Hydrogen Storage System Modeling:

Public Access, Maintenance, and Enhancements

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NREL Transforming ENERGY

Pacific Northwest NATIONAL LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

DOE Hydrogen Program

2022 Annual Merit Review and Peer Evaluation Meeting

June 6–8, 2022

Project ID: ST008

DOE WBS #: NREL – 4.2.0.502

PNNL – 4.2.0.702   SRNL – 4.2.0.902

Project Goal

The overall vision of this project is to provide ownership and support for maintaining existing material-based hydrogen storage systems models. This incudes 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 DOE vehicle-level targets. Key elements for FY22:

- 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- and heavy-duty vehicles and mining and agricultural vehicles.
- Model alternatives to material-based systems including compressed and liquefied H_2.

HyMARC
Hydrogen Materials Advanced Research Consortium

Overview

Timeline

- Start: October 1, 2015
- End: September 30, 2022*

Budget

- Total DOE Funds Received to Date**: $2,387,000
  - 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

Partners

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

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

Relevance

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 light-, medium-, and heavy-duty vehicles relative to the available DOE Technical Targets.**

Relevance – Addressing Barriers with Models

Barriers	Model Addressing Barrier
A. System Weight and Volume	System Estimators
B. System Cost	System Estimators Tank Volume/Cost Model
C. Efficiency	Framework Model - Onboard Efficiency - Fuel Economy Round Trip Efficiency Estimator
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

Relevance – Improving Model Utilities for Materials Researchers

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

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Isotherm Fitting Tool

Dubinin-Astakhov
Parameters

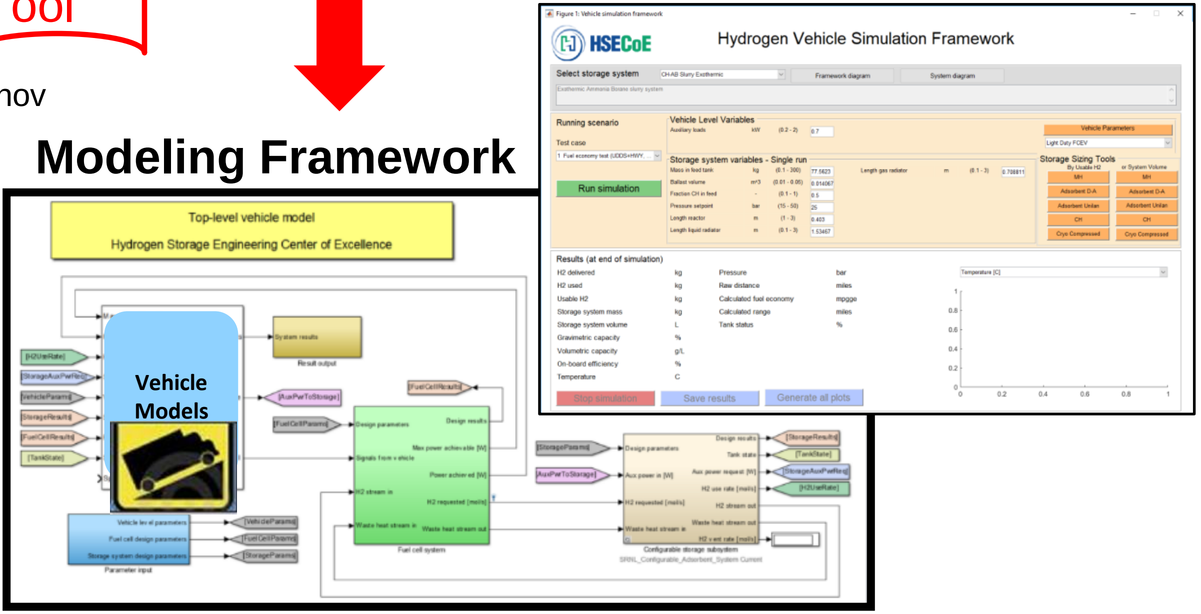
Stand-Alone System Design Tools

Component and
System Mass and
Volume

Stand-Alone Values

Estimated Gravimetric and Volumetric Capacity

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

Modeling Tools Available or In Progress

Note: Updates in blue text

Framework Model with:

• Physical Storage	UTRC/NREL	Light-, medium-, and heavy-duty vehicles FY22: Plans to expand to agricultural and mining vehicles
• 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	FY22: Plan to expand to liquid H_2

Stand-Alone System Design Tools:

• Adsorbent (AD)	SRNL	Light-, medium-, and heavy-duty vehicles MH includes high temperature alloys
• Chemical Hydrogen (CH)	PNNL	
• Metal Hydride (MH)	PNNL	
• Compressed/Cryo-Compressed H_2	SRNL	

Additional Tools/Models:

• MH Acceptability Envelope (MHAE)	SRNL	
• Tank Volume/Cost Model (Tankinator)	PNNL	High T alloys and flags to maintain in bounds
• AD Isotherm Fitting Tool	SRNL	
• MH Refueling Model	PNNL	Model developed and validated with $NaAlH_4$
• Round-Trip Efficiency Estimator	PNNL	Preliminary model developed

Finite Element Models:

• Metal Hydride (MH) Finite Element (MHFE)	SRNL
• Adsorbent (AD) – HexCell and MATI	SRNL

UTRC: United Technologies Research Center

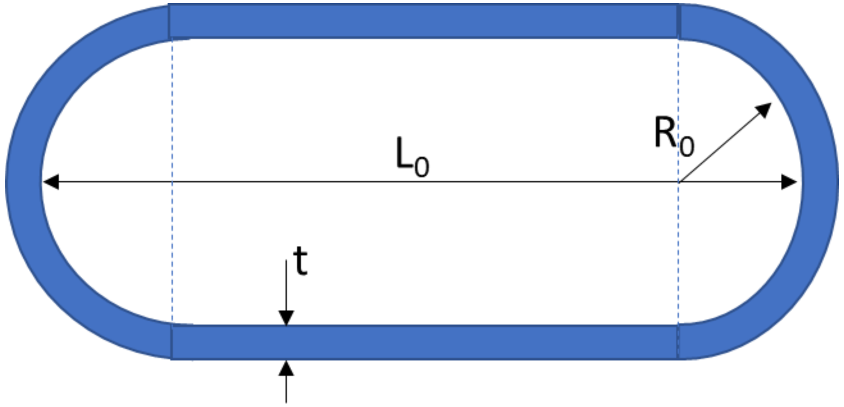
Accomplishments and Progress – Design Tools and Framework Estimate Allow Evaluation of Hydrogen Storage Systems

Capabilities:

- Expanded Tankinator to include additional high temperature alloys and flags to ensure the inputs and outputs are within range
- Developed a refueling model for metal hydrides to understand the interplay between heat transfer and kinetics in the H_2 storage tank
- Updated the storage models in the Framework to include medium- and heavy-duty vehicles
- Updated stand-alone models to include combined light/medium/heavy-duty vehicles and volume- and usable H_2 mass-based sizing
- Developed a spreadsheet-based round trip efficiency calculator

Accomplishments and Progress – Tankinator Model Update

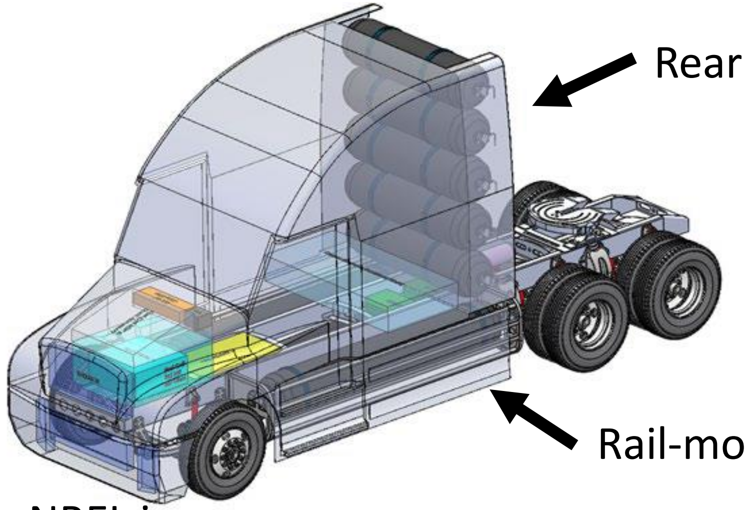
- **The current release version of Tankinator is v3.0**
  - This version is in use by researchers worldwide
  - Only Al 6061 and 316SS had temperature dependency
- **Expanding Tankinator capability to estimate Type 1 tanks at elevated temperature (up to 350°C, depending on material)**
  - Use to reduce tank mass for high temperature metal hydrides
  - Increased number of material options and the temperature-dependent data for the existing material options
- **Developing a new formal release version of Tankinator (v4.0)**
  - Will have realistic end cap geometries
  - Automatic recognition of cases that are "out of bounds" for a reasonable estimate



