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

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Savannah River National Laboratory

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Hydrogen Storage Engineering CENTER OF EXCELLENCE

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Project ID# ST008

SRNL-STI-2016-00220

Overview

Timeline

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

Barriers

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

Budget

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

Partners

NREL National Renewable Energy Laboratory

SRNL Savannah River National Laboratory

Pacific Northwest National Laboratory

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).

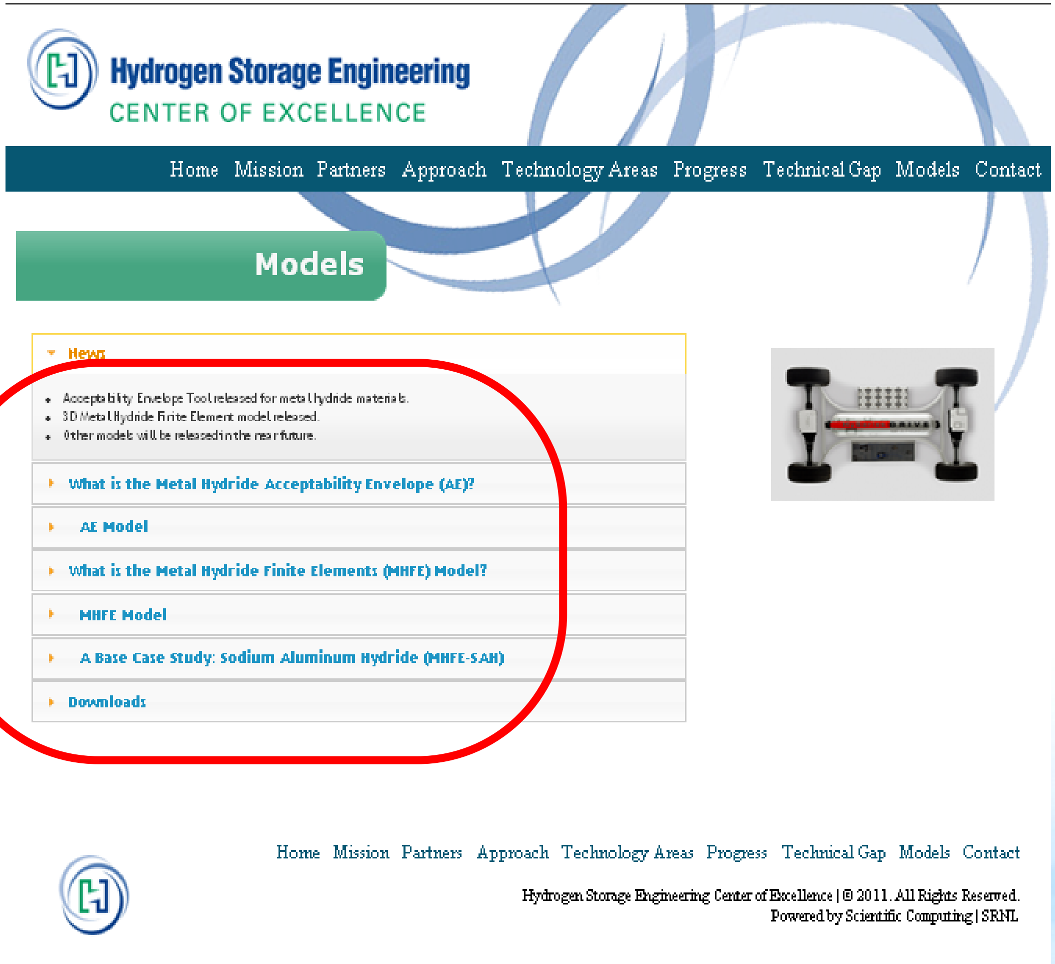
- Manage the **HSECoE model dissemination** web page.
- Manage, update, and enhance the **HSECoE modeling framework**.
- Maintain, enhance, and update the **specific storage system models** developed by the HSECoE.
- **Ultimate Goal:** Provide models that will **accept direct materials property inputs**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

