

# Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements

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- Sam Sprik, NREL

**Savannah River National Laboratory**

**June 9, 2016**



# Overview

## Timeline

- **Start: October 1, 2015**
- **End: September 30, 2018**
- **17% Complete (as of 4/1/16)**

## Budget

- **Total Project Funding: \$1,100,000**
  - **FY16 Funding: \$336,000**
  - **FY17 Funding: \$389,000**
  - **FY18 Funding: \$375,000**

## Barriers

- A. System Weight and Volume**
- B. System Cost**
- C. Efficiency**
- E. Charging/Discharging Rates**
- I. Dispensing Technology**
- K. System Life-Cycle Assessment**

## Partners



# Models on the Web Technical Objectives

Collaborative effort to **manage, update, and enhance** hydrogen storage system models developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE).

- Manage the **HSECoE model dissemination** web page.
- Manage, update, and enhance the **HSECoE modeling framework**.
- Maintain, enhance, and update the **specific storage system models** developed by the HSECoE.
- **Ultimate Goal**: Provide models that will **accept direct materials property inputs** as advancements in materials research are achieved.

## Model Access Website and Support

HSECoE website:

<http://hsecoe.org/>

Model support:

[HSECoE@nrel.gov](mailto:HSECoE@nrel.gov)

### Model access/description sub-page



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Home



The Hydrogen Storage Engineering Center of Excellence (HSECoE) is working to help reduce our Nation's dependence on foreign energy sources by changing the way we power our cars, homes, and businesses. The HSECoE was selected through a competitive, merit reviewed solicitation process by DOE.



The Center addresses the significant engineering challenges associated with developing lower-pressure, material-based, hydrogen storage systems for hydrogen fuel cell and internal combustion engine light-duty vehicles.

This project is incorporated into the DOE's Fuel Cell Technology Program, which consists of applied research and development activities, conducted through Center of Excellence materials and engineering teams, and independent projects focusing on materials and concepts, testing, and system analysis.



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Models

News

- Acceptability Envelope Tool released for metal hydride materials.
- 3D Metal Hydride Finite Element model released.
- Other models will be released in the near future.

What is the Metal Hydride Acceptability Envelope (AE)?

AE Model

What is the Metal Hydride Finite Elements (MHFE) Model?

MHFE Model

A Base Case Study: Sodium Aluminum Hydride (MHFE-SAH)

Downloads



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# Accomplishments and Progress

# Model Access Website

## Model documentation and downloads

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### Models

News

What is the Metal Hydride Acceptability Envelope (AE)?

The design and evaluation of vehicle based hydrogen storage systems require the use of detailed numerical models to evaluate performance and determine vehicle level performance. The design team is currently developing a design tool to assess vehicle coupled storage and storage vessel systems capable of achieving selected performance targets.



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### Models

- News
- What is the Metal Hydride Acceptability Envelope (AE)?
- AE Model
- What is the Metal Hydride Finite Elements (MHFE) Model?
- MHFE Model
- A Base Case Study: Sodium Aluminum Hydride (MHFE-SAH)
- Downloads

**Metal Hydride Acceptability Envelope (AE)** The AE 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. The file **AEHSC** refers to the rectangular coordinate model, while **AEHCC** refers to the cylindrical coordinate model.

**Metal Hydride Finite Element - Sodium Aluminum Hydride (MHFE-SAH)** MHFE-SAH is a 3D model, developed under COMSOL 4.2a, which allows the user to see the thermo-chemical 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 UTRC prototype.

Please enter your email address. We will use your information to send the number of views. We do not share any third parties.

Email \*

## User's manual

## H<sub>2</sub> Vehicle Simulation Framework

### MODEL DESCRIPTION AND USER MANUAL

Hydrogen Storage Engineering Center of Excellence  
José Miguel Pasini United Technologies Research Center  
Jon Cosgrove National Renewable Energy Laboratory

April 21, 2014

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The screenshot shows the user manual for the H<sub>2</sub> Vehicle Simulation Framework. It includes a table of contents with page numbers, a model description section, and a drive cycles section. The model description section includes a table with columns for 'Model description', 'Drive cycles', 'Vehicle model', 'Fuel cell system', 'Hydrogen storage systems', 'User manual', 'Introduction', 'System requirements', 'Installation', 'Creating the UTRC and setting up the simulation', 'Selecting the storage system', 'Selecting the parameters for the user', 'Running a single simulation', 'Plotting and saving the results', and 'Biography'. The drive cycles section includes a table with columns for 'Model description', 'Drive cycles', 'Vehicle model', 'Fuel cell system', 'Hydrogen storage systems', 'User manual', 'Introduction', 'System requirements', 'Installation', 'Creating the UTRC and setting up the simulation', 'Selecting the storage system', 'Selecting the parameters for the user', 'Running a single simulation', 'Plotting and saving the results', and 'Biography'.

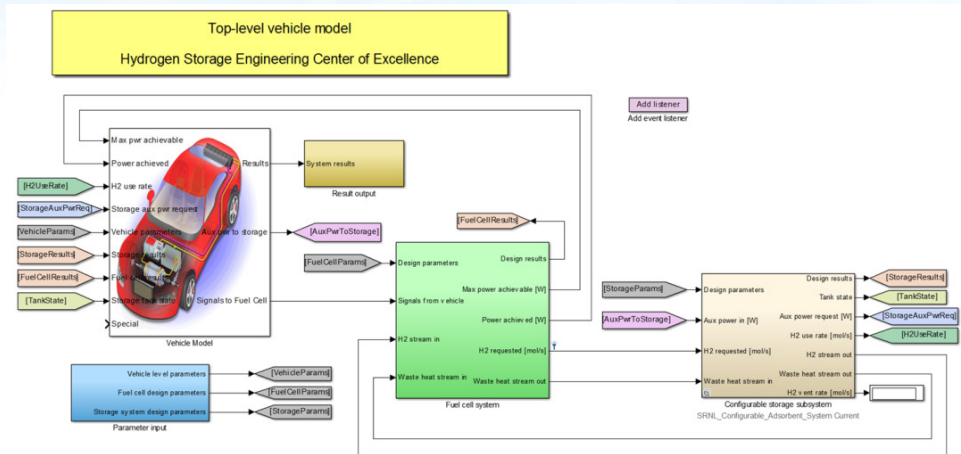




## Recent Model Updates

### Vehicle Framework Updates:

- Completed adsorbent model updates and integration.
  - Validated adsorbent models based on 2-liter Prototype experimental results.
- Adjusted CH tank size to ensure 5.6 kg of usable hydrogen.
- Troubleshooting of compiler and software versions.
- Updated and posted newest version of the documentation (as of January, 2016).
- Working on adding model and sub-model validation references to the web page.



### Ongoing/Future Activities:

- Web support for publicly available models.
- Tracking and monitoring Web activity and downloads.
- Develop storage system sizing pre-processor (CH storage system).
  - Update/improve adsorbent storage system sizing pre-processor.
- Develop a stand-alone isotherm data fitting routine to convert raw excess hydrogen adsorption data into D-A parameters for use in the vehicle model.
- Framework beta testing for new releases.