Tankinator v3.5
Type 1 Material List

1. 6061_T6_Aluminum
2. A2618_Aluminum
3. A4032_Aluminum
4. NASA_380_Aluminum
5. Al-MS89_Aluminum
6. 316_Stainless_Steel
7. 4340_Alloy_Steel

Targeted Applications: Light/Medium/Heavy-Duty Vehicle Application



NREL image

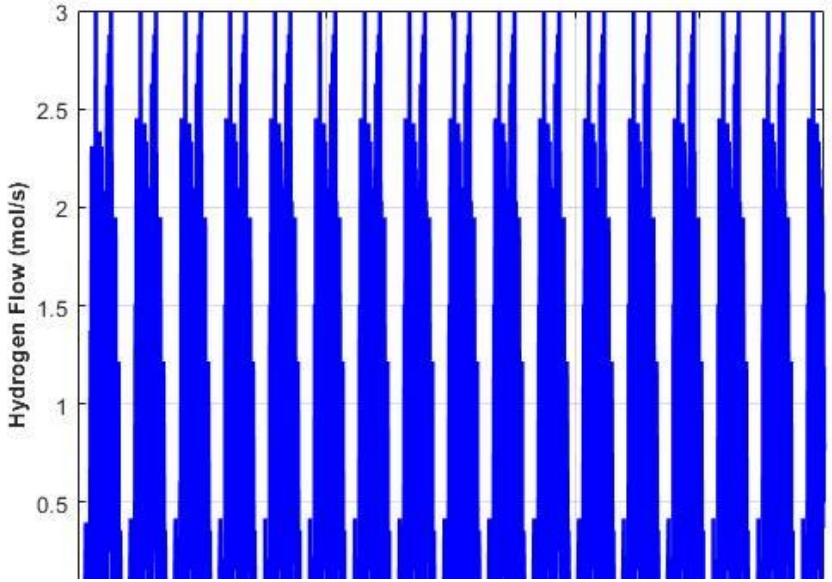
System Configuration	H_2 Required (kg)	$NaAlH_4$ Needed (kg)	Internal/ Saddle Tanks	Rear Tanks	System Volume (L)
Light-Duty	5.6	131	1	0	405
Medium-Duty	20	471	2	0	1330
Heavy-Duty	60	1413	2	2	3910

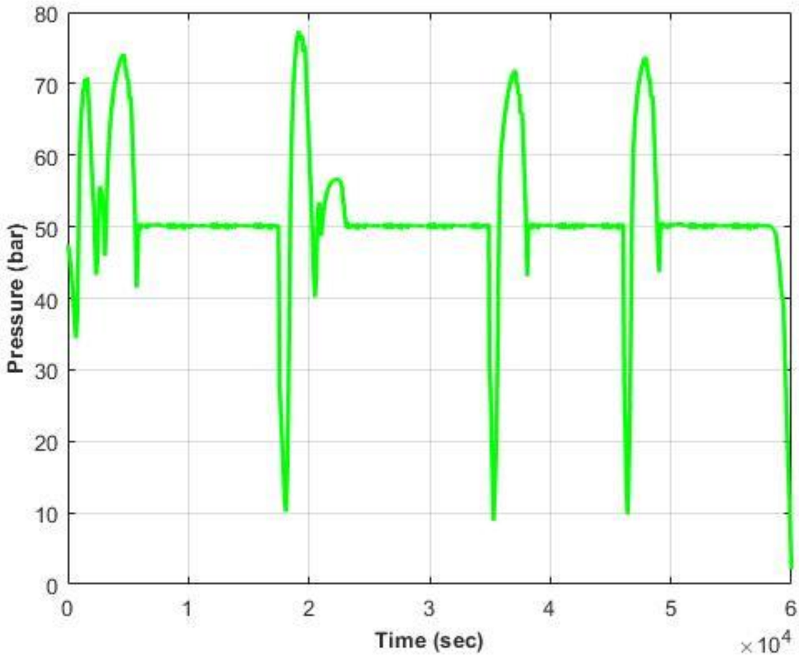
Accomplishments and Progress – Framework Estimate Allows Evaluation of Hydrogen Storage Systems

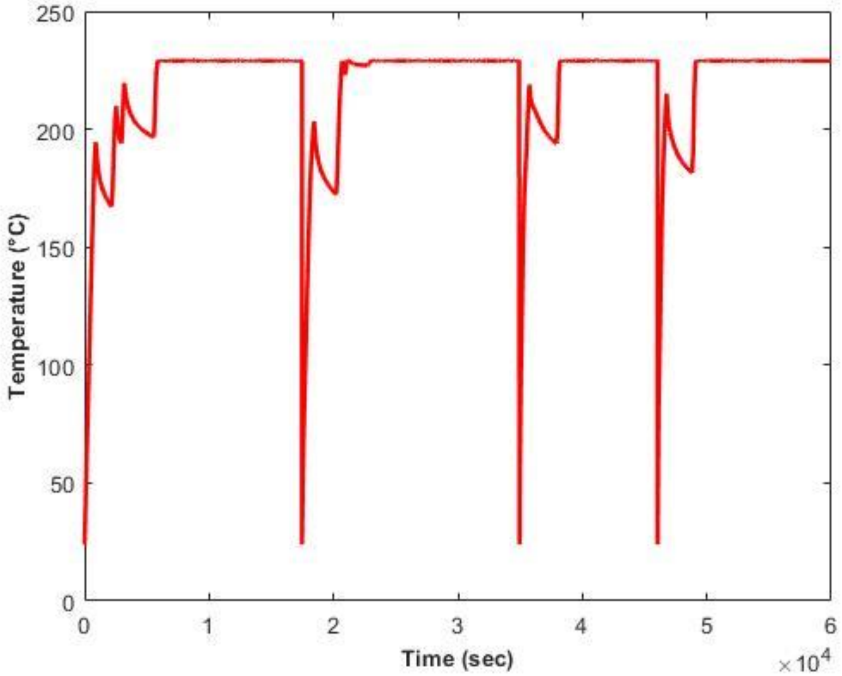
Framework Results: Heavy-Duty Vehicle

- Drive Cycle: HHDDT composite (300 kW max)
- System: 2 saddle tanks, 2 rear tanks
  - Pressure and temperature spike after one tank is empty and as the next begins heating
  - Pressure cannot drop below 5 bar or the drive cycle stops

Result	Value	Units
Useable H_2	55.5	kg
Onboard efficiency	69%	--
Distance traveled	430	miles
Fuel economy	5.3	mpgge