Model Access Website and Support

HSECoE website:
http://hsecoe.org/

Model support:
HSECoE@nrel.gov

Model access/description sub-page

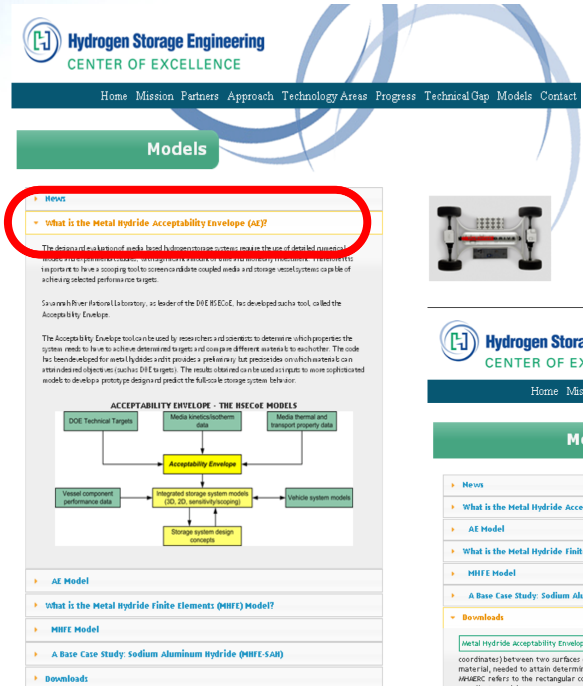


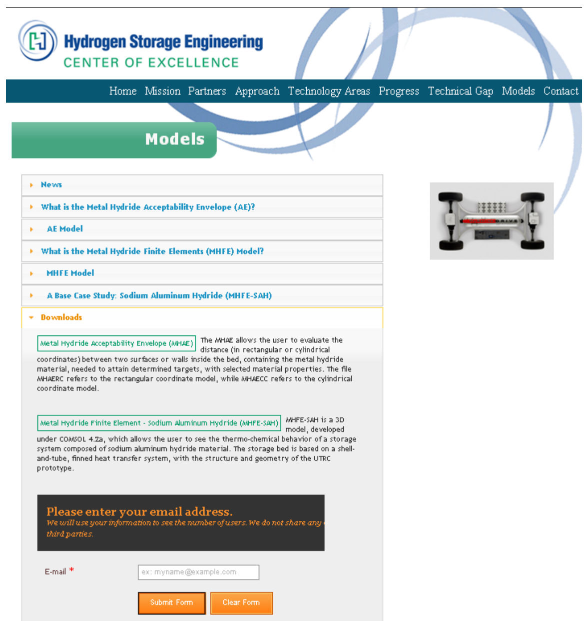
HSECoE

Accomplishments and Progress

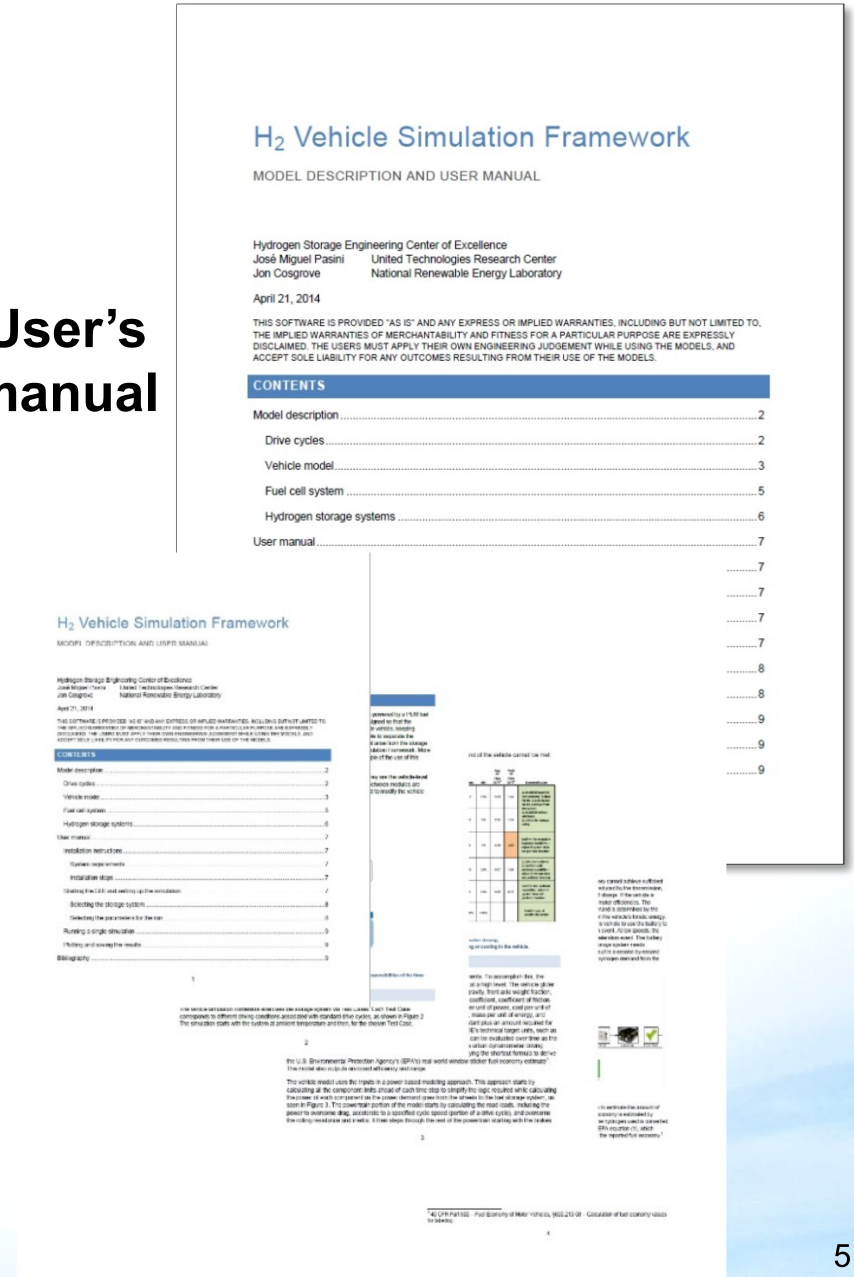
Model Access Website

Model documentation and downloads



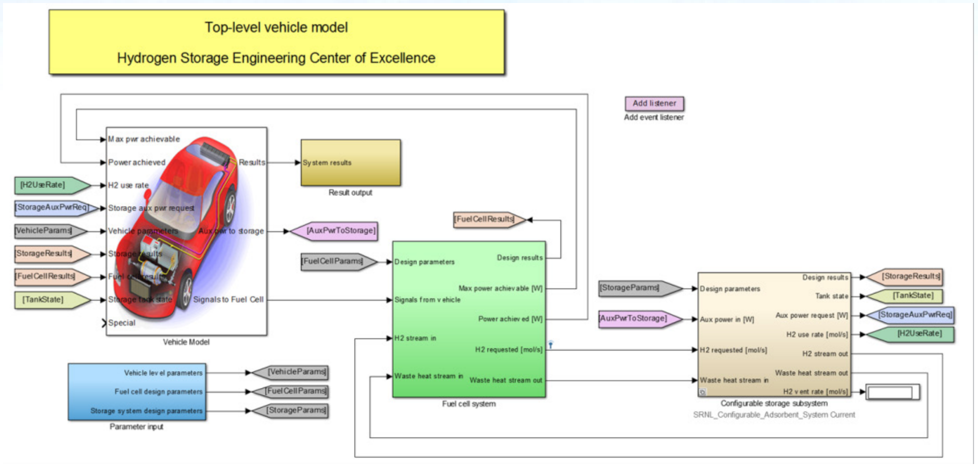


User's manual



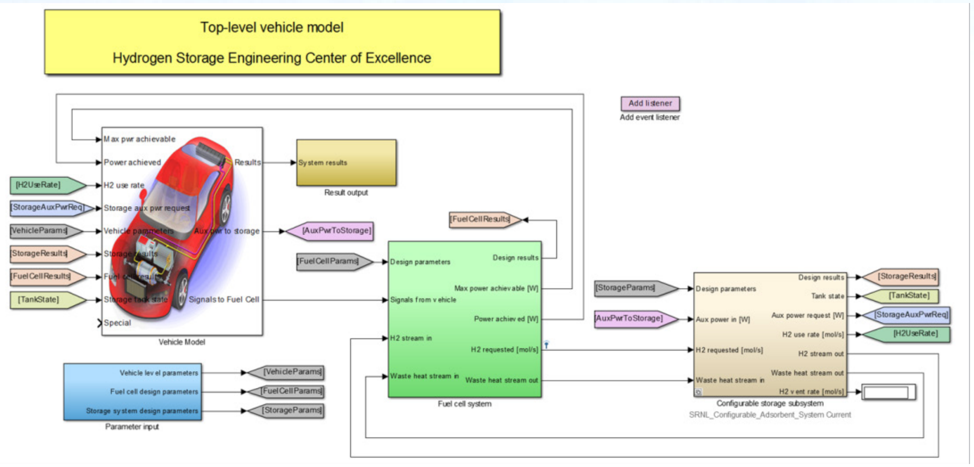
Accomplishments and Progress

Model Posting Status



MH Acceptability Envelope	SRNL	Complete
MH Finite Element Model	SRNL	Complete
Framework Model w/ Phy. Stor.	UTRC/NREL	Complete
Framework Model w/ MH	UTRC/SRNL/NREL	Complete
Tank Volume/Cost Model	PNNL	Complete
Framework Model w/ CH	PNNL/NREL	Complete
Framework Model w/ AD	SRNL/NREL	Beta Release Complete – 4/16
AD Finite Element Model	SRNL	Projected Release – 6/16

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-along 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 ±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_{H2})
- Reaction Parameters (e.g. E_a, ΔH_{rxn})
- Slurry Properties (e.g. wt% inert, Cp, ρ)

Parameters Normally Measured by Material Developers

↓

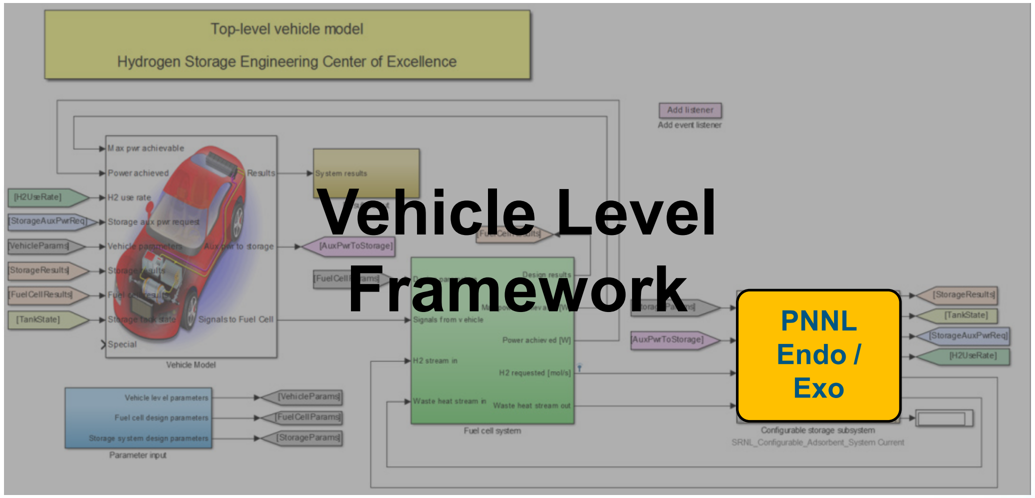
Preprocessor

↓

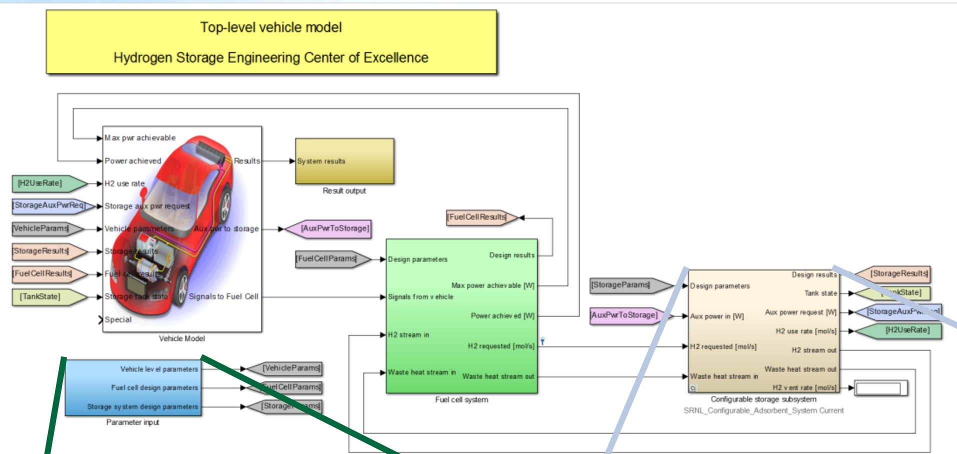
Preprocessor Output:

- Mass of CH in Feed Tank
- Liquid/Gas Radiator Length
- Reactor Length
- Ballast Tank Volume
- Recuperator Length

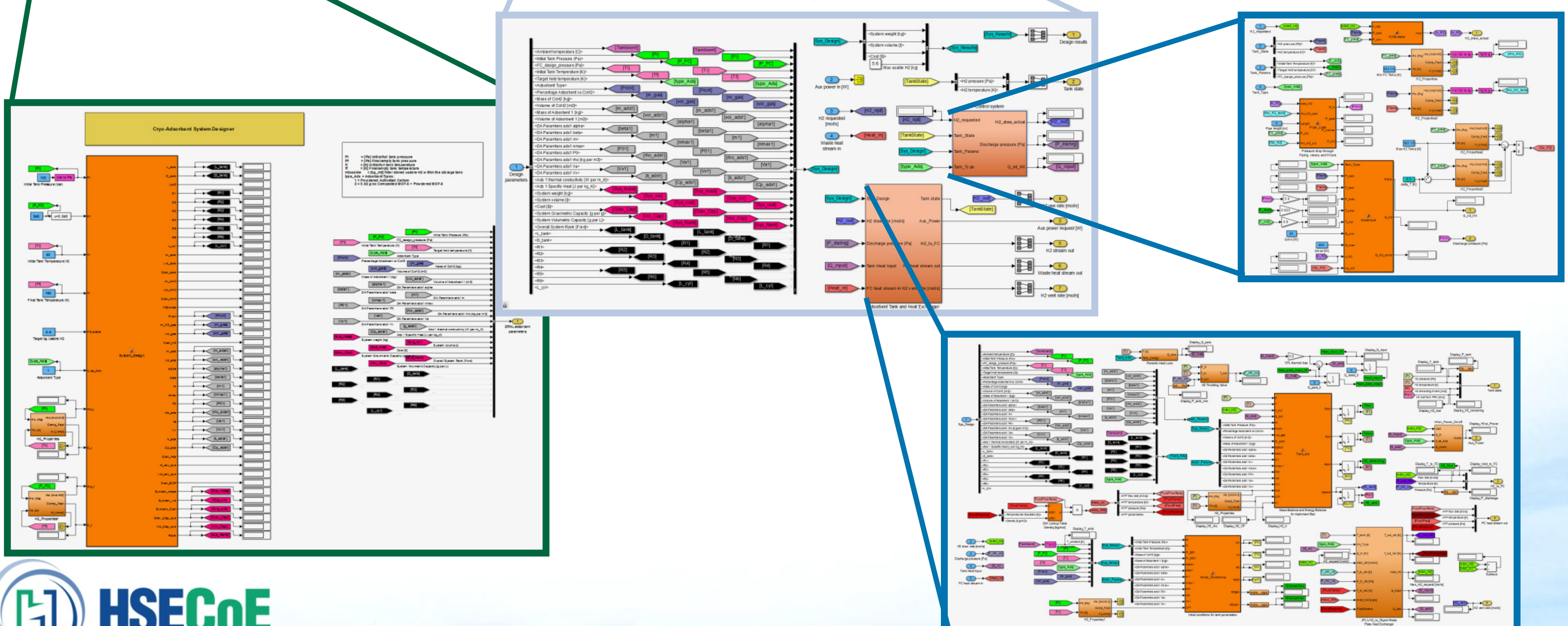
Parameters Needed as Input to the Model



Adsorbent Storage System Model Updates



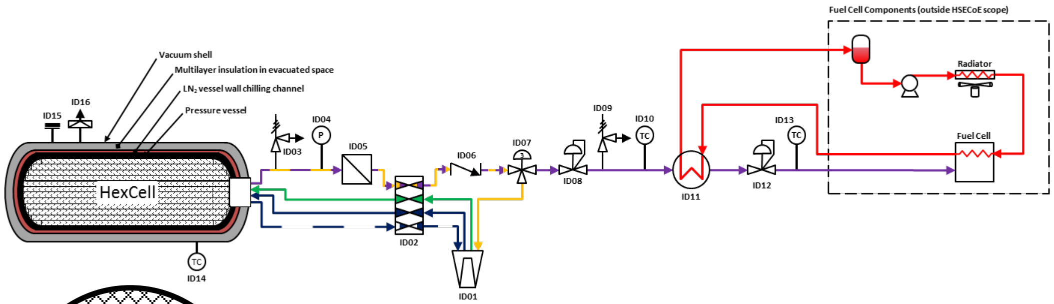
- Finished the most recent set of adsorbent storage system model updates.
  - Integrated it into the full vehicle model.
  - Continued to beta-test this newly integrated adsorbent model.
- Created an updated version of the “Fully Configurable Adsorbent Parameters” module.
  - Finished this first step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

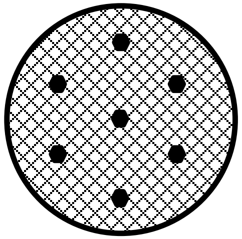


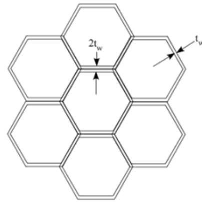
Adsorbent Storage System Model Description

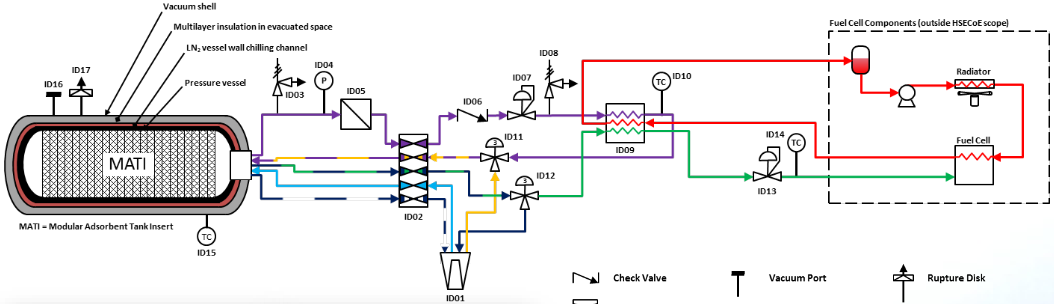
Adsorbent Module Controls:

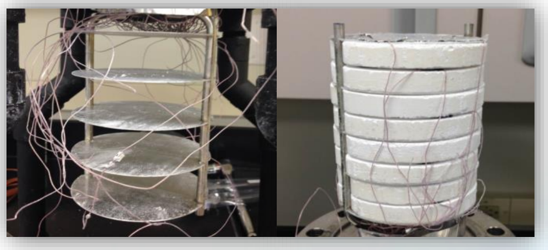
- Full tank pressure
  - 10 bar ≤ P_{tank} ≤ 100 bar
- Full tank temperature
  - 77 K ≤ T_{tank} ≤ 300 K
- Target empty tank temperature
  - 77 K ≤ T_{tank} ≤ 300 K
  - Model was tuned toward a temperature increase of 80 K
- Target usable hydrogen
  - 0.5 kg ≤ $H_{2,usable}$ ≤ 12 kg
- Type of Adsorbent / 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