# CH and Tank Volume/Cost Model Updates Completed

## Chemical Hydrogen (CH) Storage Model in the Vehicle Level Model:

- Integrated into the framework, documented and released models to the public.
  - Exothermic (Ammonia Borane) and Endothermic (Alane) Models.
- Continued beta testing models identified issues.
  - Adjusted tank size to ensure 5.6 kg of usable hydrogen available to the vehicle.
- Developing a preprocessor to convert kinetic and thermodynamic data from material developers into input parameters in the model.
  - Preprocessor helps size the system and determine the appropriate parameters in the setup file.
  - Simplifies the use of alternative materials.

## Tank Volume/Cost Model:

- Completed Model Documentation.
  - Mass compared to actual within  $\pm 10\%$ .
  - Costs are for comparison only – cost of raw materials but not fabrication.



# Tank Volume/Cost Model: Comparison to American CNG Tanks

- **Type-I Tank Chromoly Steel Tank TYPE1-CP1459**

- 120 liter tank 14" diameter x 59" long, working pressure 248 bar = **297 lbs**.
- Tankinator estimate = **307 lbs** based on tank dimensions and pressure (**3.4%** difference for a tank volume prediction of 137 liters).

- **Type-III AME1945E**

- 140 liter tank, 19" diameter x 45" long, working pressure 304 bar = **151 lbs**.
- Tankinator estimate = **144 lbs** based on tank dimensions and pressure (**5%** difference).

- **Type-IV QT2560**

- 234 L tank, 25" diameter x 40" long, working pressure 311 bar = **117 lbs**.
- Tankinator estimate = **121 lbs** based on tank dimensions and 300 bar (**3.2%** difference).

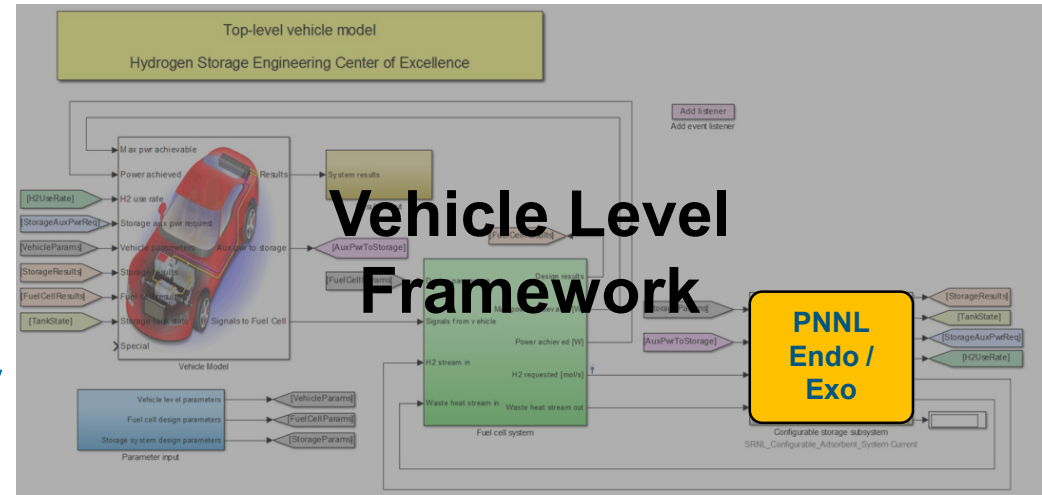
# Purpose of the Chemical Hydrogen Preprocessor

**User Input Data:**  
Material Properties (e.g. MW,  $x_{H_2}$ )  
Reaction Parameters (e.g.  $E_a$ ,  $\Delta H_{rxn}$ )  
Slurry Properties (e.g. wt% inert,  $C_p$ ,  $\rho$ )

**Parameters Normally Measured  
by Material Developers**

Preprocessor

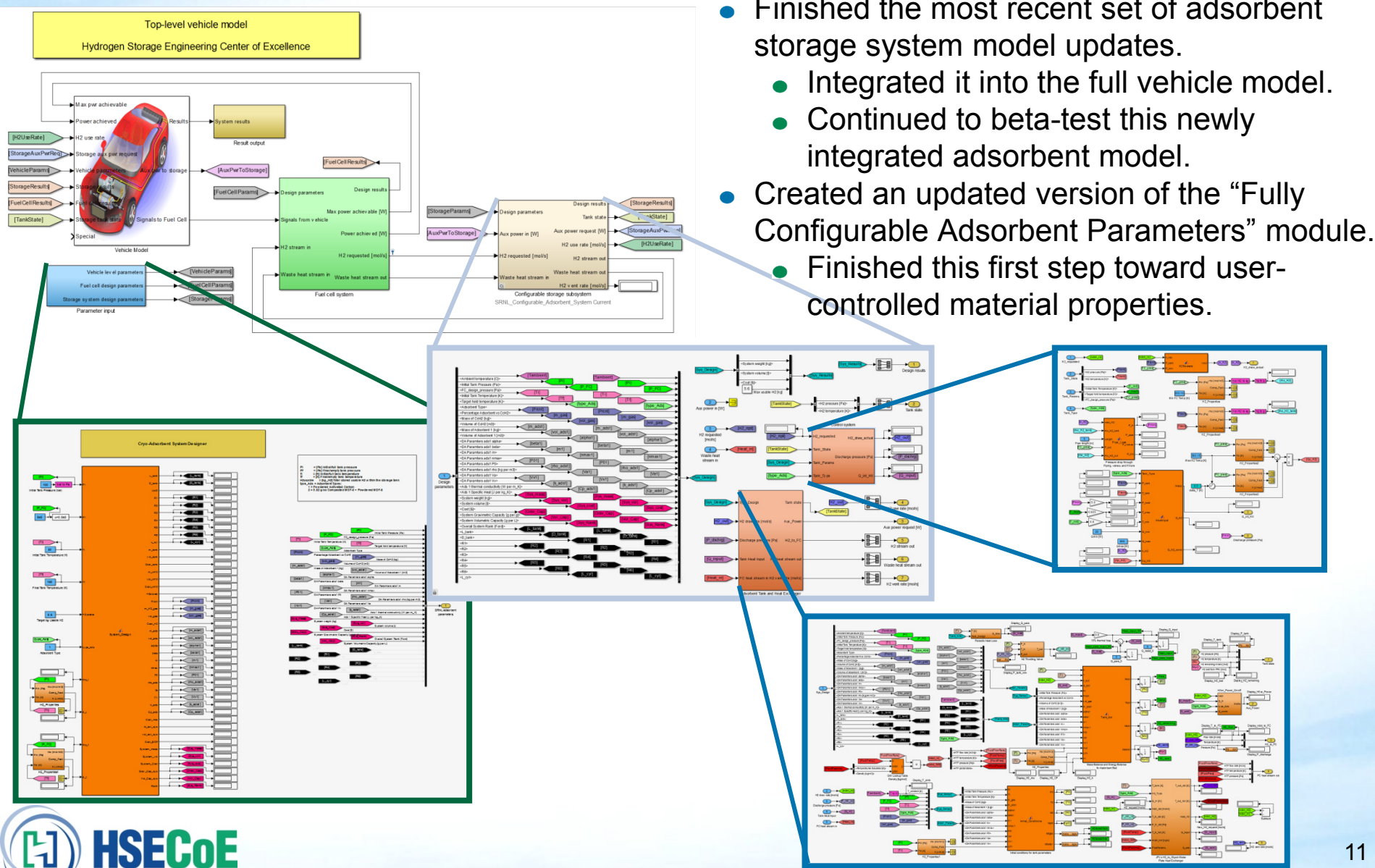
**Preprocessor Output:**  
Mass of CH in Feed Tank  
Liquid/Gas Radiator Length  
Reactor Length  
Ballast Tank Volume  
Recuperator Length