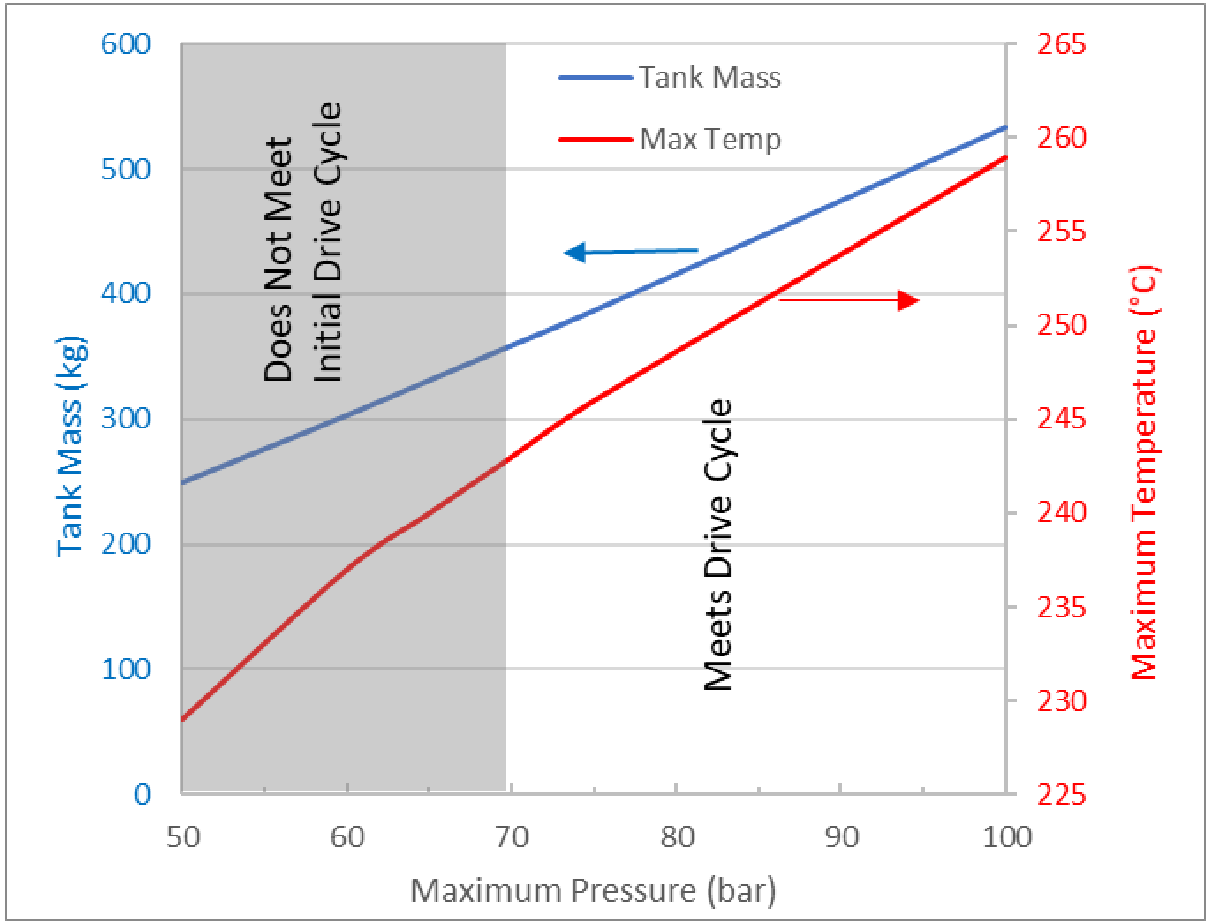




Accomplishments and Progress – Framework Estimate Allows Evaluation of Hydrogen Storage Systems

Framework Results: Light-Duty Vehicle

- System design is driven by start-up of each MH tank
  - Higher pressure allows longer start-up time to meet drive cycle
  - Higher pressure increases the temperature, resulting in a heavier system
  - Temperature/pressure relationship determined by thermodynamics/kinetics



Accomplishments and Progress – Stand-Alone Model and Framework Allow Evaluation of Hydrogen Storage Material

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

Accomplishments and Progress – MH Refueling Model

- **Purpose**: Estimate time and temperature profile of the tank during refueling
- **How it works:**
  - For a given feed pressure and initial temperature
  - Calculate H_2 uptake, temperature, and heat flux as a function of time
  - Based on 4th-order Runge-Kutta integration
  - Lumped capacitance model with heat transfer hA term (W/K)
  - Provide heating/cooling reach appropriate temperatures but remove excess heat
- **Model $NaAlH_4$ first step hydrogenation**
  - 60 kg MH
  - 100 bar pressure
  - 38°C initial temperature

- **Van't Hoff Equilibrium pressure and temperature drive the refueling process**

$$P_{eq,A} = P_{ref} exp\left[\frac{\Delta H_A}{RT} - \frac{\Delta S_A}{R}\right]$$

- **Kinetic rate sufficient to absorb the hydrogen**

$$r_{H2} = k_A(T) f_{yA}(y)\, f_{pA}(P)$$

$$where:$$

Absorption: $k_A = K_A\, exp\left[\frac{-E_A}{RT}\right]$

Concentration Driving Force: $f_{yA}(y) = (y_{eA} - y)^{\alpha_A}$

Pressure Driving Force: $f_{pA}(P) = ln\left(\frac{P}{P_{eq,A}}\right)$

- **Heat sufficiently for kinetics but not high enough to possibly damage MH**

Energy Balance: $\frac{dT}{dt} = \frac{hA}{M_{final} C_p}(T_{HT} - T) - \frac{1}{2}\frac{\Delta H_A}{100 * MW_H C_p}\frac{dy}{dt}$

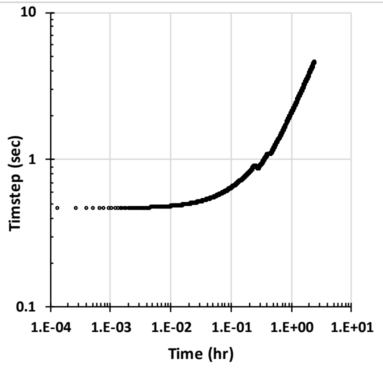
Accomplishments and Progress – MH Refueling Model

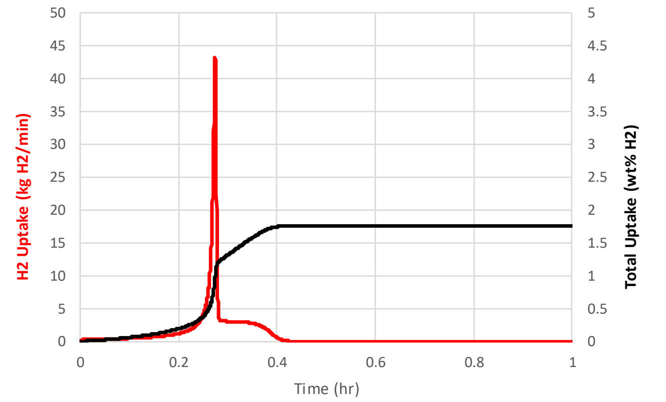
	0.005	fraction of time constant to use for initial timestep	factor of range on limits, f_v	0.5 set to < 1
set to >= 1	1.0005	f_t, factor by which to modify timestep relative to preceding step	max accepted ΔT, K per step	0.5
set to >= 1	200	f_{tmax}, max timestep, relative to initial timestep	max accepted Δy, wt% per step	0.05
			reference T for time constants, T_{ref}	110 C

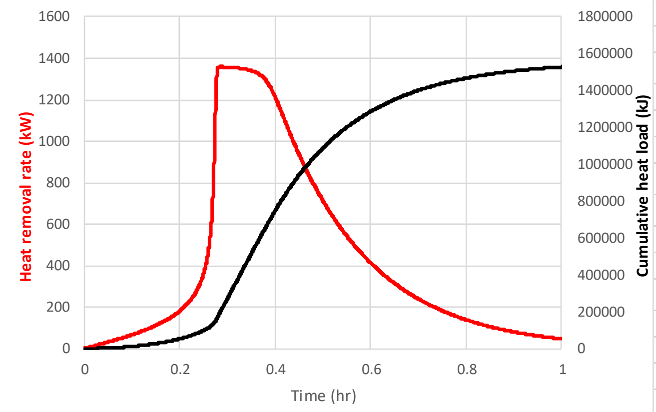
R =	8.314	J/gmol gas K
	2.016	g hydrogen/gmol H2
	100000	Pa / bar
	1.01325	bar / atm
y at minimum hydriding, y_{eD}	0	H as wt% of maximally-hydrided material including inactive mass
y at maximum hydriding, y_{eA}	1.76	H as wt% of maximally-hydrided material including inactive mass
Desired H mass	60	kg
M_{final}	3409.091	kg maximally hydrided material
Packed bed density	620	kg/m3
Bed bulk volume	5.498534	m3
Heat capacity C_p	1200	J/kg K
Bulk thermal conductivity k_{HT}	0.4	W/m K
Heat transfer coefficient h	31	W/m2 K
eat transfer medium temperature T_{HT}	35	C = 308.15 K
Heat transfer area A	200	m2
Feed pressure P	100	bar
Initial bed temperature T_0	35	C = 308.15 K
T_{limit}	135	C = 408.15 K