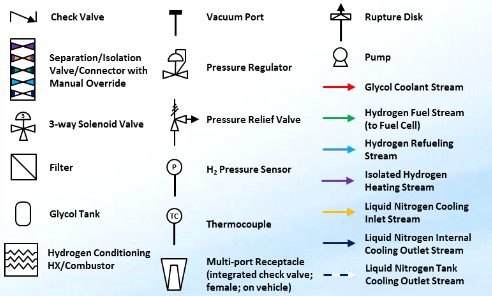




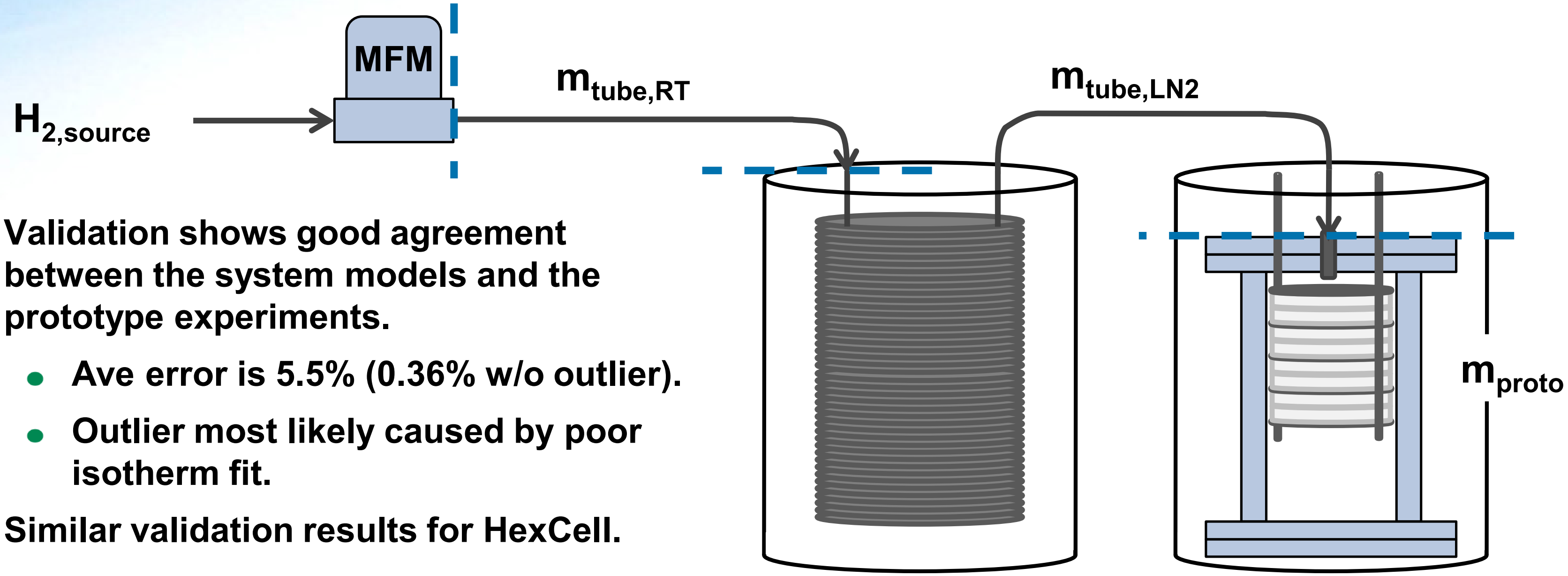








MATI Adsorbent Storage System Validation

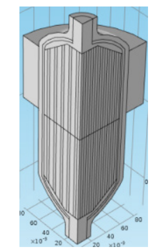


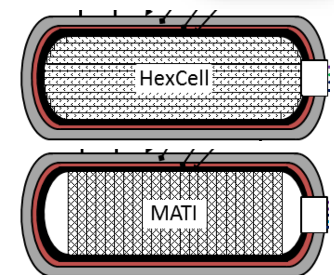
- Validation shows good agreement between the system models and the prototype experiments.
  - Ave error is 5.5% (0.36% w/o outlier).
  - Outlier most likely caused by poor isotherm fit.
- Similar validation results for HexCell.

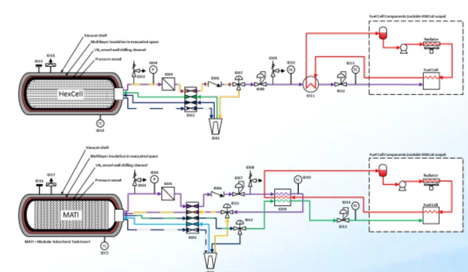
Op. Conditions	$H_{2,in}$	$m_{tube,tot}$	$m_{proto,exp}$	$m_{proto,model}$	%-Diff
(1.07 bar, 83.7 K) → (60.0 bar, 91.3 K)	86.85 g	41.69 g	45.16 g	45.45 g	0.639%
(1.09 bar, 83.7 K) → (100.0 bar, 84.5 K)	140.54 g	72.56 g	67.99 g	68.09 g	0.158%
(5.05 bar, 84.0 K) → (60.5 bar, 106.6 K)	59.55 g	28.51 g	31.04 g	24.57 g	**-20.86%**
(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

	Powder MOF-5 HexCell HX	Compact MOF-5 MATI HX
Measured 2-liter Prototype (material + $HX_{internal}$)	(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 + $HX_{internal}$)	(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