**Parameters Needed  
as Input to the Model**

## Adsorbent Storage System Model Updates

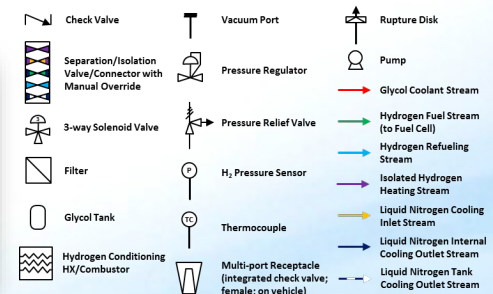
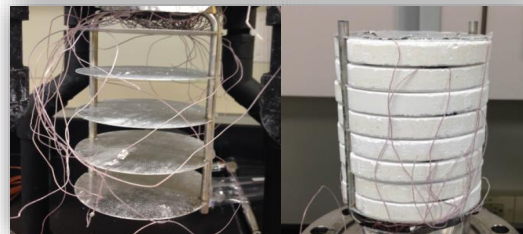
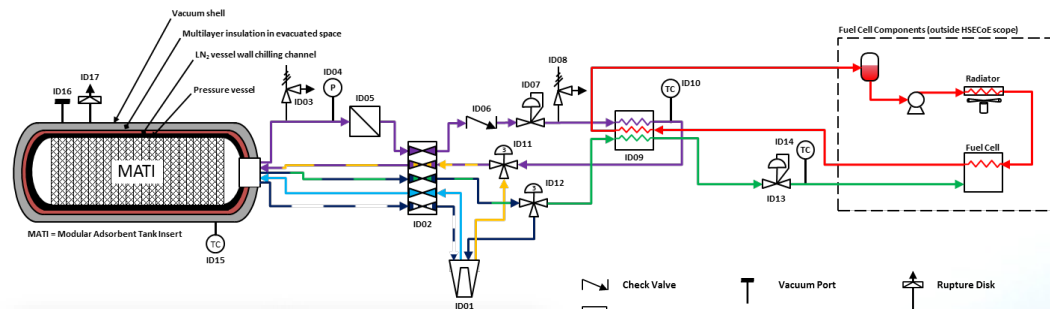
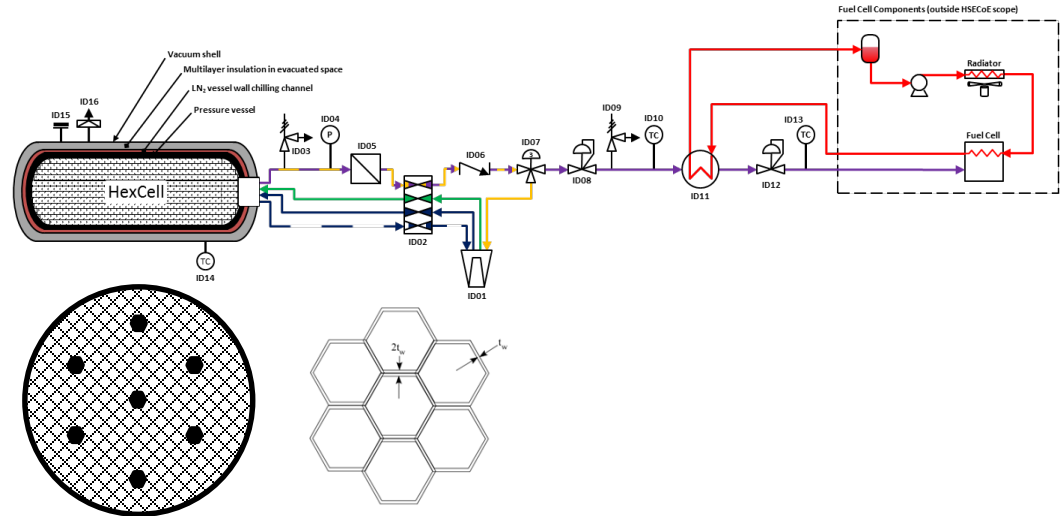
- Finished the most recent set of adsorbent storage system model updates.
  - Integrated it into the full vehicle model.
  - Continued to beta-test this newly integrated adsorbent model.
- Created an updated version of the “Fully Configurable Adsorbent Parameters” module.
  - Finished this first step toward user-controlled material properties.



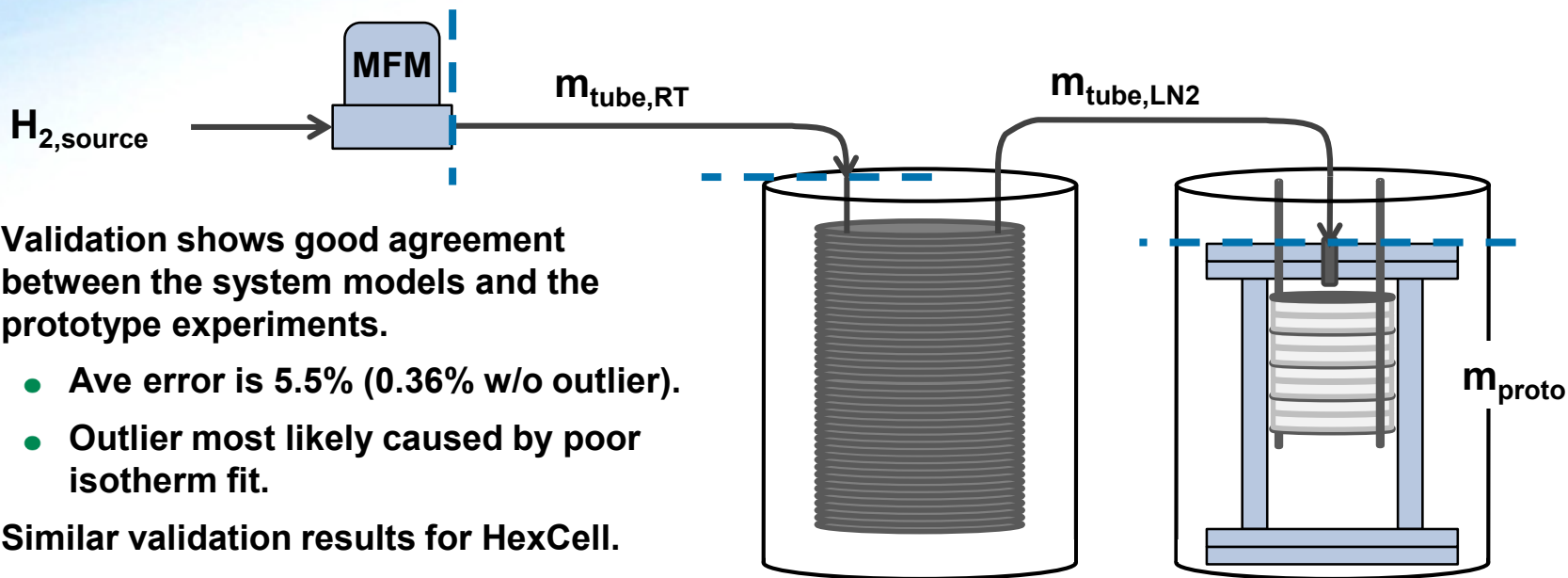
## Adsorbent Storage System Model Description