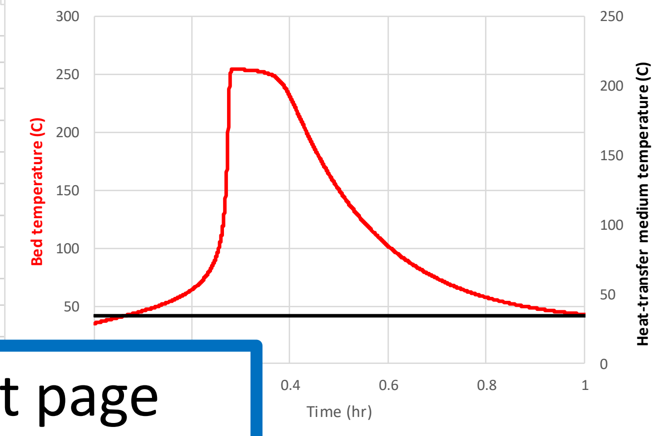
-6300	$\Delta H_A/R$, units K -- gives P in atm	0.019359 atm at T_0
-16.5	$\Delta S_A/R$, unitless -- gives P in atm	2.899384 atm at T_{limit}
-52378.2	ΔH_A, J/mol H_2	
1.02E+08	K_A units are 1/hour	
56200	E_A, J/mol	
1	α_A, order of reaction for absorption	
y	Use logarithmic pressure driving force? (leave blank if arithmetic ratio is to be used)	
	β_A, exponent on the arithmetic ratio (if used) for pressure driving force	

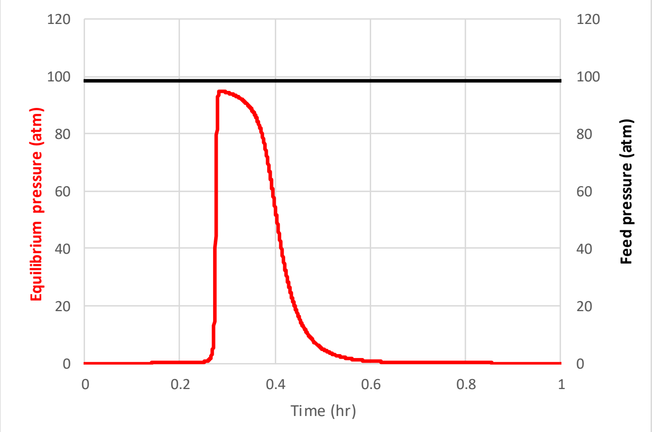
max observed abs. ΔT (K) =	3.788773					
max observed abs. Δy (wt% H) =	0.018558					
Summary for absorption						
wt% H =	1.760	by	2.4	hr		
maximum T	254.2	C				
maximum H2 feed rate	43.1994	kg/min		total fed H2	60.000	kg
maximum heat rate	1359.078	kW		total heat	1559169	kJ
wt% H =	1.760	at	1	hr, or	100%	conversion







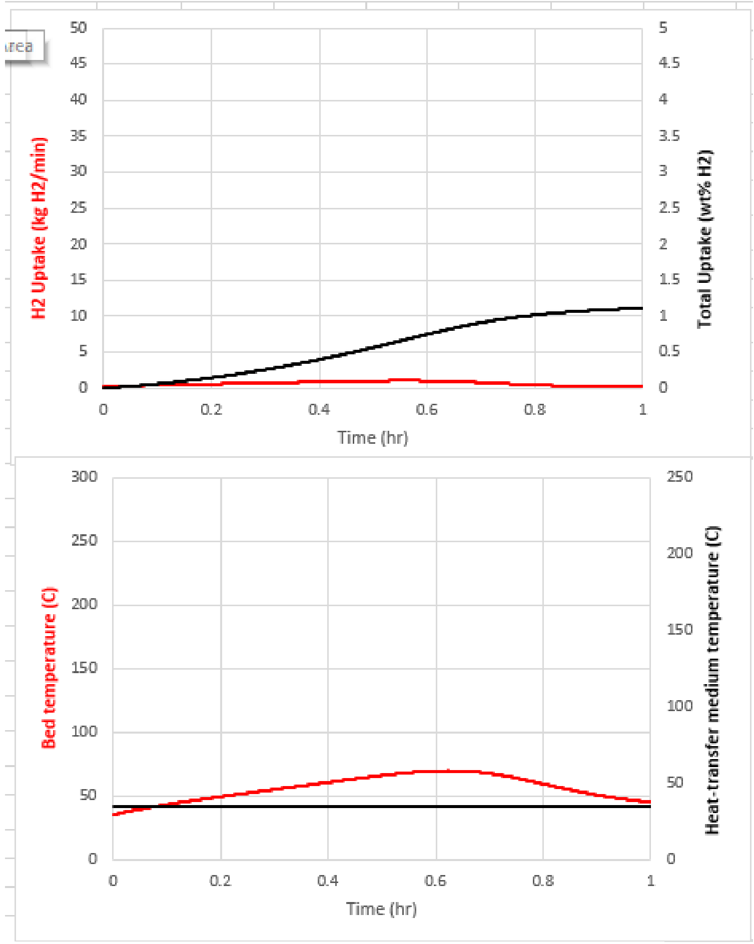




Model interface: input/output page

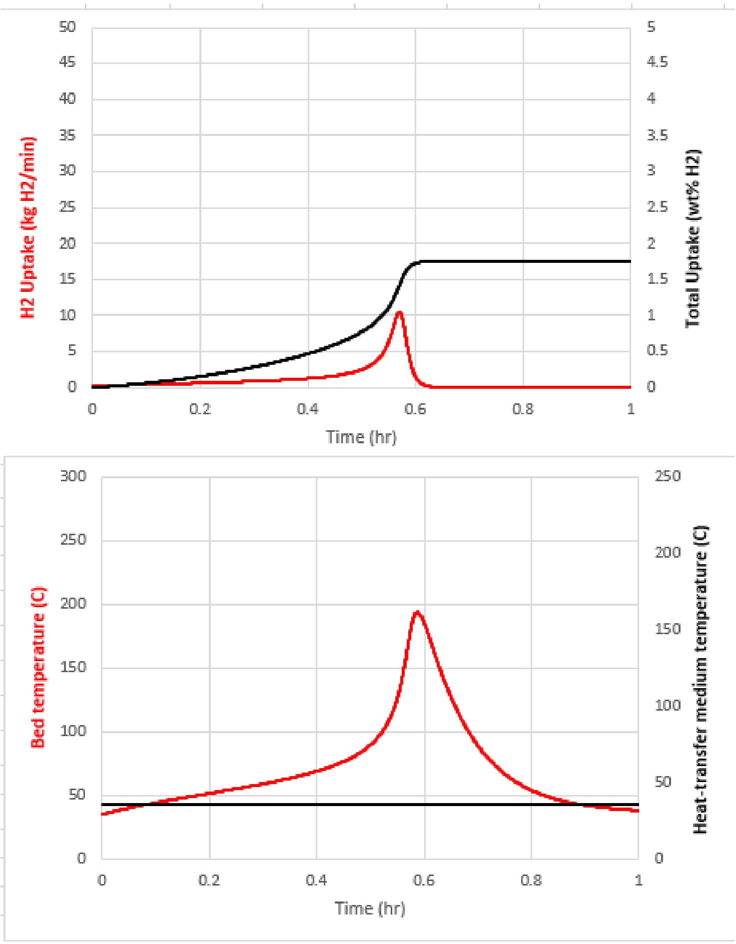
Accomplishments and Progress – MH Refueling Model