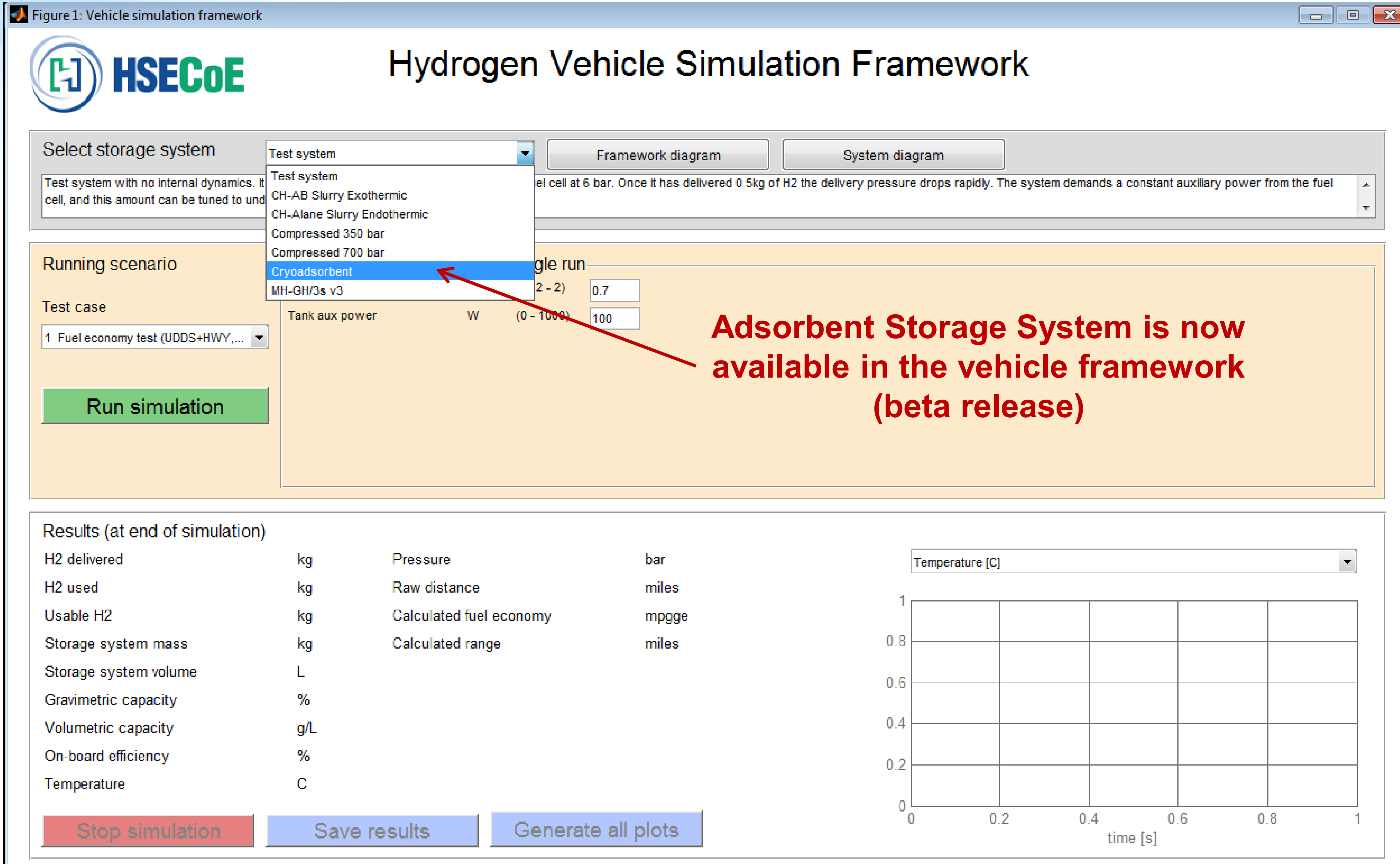






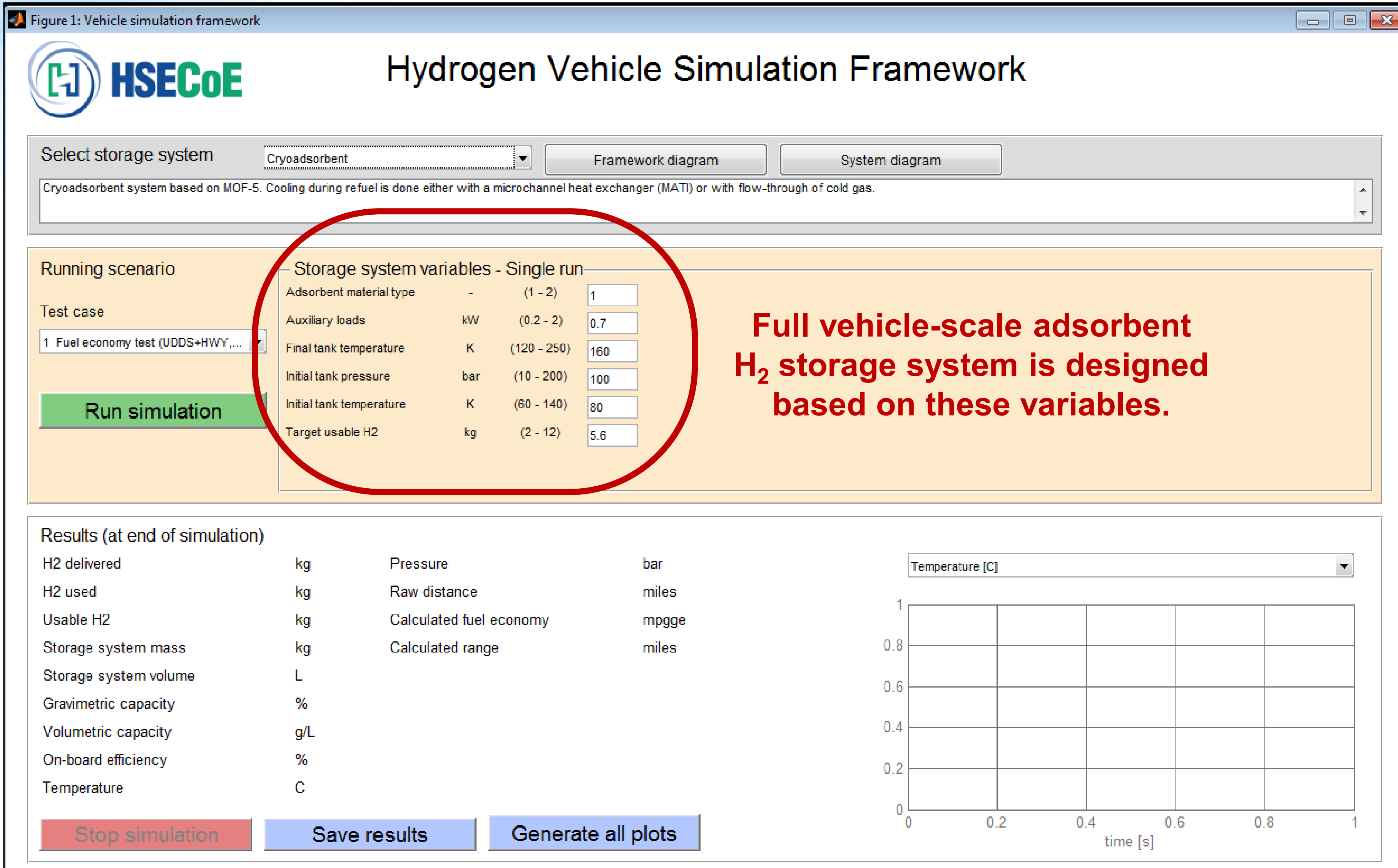
Accomplishments and Progress

Hydrogen Vehicle Simulation Framework

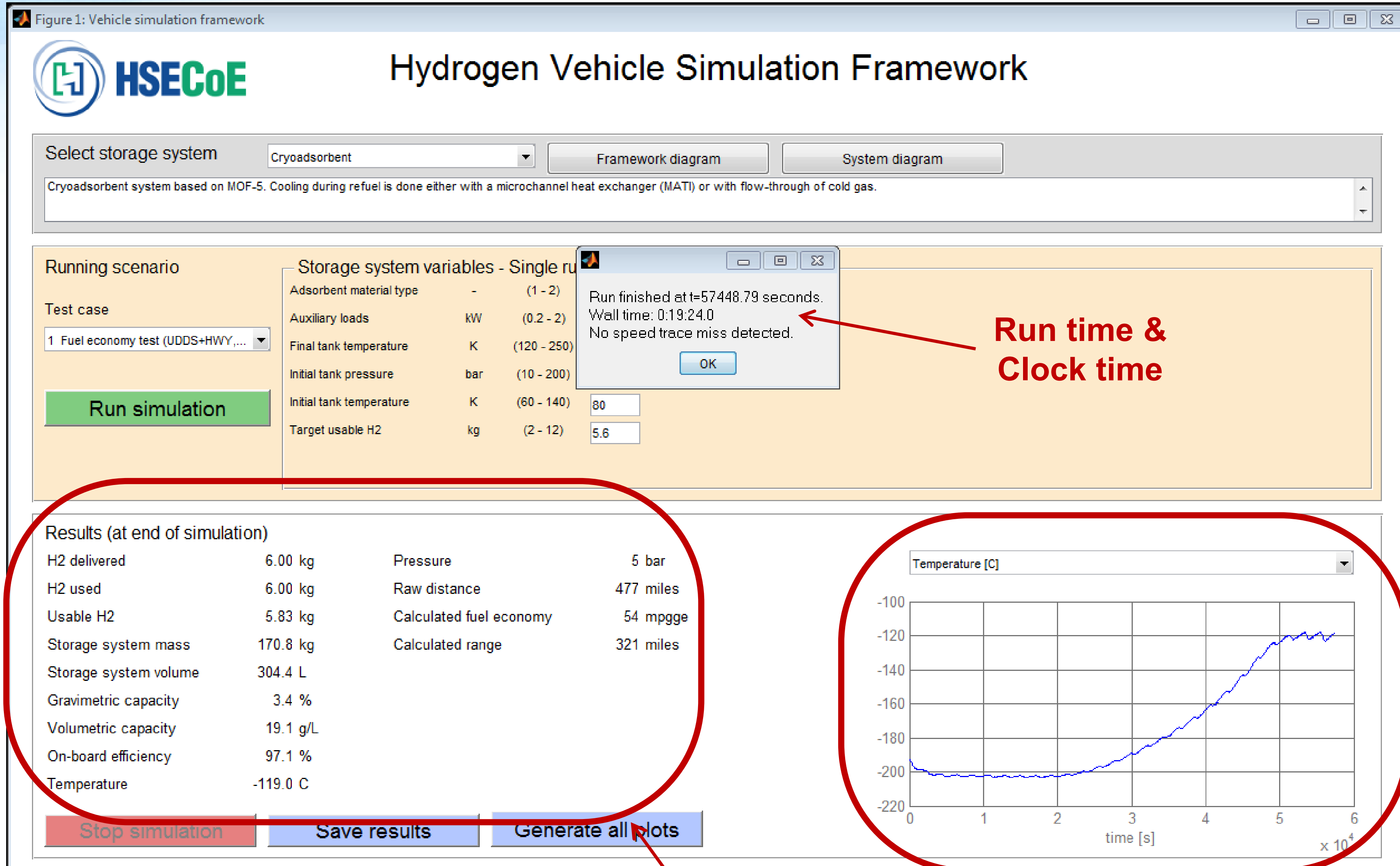


HSECoE

Hydrogen Vehicle Simulation Framework

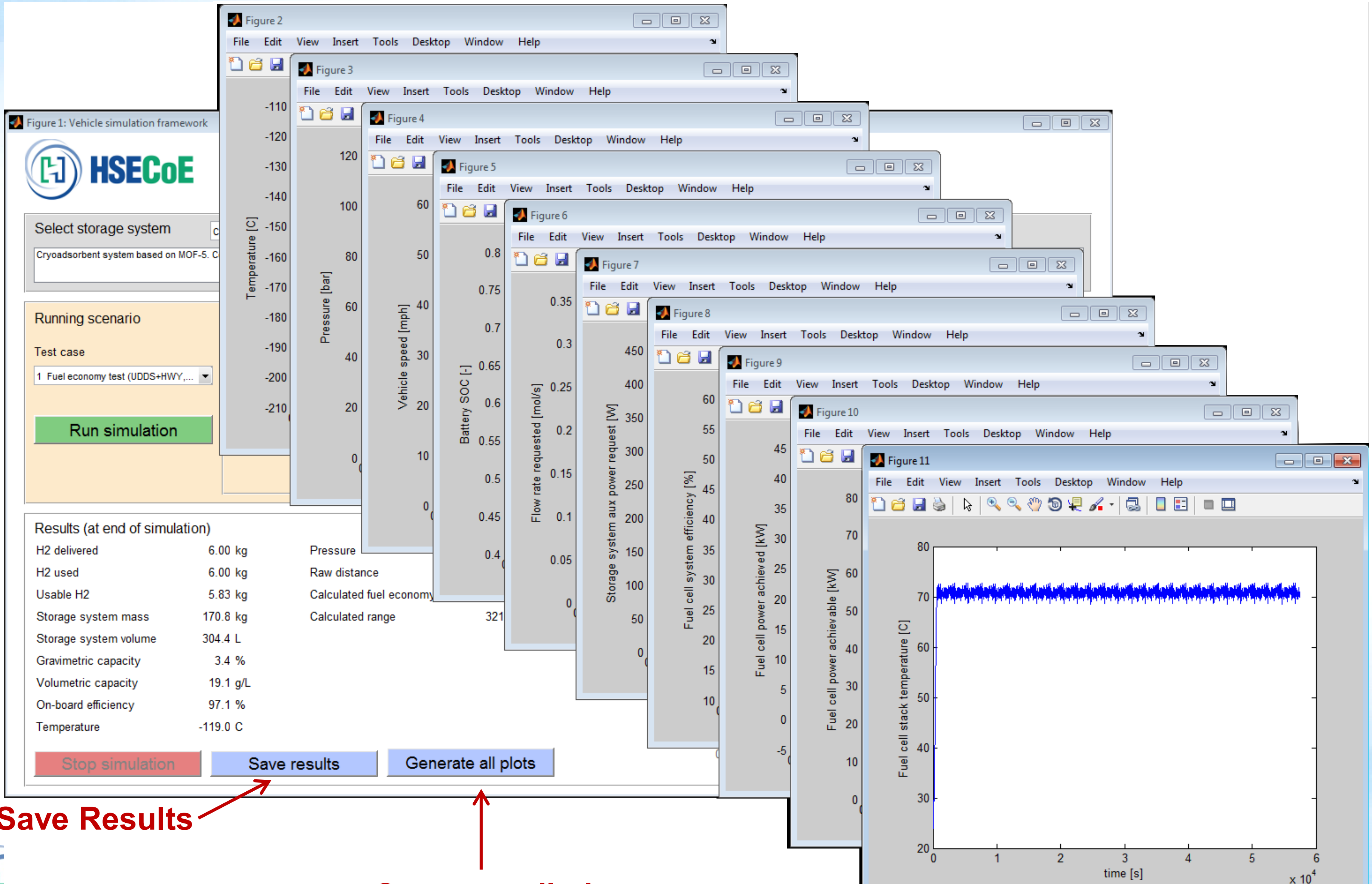


Hydrogen Vehicle Simulation Framework



End of Simulation Results & Plots