### Adsorbent Module Controls:

- Full tank pressure
  - $10 \text{ bar} \leq P_{\text{tank}} \leq 100 \text{ bar}$
- Full tank temperature
  - $77 \text{ K} \leq T_{\text{tank}} \leq 300 \text{ K}$
- Target empty tank temperature
  - $77 \text{ K} \leq T_{\text{tank}} \leq 300 \text{ K}$
  - Model was tuned toward a temperature increase of 80 K
- Target usable hydrogen
  - $0.5 \text{ kg} \leq H_{2,\text{usable}} \leq 12 \text{ kg}$
- Type of Adsorbent / System
  - Adsorbent/System # 1 – Powder MOF-5 (0.18 g/cc) in a HexCell heat exchanger
  - Adsorbent/System #2 – Compacted MOF-5 pucks (0.4 g/cc) in a MATI isolated-fluid heat exchanger



# MATI Adsorbent Storage System Validation



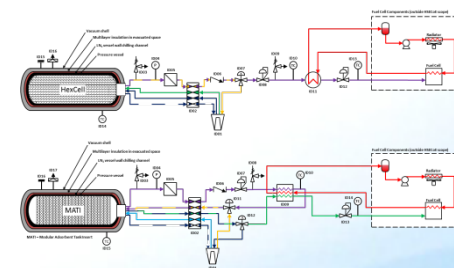
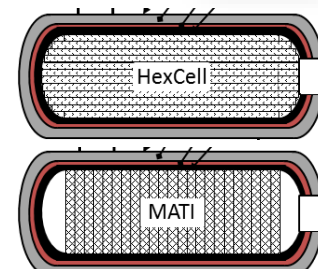
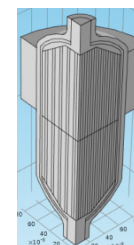
- Validation shows good agreement between the system models and the prototype experiments.
  - Ave error is 5.5% (0.36% w/o outlier).
  - Outlier most likely caused by poor isotherm fit.
- Similar validation results for HexCell.

Op. Conditions	$H_{2,in}$	$m_{tube,tot}$	$m_{proto,exp}$	$m_{proto,model}$	%-Diff
(1.07 bar, 83.7 K) → (60.0 bar, 91.3 K)	86.85 g	41.69 g	45.16 g	45.45 g	0.639%
( 1.09 bar, 83.7 K) → (100.0 bar, 84.5 K)	140.54 g	72.56 g	67.99 g	68.09 g	0.158%
(5.05 bar, 84.0 K) → (60.5 bar, 106.6 K)	59.55 g	28.51 g	31.04 g	24.57 g	<b>-20.86%</b>
( 5.23 bar, 83.2 K) → (100.2 bar, 102.4 K)	107.24 g	58.10 g	49.14 g	49.00 g	-0.285%



## Ads. Validation Results to Full-Scale Projections

	<b>Powder MOF-5 HexCell HX</b>	<b>Compact MOF-5 MATI HX</b>
Measured 2-liter Prototype (material + HX <sub>internal</sub> )	(90 K, 80 bar) → (85 K, 1.7 bar)	(84.5 K, 100 bar) → (83.7 K, 1.1 bar)
Gravimetric Capacity	0.112 g/g	0.092 g/g
Volumetric Capacity	23.6 g/l	37.2 g/l
Full-scale 5.6 kg System model (material + HX <sub>internal</sub> )	(80 K, 100 bar) → (160 K, 5.0 bar)	(80 K, 100 bar) → (160 K, 5.0 bar)
Gravimetric Capacity	0.125 g/g	0.100 g/g
Volumetric Capacity	32.9 g/l	44.4 g/l
Full-scale 5.6 kg System model (full system)	(80 K, 100 bar) → (160 K, 5.0 bar)	(80 K, 100 bar) → (160 K, 5.0 bar)
Gravimetric Capacity	0.0321 g/g	0.0315 g/g
Volumetric Capacity	18.9 g/l	21.0 g/l





## Hydrogen Vehicle Simulation Framework

Figure 1: Vehicle simulation framework

**Hydrogen Vehicle Simulation Framework**

Select storage system: Test system (dropdown menu open)

- Test system
- CH-AB Slurry Exothermic
- CH-Alane Slurry Endothermic
- Compressed 350 bar
- Compressed 700 bar
- Cryoadsorbent** (highlighted)
- MH-GH/3s v3

Running scenario: 1 Fuel economy test (UDDS+HWY, ...)

Run simulation

Results (at end of simulation)