hA = 12400 W/K, T = 35°C



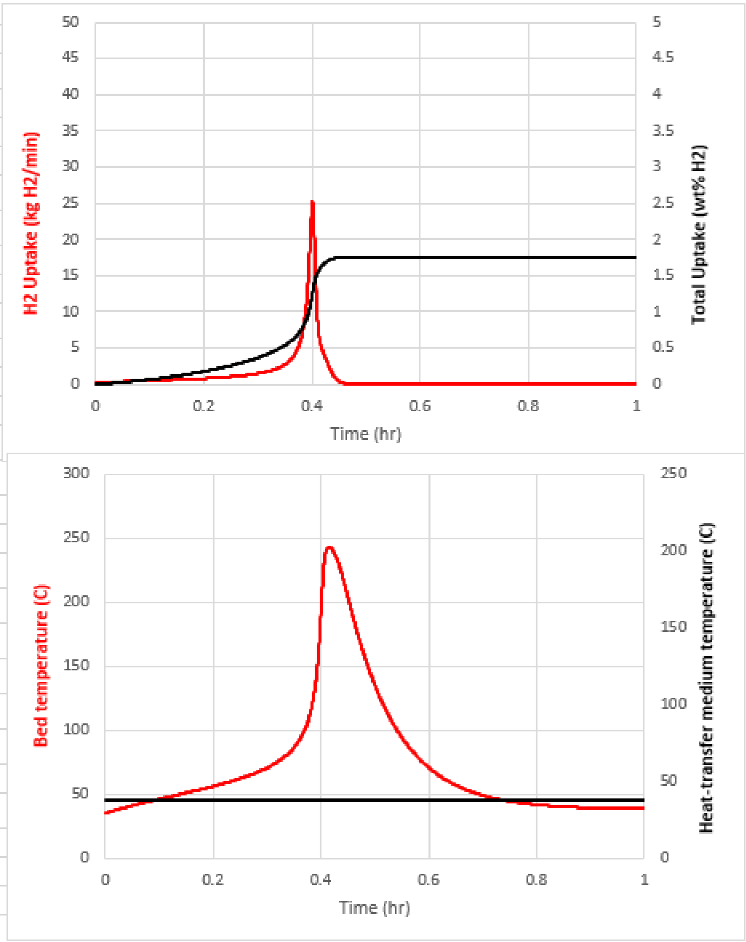
Bed Temp <70°C
Reduced hydrogenation @ 1 h

hA = 12400 W/K, T = 36°C



Bed Temp <200°C
Full hydrogenation @ 36 min

hA = 12400 W/K, T = 38°C



Bed Temp exceeds 200°C
Full hydrogenation @ 24 min

Learnings from MH Refueling Model

- **H_2 adsorption is slow until there is a sharp increase in hydrogen uptake as the bed temperature exceeds 75°C**
- **Small changes in coolant temperature and heat transfer coefficient result in:**
  - – A potential spike in temperature beyond melting point ***or***
  - – Suppressed hydrogenation reaction
  - – Balance of kinetics and thermodynamics
- **Model helps understand the interplay between coolant heat transfer, reaction rate, feed pressure, and their impact on bed temperature, H_2 uptake, and heat removal**

Accomplishments and Progress – Round Trip Efficiency Estimator

- **Excel Spreadsheet Model**
- **Compare the cost of utilizing hydrogen carriers to directly transporting compressed hydrogen. Includes cost of:**
  - Acquiring the H_2 carrier
  - Hydrogenation (and cooling requirements)
  - Transportation of the carrier to the point of use (truck or cargo ship options)
  - Dehydrogenation (and heating/compression requirements)
  - Return of spent carrier
- **Inputs/Assumptions**
  - Initial temperature and pressure
  - Loss per trip
  - Carrier properties
  - Shipping capacity (8,550 gallons liquid organic hydrogen carrier vs. 300 kg gaseous H_2)

Accomplishments and Progress – Round Trip Efficiency Estimator

Inputs

	A	B	C	H	I	J	K
1	**Inputs**						
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				
16	**Legend:**						
17	Can be changed						
19	**Hydrogenation Inputs**			**Dehydrogenation Inputs**			
21				Recuperator Efficiency	0.7		
22	Fraction Unreacted	0.01		Fraction Unreacted	0.01		

Descriptions | Inputs | Carrier Properties | Calculations | Outputs

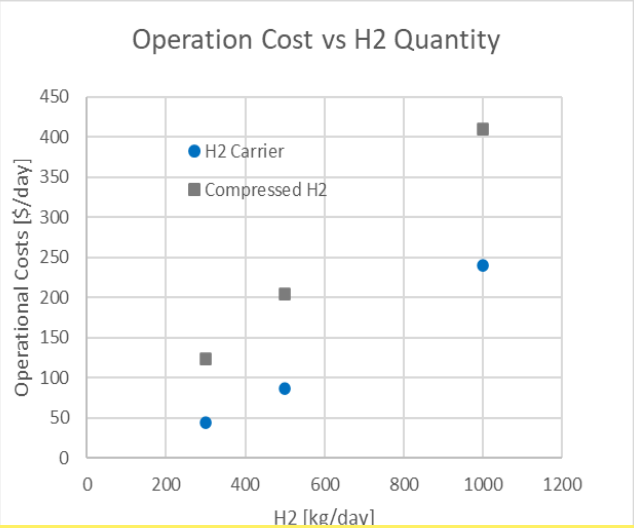
Initial values:
- 500 kg H_2/day
- 50 miles via truck
- 2% losses

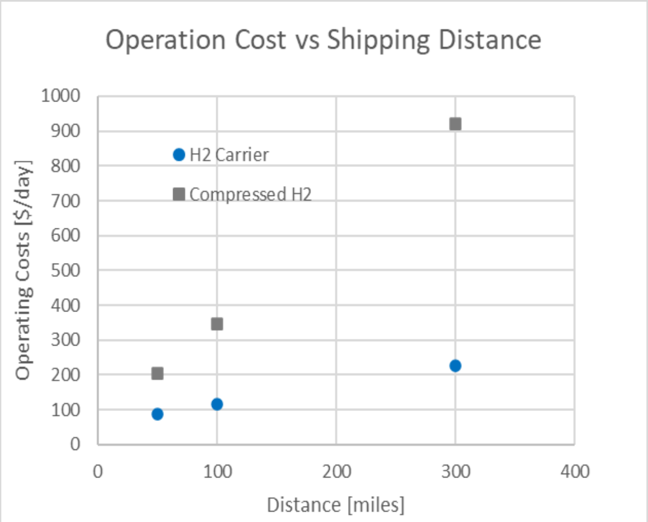
Outputs

	A	D	E	H	L	M
1	**Outputs**					
3	**General Outputs**			**Shipping Costs**		
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	
15				Compressed Hydrogen shipments		
16				Number of trucks needed	2	
17				Days between shipments	0.6	
19				Cost per shipment	$85.77	
20				Cost per day	$142.95	
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
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
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
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