Hydrogen Vehicle Simulation Framework

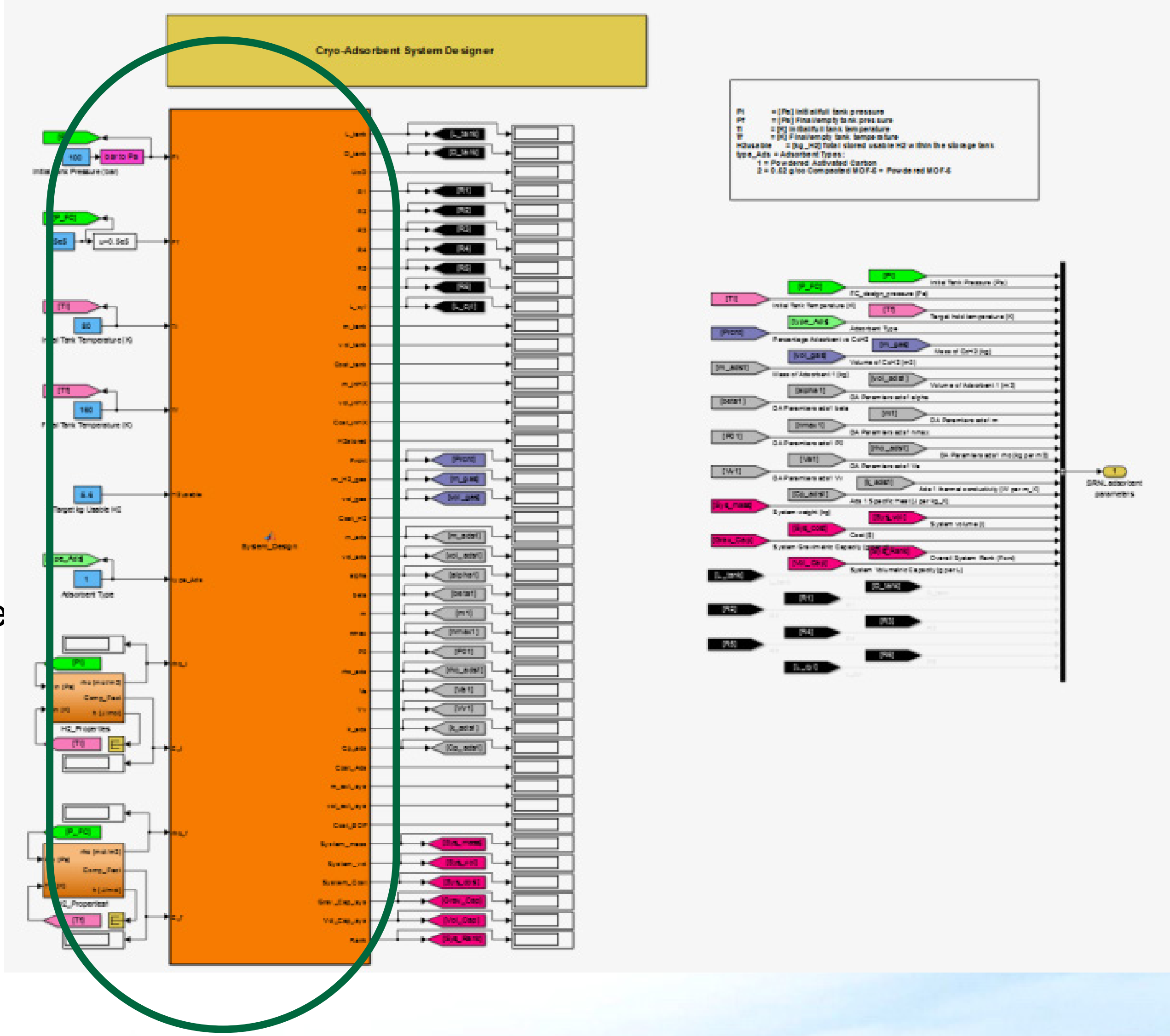


Save Results

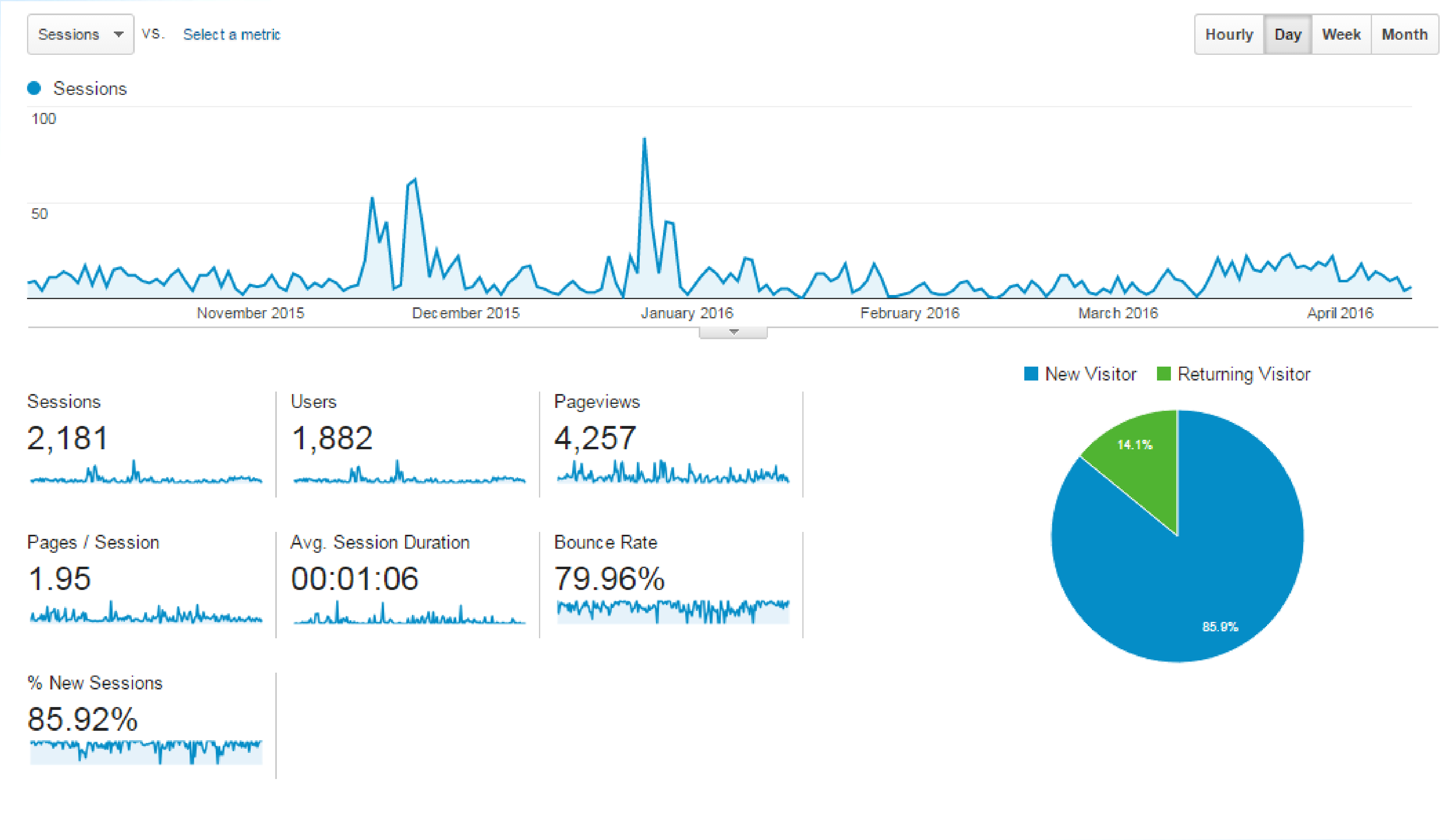
Generate all plots

AD Module Update – "Fully Configurable Ads. Param."

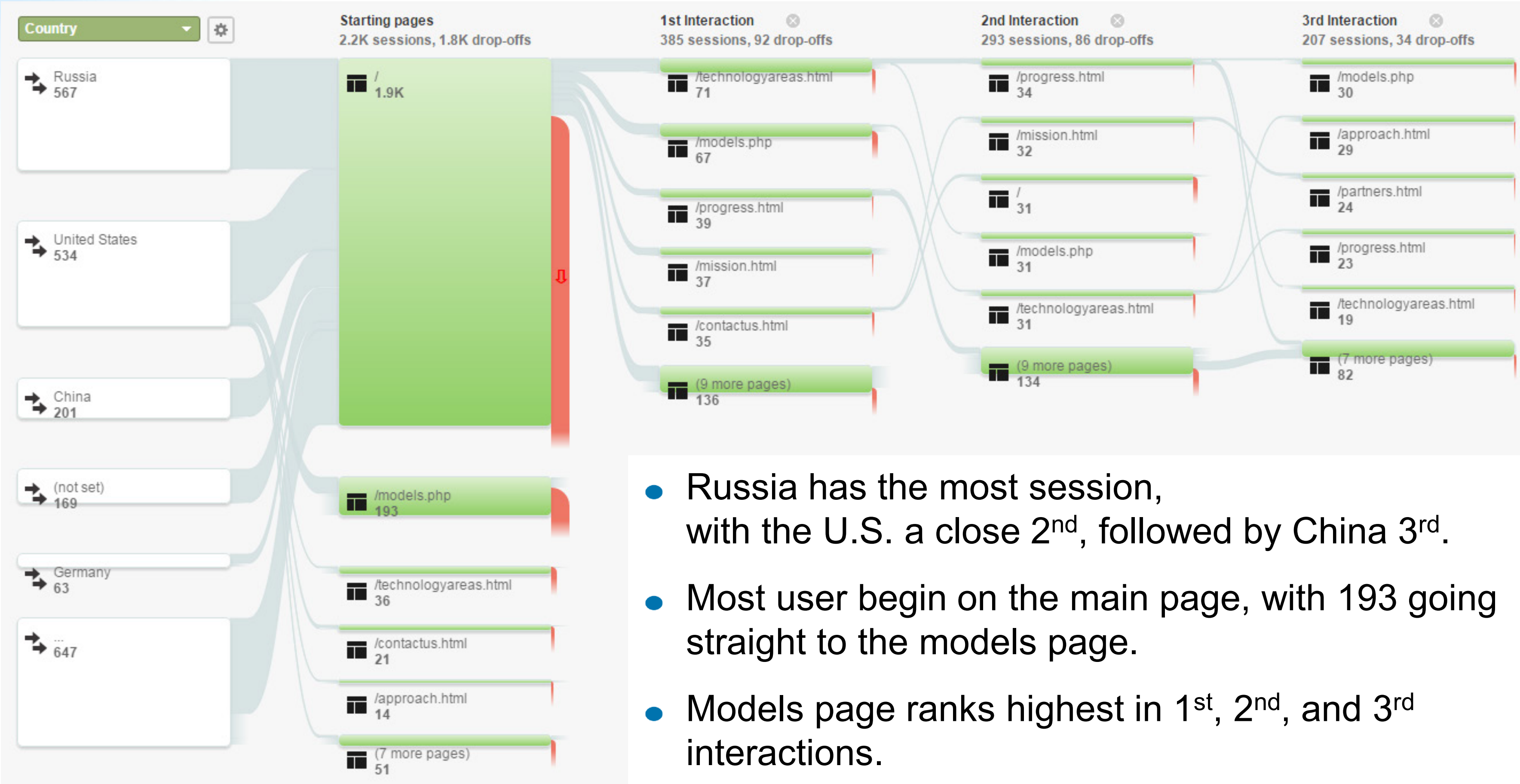
- Module designed to create an adsorbent storage system based on the target H_2 storage and the operating conditions.
- Embedded MatLab script has been moved outside of the Simulink code:
    - GUI calls the adsorbent storage system creation script directly.
    - Gives user full control of what values / properties are passed into the storage module.
- Adsorbent material properties database is also part of the MatLab script.
    - This is the beginning of a user-controlled material properties input.