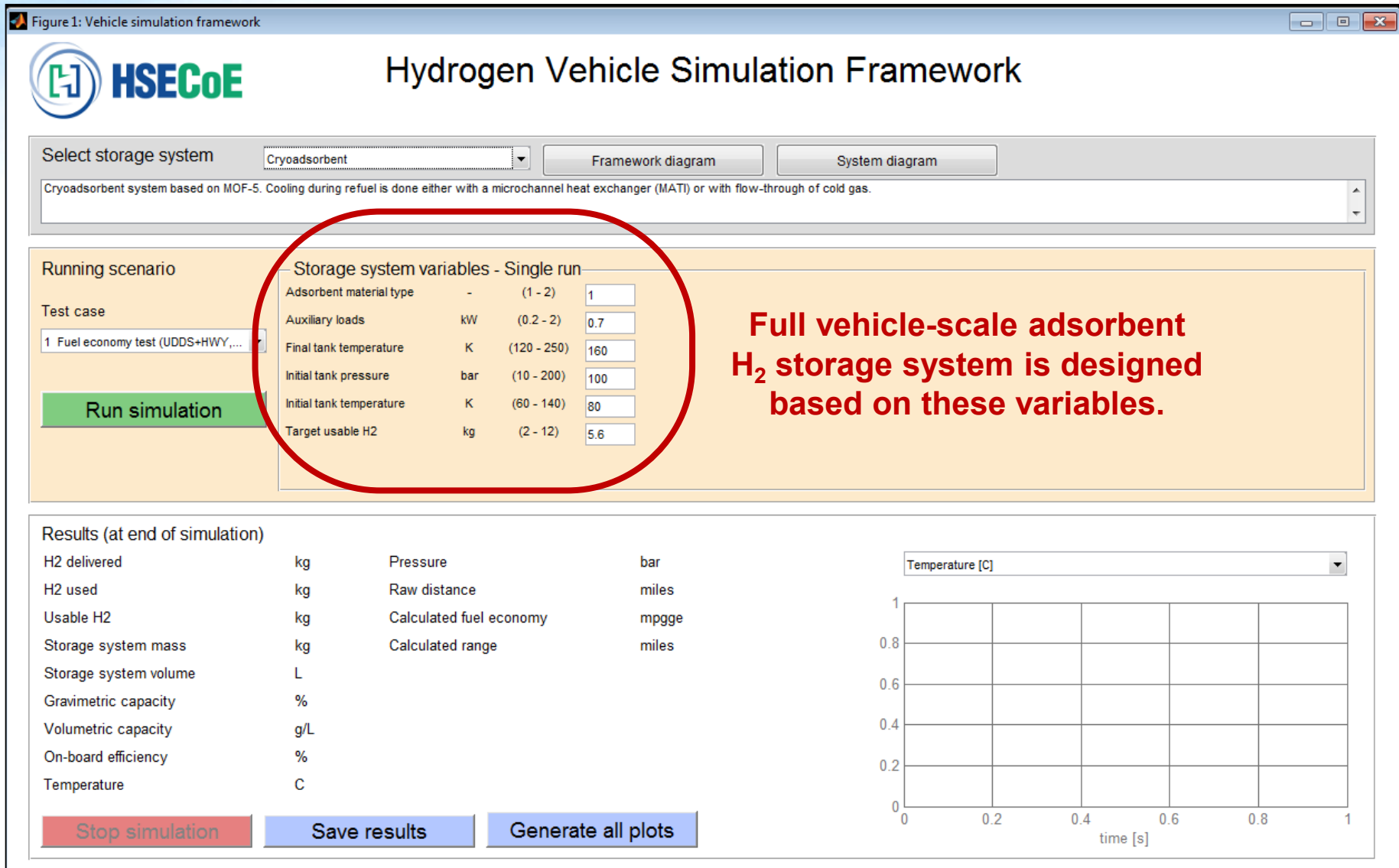
H2 delivered	kg	Pressure	bar
H2 used	kg	Raw distance	miles
Usable H2	kg	Calculated fuel economy	mpgge
Storage system mass	kg	Calculated range	miles
Storage system volume	L		
Gravimetric capacity	%		
Volumetric capacity	g/L		
On-board efficiency	%		
Temperature	C		

Temperature [C] plot: 0 to 1 on both axes, time [s] on x-axis.

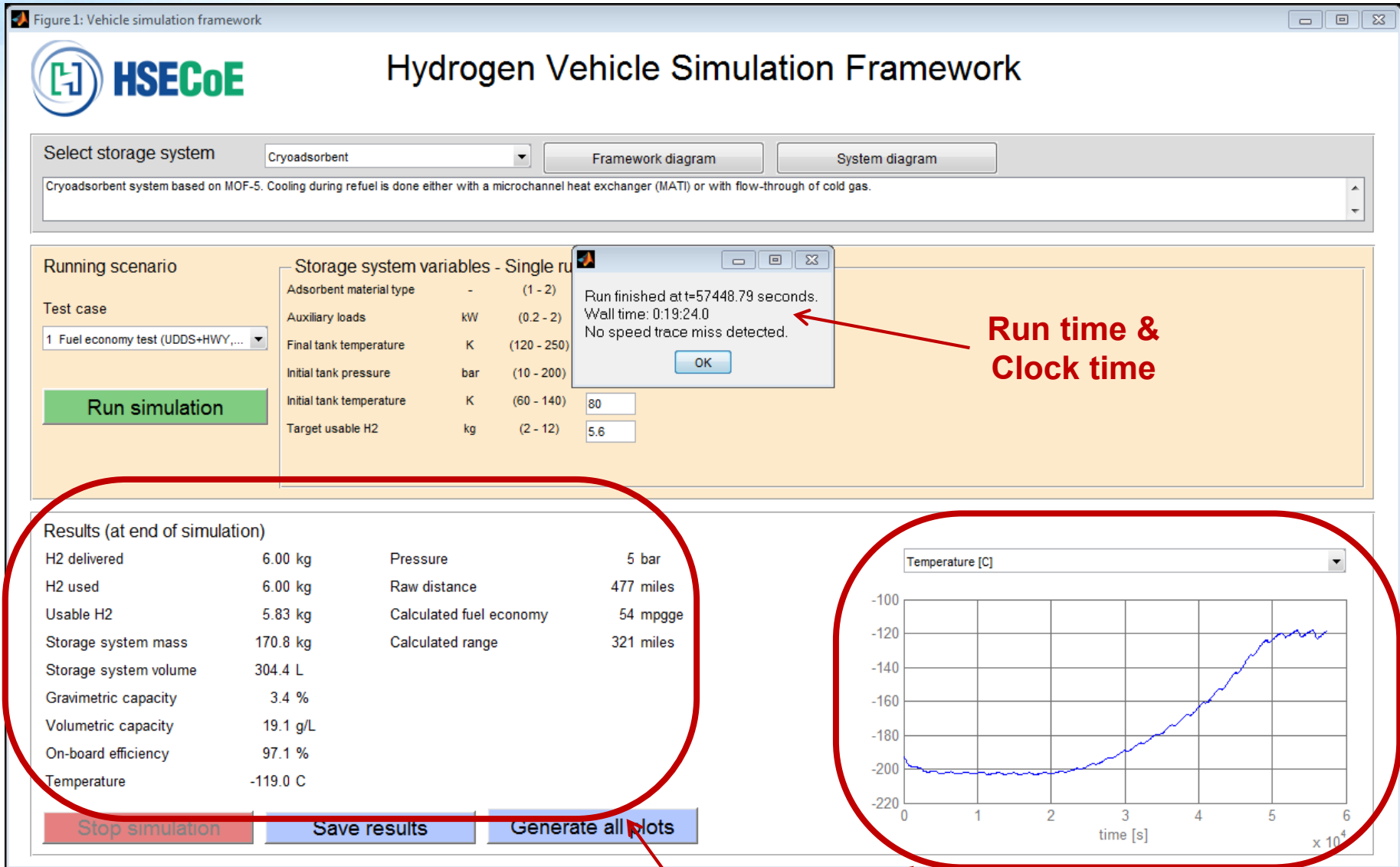
Stop simulation | Save results | Generate all plots