Descriptions | Inputs | Carrier Properties | Calculations | Outputs

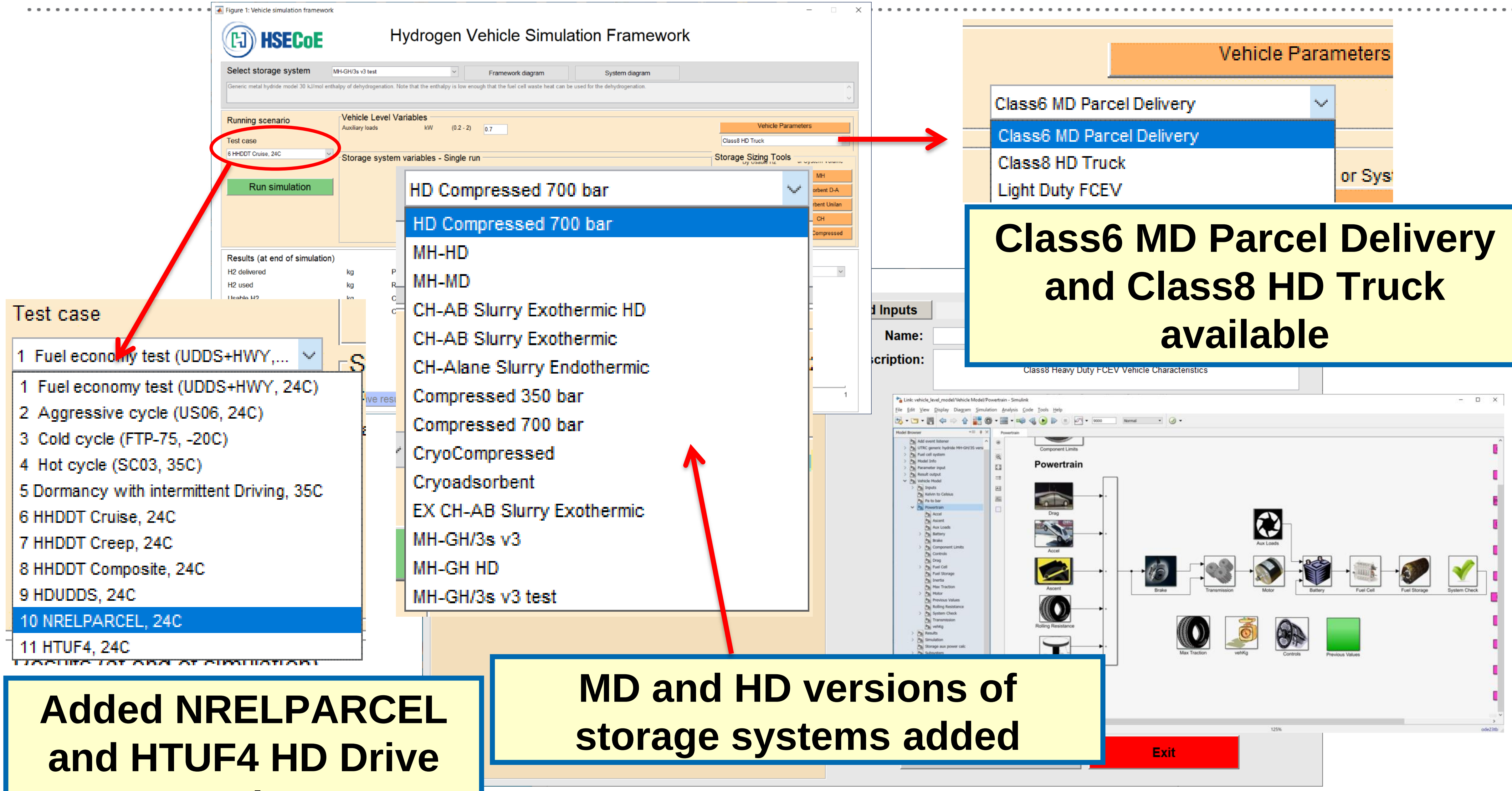
Sample Results





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

Accomplishments and Progress – Vehicle Framework Graphical User Interface



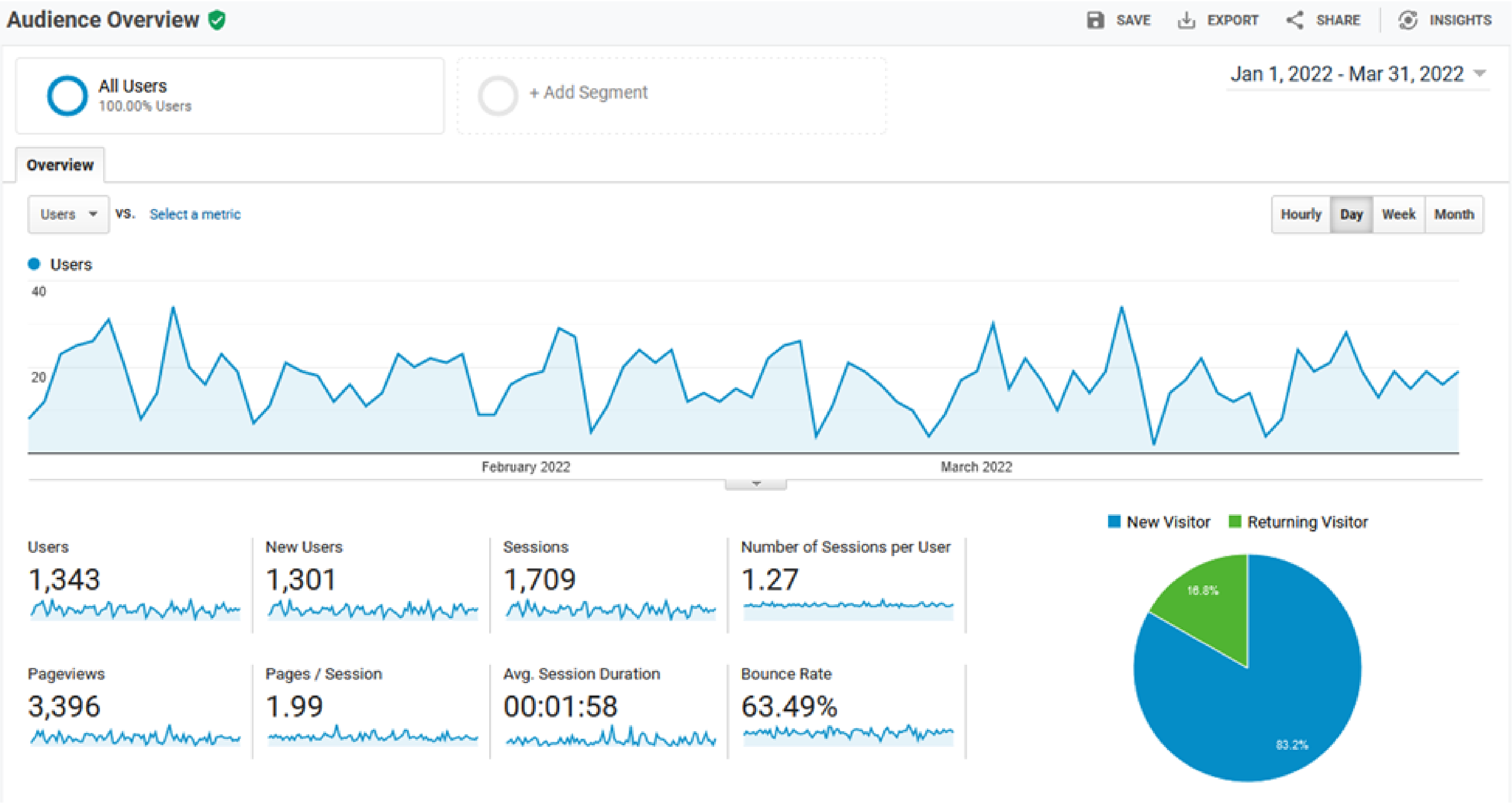
Class6 MD Parcel Delivery and Class8 HD Truck available

