
35	Cooling efficiency	-2.74	%	Total cooling requirements	-543.544	kWh
36	Cooling cost difference	$0.28	/day	Total cooling cost	$10.63	/day
37						
38				Hydrogen		
39				Compression Energy	535.4	kWh
40				Compression Cost	$35.87	$/day
41				Cooling Energy	-529.0	kWh
42				Cooling Cost	$10.34	$/day
43						
44						
45				Dispensing Energy		
46				Expander energy	-263.2	kWh
47				Expander cost	$0.00	$/day
48				Possible savings via recovered energy	$17.63	$/day
49				Heater energy	256.2	kWh
50				Heater cost	$15.48	$/day
51						
52						

Outputs