**Adsorbent Storage System is now available in the vehicle framework (beta release)**

## Hydrogen Vehicle Simulation Framework

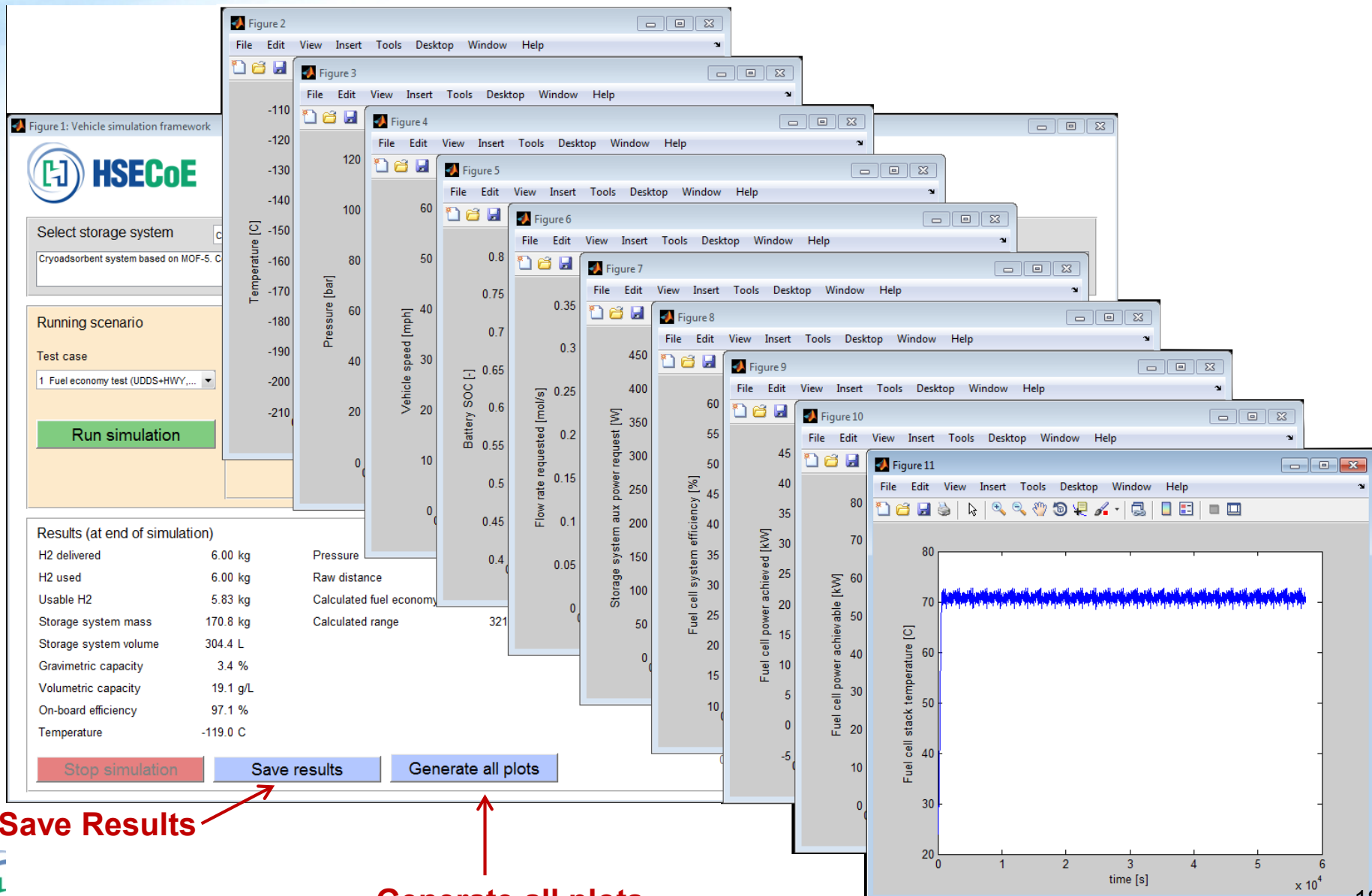


## Hydrogen Vehicle Simulation Framework



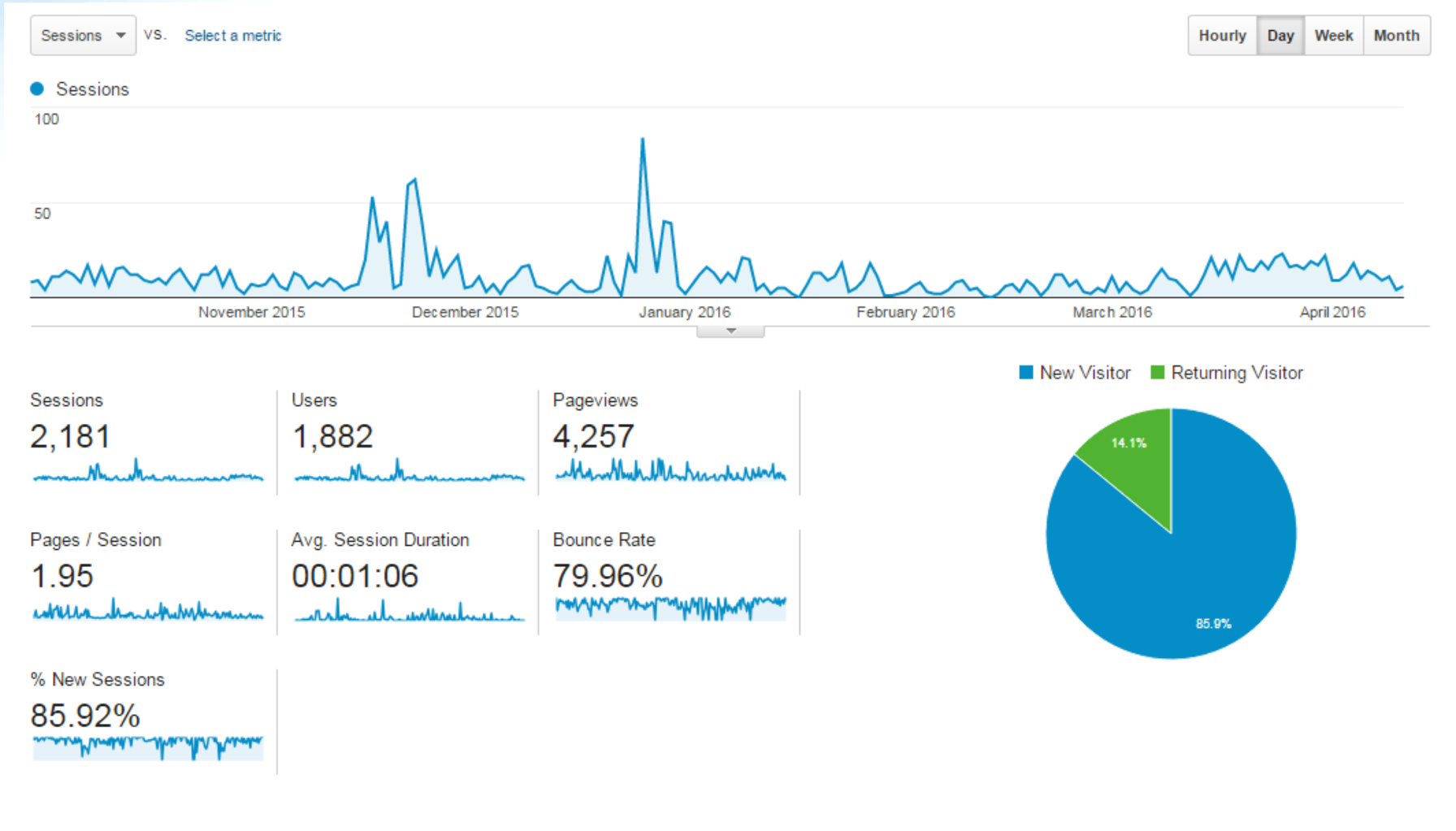
End of Simulation Results & Plots

## Hydrogen Vehicle Simulation Framework



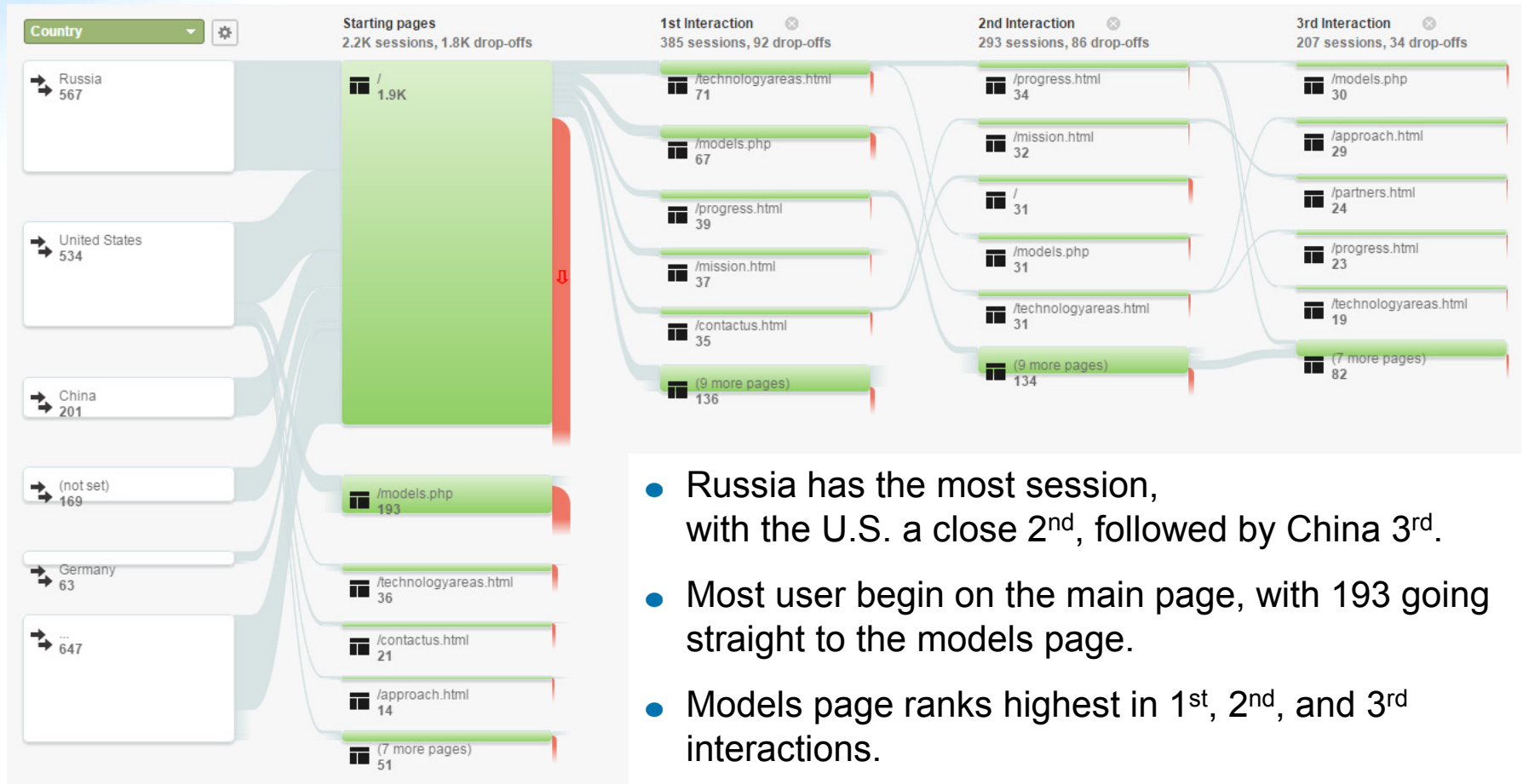