Added NRELPARCEL and HTUF4 HD Drive Cycles

MD and HD versions of storage systems added

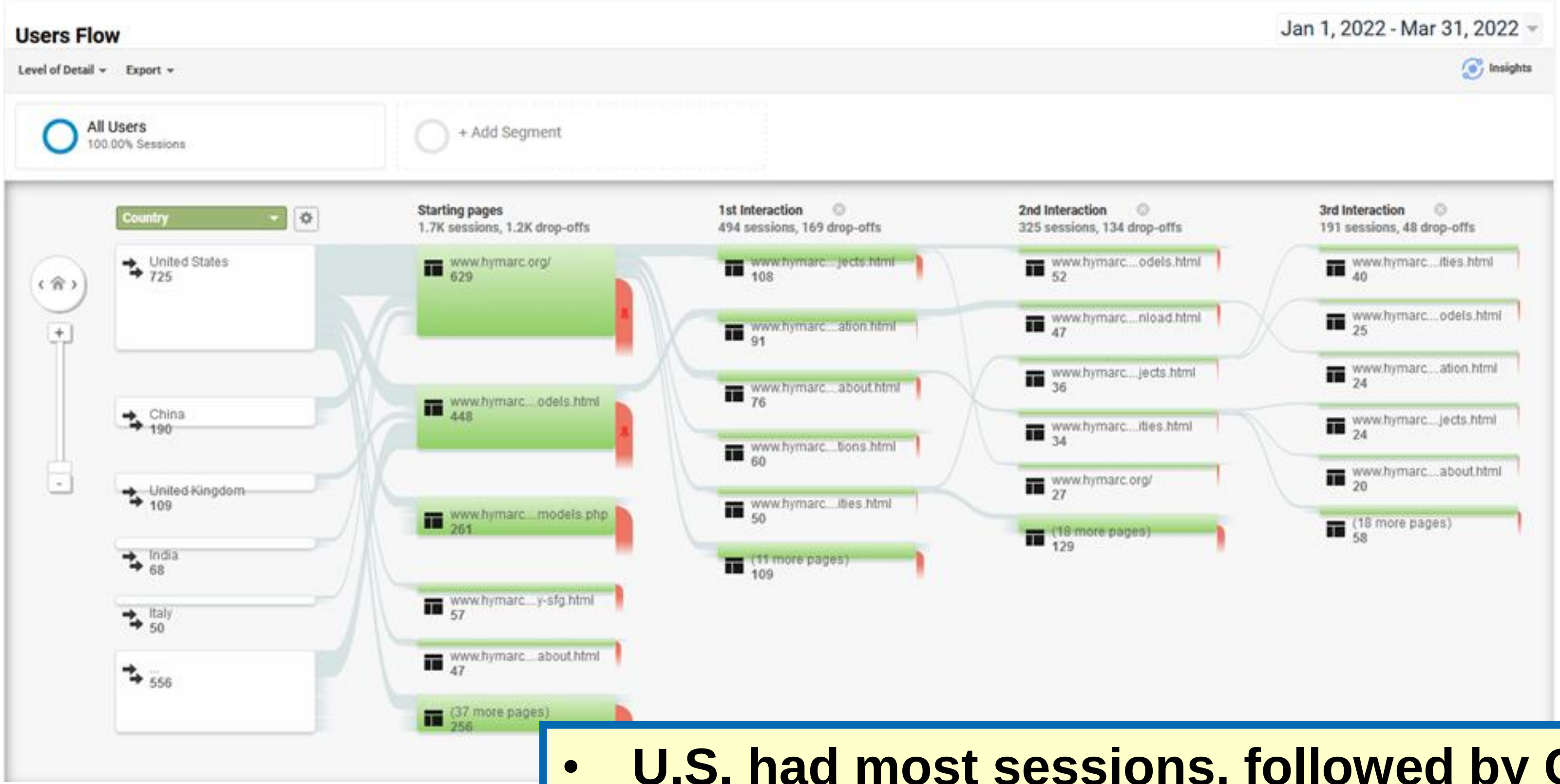
MD: medium-duty, HD: heavy-duty

Accomplishments and Progress – Model Website Analytics: Most Recent Activity (January 1, 2022–March 31, 2022)



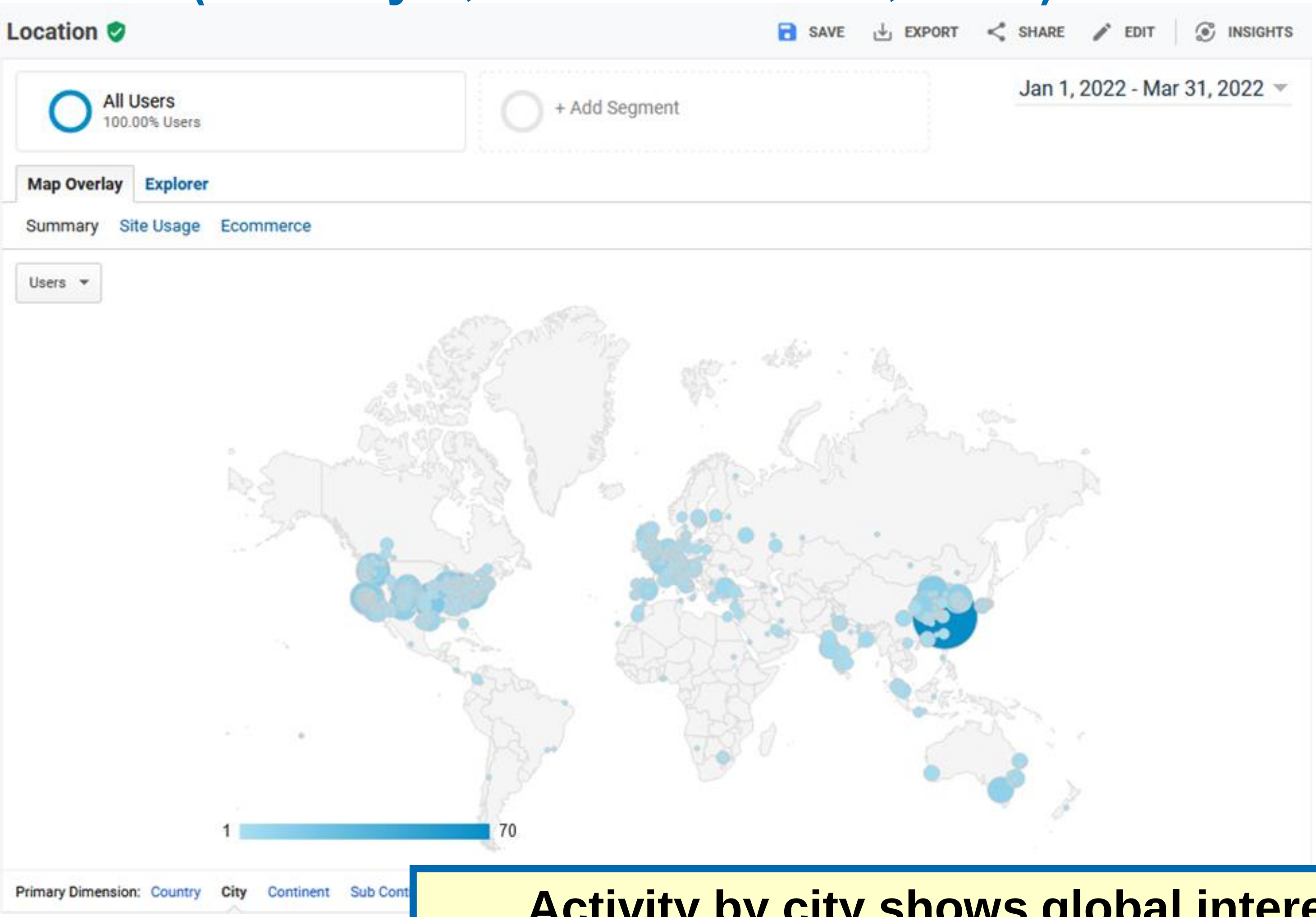
Activity every week; 83% of sessions were by new visitors

Accomplishments and Progress – Model Website Analytics: Web Flow (January 1, 2022–March 31, 2022)



- U.S. had most sessions, followed by China and UK
- Starting on HyMARC or Models page
- Models page had 1st and 2nd highest number of sessions by the 2nd and 3rd interaction

Accomplishments and Progress – Model Website Analytics: Locations (January 1, 2022–March 31, 2022)