Model Website Analytics October-April



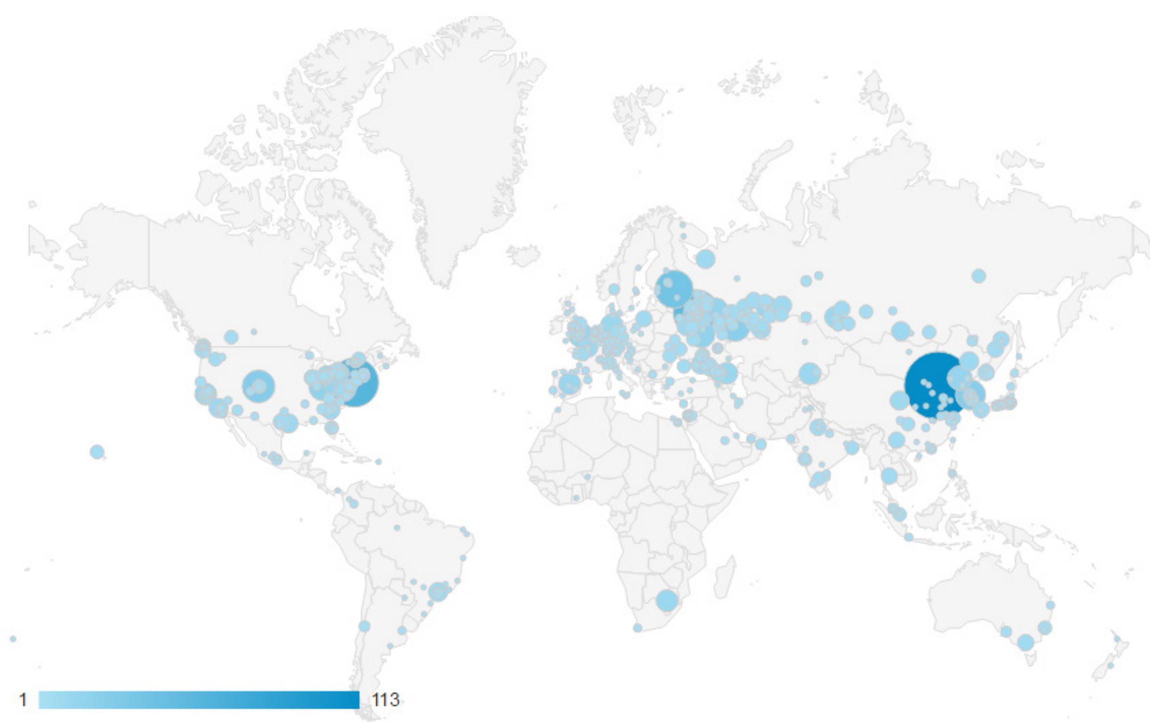
Model Website Analytics Web Flow



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

HSECoE

Model Website Analytics



MODEL	DOWNLOAD COUNT (Q2)
H_2 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

Partner	Project Roles
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 exiting 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
SMART milestone – Develop a stand-alone isotherm data fitting routine to convert raw excess adsorption H_2 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
SMART milestone – 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
SMART milestone – 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.

HSECoE

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

HSECoE

Chemical Hydrogen Storage Model Validation

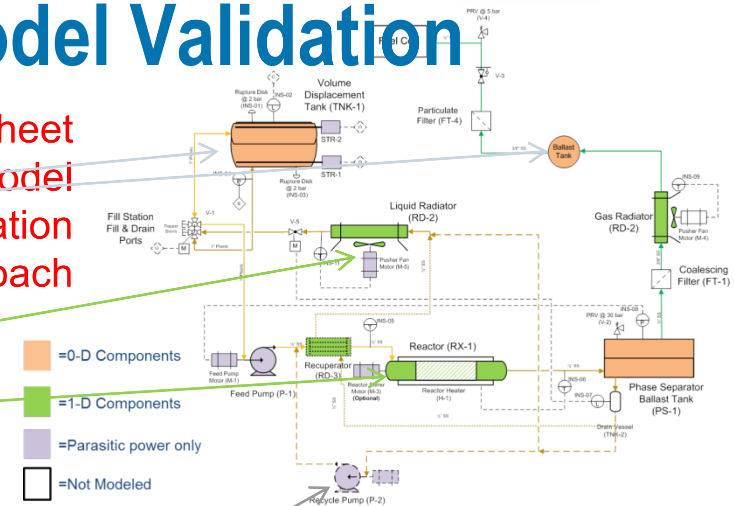
Individual component validation

- **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

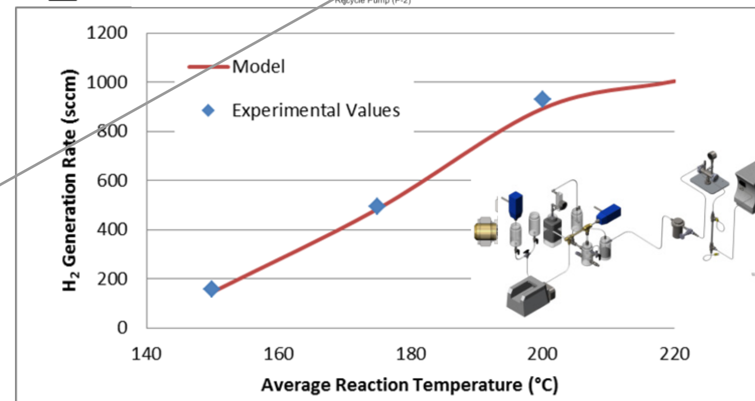
Overall system validation

- **Mass balance**
  - Chemical hydrogen in vs. hydrogen out

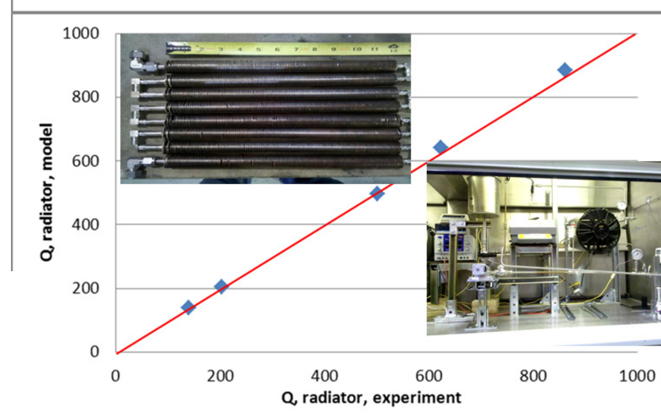
Flowsheet with Model Validation Approach



Reactor Validation: LANL Data



Radiator Validation: PNNL Data



HSECoE

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.**