## Model Website Analytics October-April



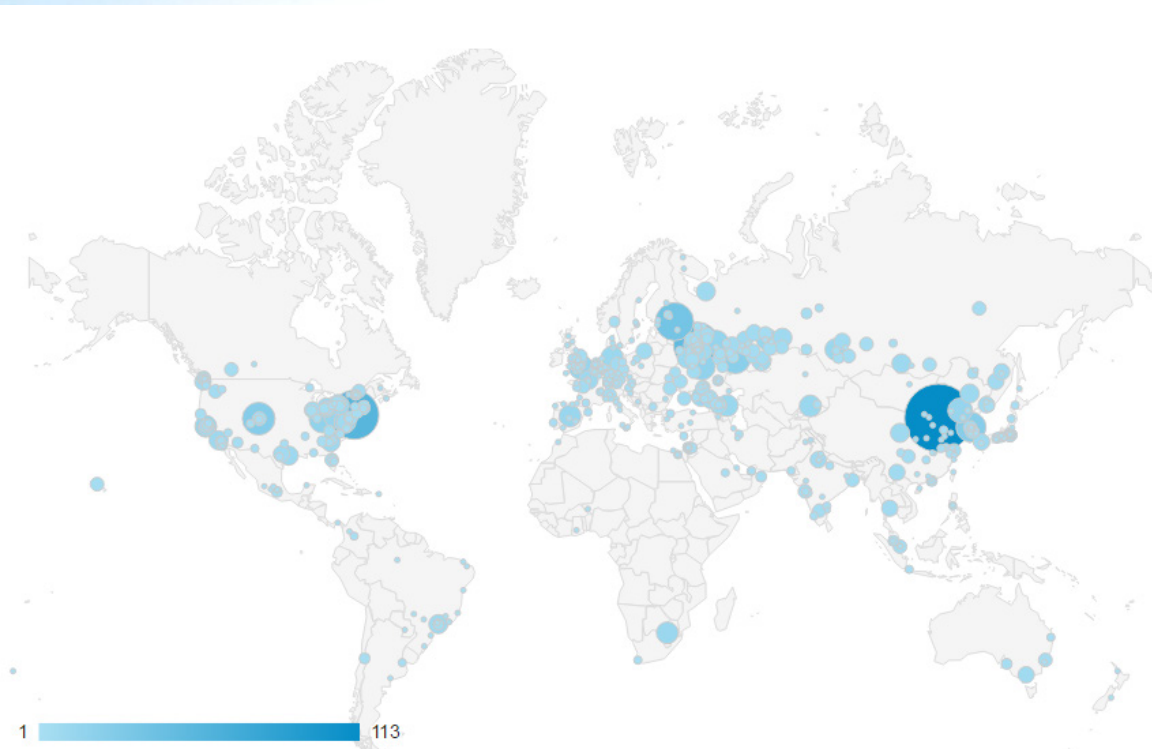


## Model Website Analytics Web Flow



- Russia has the most session, with the U.S. a close 2<sup>nd</sup>, followed by China 3<sup>rd</sup>.
- Most user begin on the main page, with 193 going straight to the models page.
- Models page ranks highest in 1<sup>st</sup>, 2<sup>nd</sup>, and 3<sup>rd</sup> interactions.