Activity by city shows global interest in countries and regions including China, UK, Australia, Japan, South Korea, EU, and others

Accomplishments and Progress – Model Downloads (through March 31, 2022)

MODEL	Total	Totals AMR2021	Additional through FY22 Q2
H_2 Storage Tank Mass and Cost Model	**517**	298	219
MHAE Model	**196**	87	109
MHFE Model	**254**	131	123
Vehicle Simulator Framework Model	**376**	214	162
CH System Design Stand-Alone	**214**	59	155
Adsorbent System Design Stand-Alone	**199**	69	130
MH System Design by Usable H_2	**151**	21	130
MH System Design by System Volume	**140**	23	117

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
SRNL	Team Member	National Lab	Adsorbent and compressed gas modeling
PNNL	Team Member	National Lab	Chemical hydrogen and metal hydride modeling
HyMARC—Sandia National Laboratories	Material Research	National Lab/ Collaboration	Metal hydride data
HyMARC—Lawrence Berkeley National Laboratory	Material Research	National Lab/ Collaboration	Metal hydride data

Proposed Future Work – FY22 Milestones and Next Steps

Deliverable		Due
FY22-Q1	Complete and submit two manuscripts on the results of the project scope. Topics include Tankinator model, Rev. 4 and Adsorbents.	**Tankinator complete, Adsorbents in review**
FY22-Q2	Integrate HD/MD models into the Framework, including Adsorbents, MH, and chemical hydrogen storage. Exercise models, evaluate and validate results. Upload to website for general use.	**By AMR**
FY22-Q3	Develop and integrate an agricultural or mining vehicle duty cycle into the Vehicle Framework and demonstrate its use with Adsorbents, MH, and chemical hydrogen storage.	**6/30/2022**
FY22-Q4	In collaboration with Argonne National Laboratory, develop and integrate a liquid hydrogen storage system into the Vehicle Framework for light/medium/heavy-duty vehicles.	**9/30/2022**

Summary

Relevance	• Provide materials-based hydrogen storage researchers with models and materials requirements to assess their material's performance over a range of vehicular 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 is being expanded to increase its utility and a MH refueling modeling is being developed. • A refueling model has been developed for metal hydrides to better understand impacts of heat transfer on refueling kinetics. • A round-trip efficiency estimator has been developed to compare shipping costs between gaseous H_2 and hydrogen carriers. • Stand-alone tools and framework are being expanded beyond light-duty vehicles to medium- and heavy-duty vehicles • Stand-alone tools and framework have been used to evaluate materials for HyMARC and University of Michigan to help better understand the benefits (or not) of new materials. • Submitted one manuscript (with an additional one under review) to the ***International Journal of Hydrogen Energy***.
Collaborations	• Project team includes NREL, SRNL, and PNNL. • Consultants from industry participate in team meetings and provide input. • Material developers from HyMARC, University of Michigan, and other academic institutions have provided new material properties.
Proposed Future Research	• Expand the use of models by demonstrating their utility with other storage materials and vehicle class options and compare to storage using liquid H_2 and gaseous H_2.

Technical Backup and Additional Information

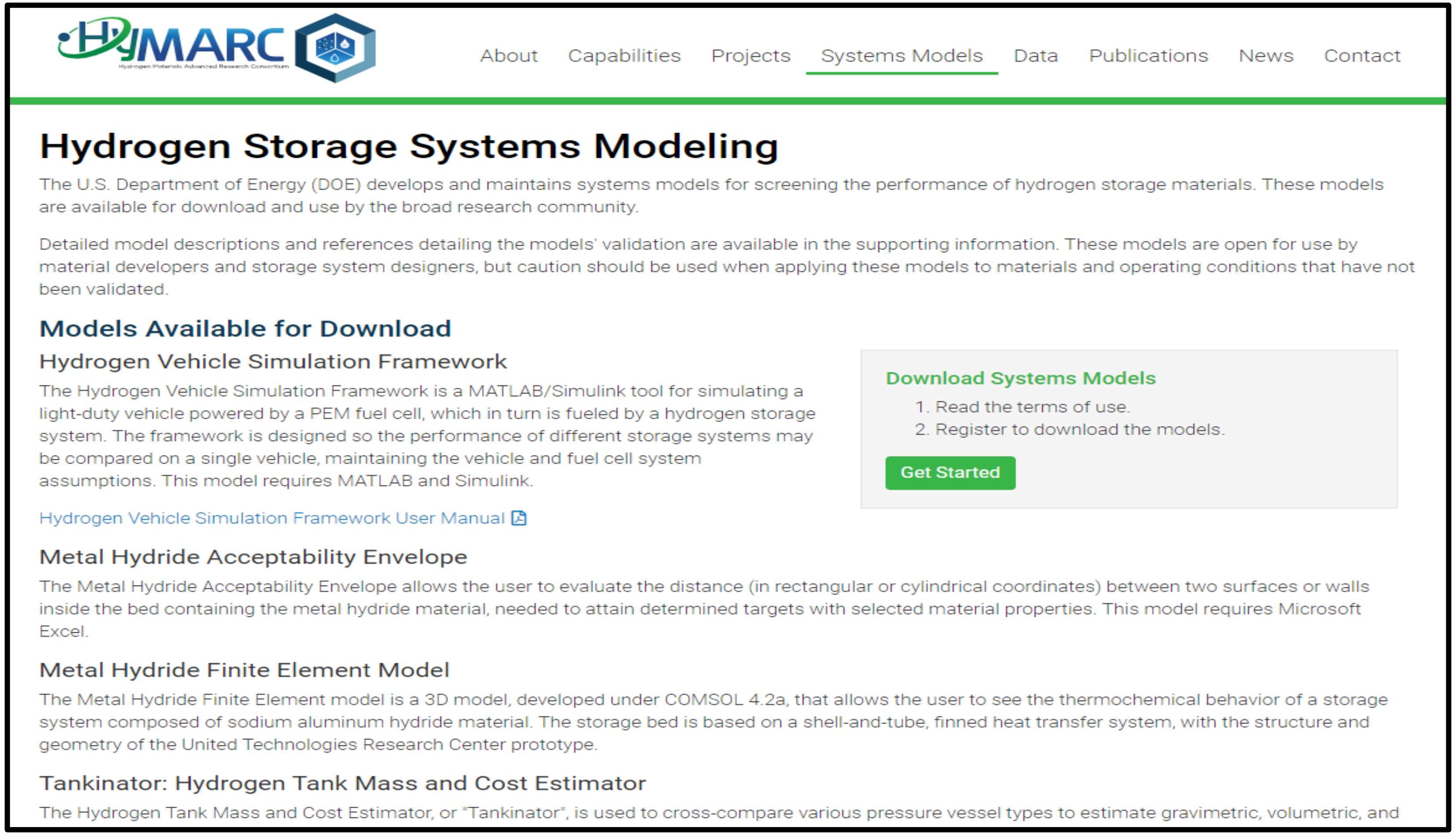
Technology Transfer Activities

- 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


HyMARC — Hydrogen Materials Advanced Research Consortium

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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.

Get Started

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

Brooks, Kriston, David Tamburello, Sam Sprik, and Matthew Thornton. 2020. “Design Tool for Estimating Metal Hydride Storage System Characteristics for Light-Duty Fuel Cell Vehicles.” *International Journal of Hydrogen Energy*, Volume 45, Issue 46, 24917–24927.

Grady, Carina, Scott McWhorter, Martin Sulic, Samuel J. Sprik, Matthew J. Thornton, Kriston P. Brooks, and David A. Tamburello, “Design Tool for Estimating Adsorbent Hydrogen Storage System Characteristics for Light-Duty Fuel Cell Vehicles,” Submitting to the *International Journal of Hydrogen Energy*, Date:TBD, Currently in review.

Klymyshyn, Nickolas, Kriston Brooks, and Nathan Barrett, “Tankinator: A Hydrogen Fuel Tank Characteristics Estimation Tool,” Submitted to the *International Journal of Hydrogen Energy*, January 2022, Currently awaiting review.