## Model Website Analytics



MODEL	DOWNLOAD COUNT (Q2)
H <sub>2</sub> Storage Tank Mass and Cost Model	101 (17)
MHAE Model	29 (6)
MHFE Model	41 (9)
Vehicle Simulator Framework Model	68 (15)

***43 new downloads of the Vehicle Simulator Framework Model since May, 2015.***

## Collaborative Activities

<b>Partner</b>	<b>Project Roles</b>
DOE	Sponsorship, steering
NREL	Project Lead, Framework Management
SRNL	Adsorbent Storage System Modeling
PNNL	Chemical Hydrogen Storage System Modeling

# Model Path Forward – Next Steps

- These activities will continue beyond the HSECoE Project.
  - Maintain and enhance existing framework models and track web activity and downloads.
  - Key enhancements will include adding sizing routines, the flexibility to accept different material properties (i.e. improve utility of the model for other materials), and consider changing to an open source code platform.
    - *Development of alternative kinetic expressions.*
    - *Reduce model size and complexity*
    - *Improve model robustness and controller algorithms*
- Finish beta testing and post the adsorbent framework models (April, 2016)
- SRNL will add an adsorbent Finite Element Analysis (FEA) Model similar to the metal hydride FEA model (June, 2016).

# Activity Deliverables / Milestones Going Forward

Deliverable	Date
Update storage system model documentation.	Completed
Update all adsorbent and CH HSECoE models based on experimental results.	Completed
Develop storage system sizing pre-processor (CH storage system).	6/2016
<b>SMART milestone</b> – Develop a stand-alone isotherm data fitting routine to convert raw excess adsorption H <sub>2</sub> data into its D-A parameters.	9/2016
Update storage system model documentation.	12/2016
Explore the possibility of changing the vehicle framework model platform to an open source code.	3/2017
Update models with any newly available data from DOE programs/literature.	6/2017
<b>SMART milestone</b> – Update the adsorbent hydrogen storage equations for additional theoretical formulations (such as UNILAN and/or 2-state Langmuir).	9/2017
Provide updates on the web portal activity.	12/2017
<b>SMART milestone</b> – Update the built-in material properties database to include new adsorbents (such as AC, HKUST-1, etc.).	3/2018
Update models with any newly available data from DOE programs/literature.	6/2018
Develop a stand-alone storage system estimator based on material properties.	9/2018

# Remaining Challenges and Barriers

- Share the models developed by the HSECoE with storage system materials developers.
- Develop storage system models that can be used by these material developers by making the models:
  - Flexible for a wider variety of storage materials.
  - Reasonable model run times.
  - Demonstration of their utility by evaluating recent experiments / material developments.
  - Consider new program environments and/or open source codes.



# Response to Previous Year Reviewer's Comments

**This project was not reviewed last year.**

# Questions?

## HSECoE Models on the WEB Team:

**Matthew Thornton**

**David Tamburello**

**Kriston Brooks**

**Jeff Gonder**

**Sam Sprik**



**With support from Bob Bowman and Mike Veenstra**

**Special thanks to the rest of the HSECoE,  
Jesse Adams, and Ned Stetson**

# Technical Backup Slides

# Chemical Hydrogen Storage Model Validation

## Individual component validation

### ● 0-D components: mass transfer only

- Feed/product tank, phase separator, ballast tank
- Approach: verify mass balance closure

### ● 1-D components: heat / mass transfer / reaction

- Reactor, radiators, recuperator
- Approach 1: compare steady state model to experimental data
- Approach 2: run model at steady state and compare to simplified models

### ● Parasitic power only components

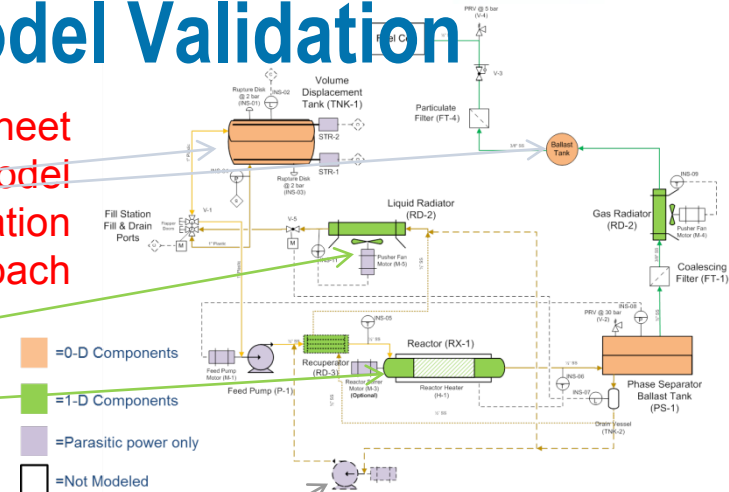
- Pumps, motors, and linear actuators

## Overall system validation

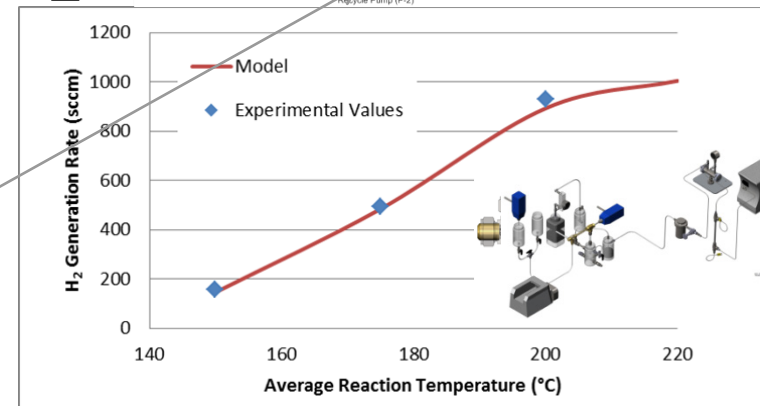
### ● Mass balance

- Chemical hydrogen in vs. hydrogen out

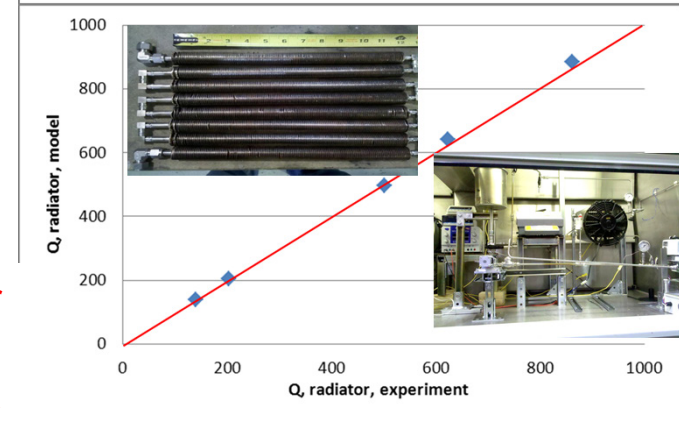
Flowsheet  
with Model  
Validation  
Approach



Reactor  
Validation:  
LANL Data



Radiator  
Validation:  
PNNL Data



# Vehicle Model Validation

**Fuel consumption for Federal Test Procedure (FTP) and highway cycles:**

- **Modeled results using a general vehicle are close to actual EPA reported data for specific vehicle classes.**
- **Provides a good estimate of relative fuel consumption for various storage systems.**

