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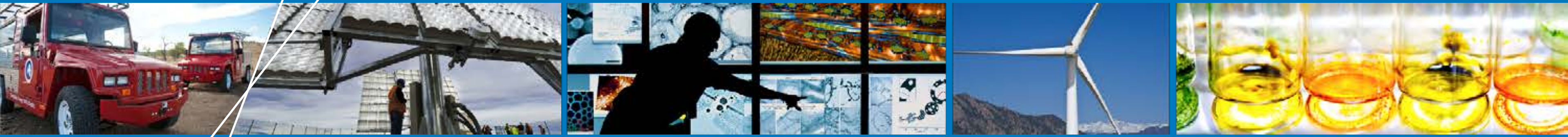
NATIONAL RENEWABLE ENERGY LABORATORY

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

System Design, Analysis, and Modeling for Hydrogen Storage Systems



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National Renewable Energy Laboratory (NREL)
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Project ID # ST008

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Overview

Timeline and Budget

Project start date: FY09

FY14 DOE funding: $125K

FY15 planned DOE funding: $125K

Total DOE funds received: $1.87M

Barriers

(A) System weight and volume

(B) System cost

(C) Efficiency

(E) Charge/discharge rate

(I) Dispensing technology

(K) System life-cycle assessments

Partners

Savannah River National Lab (SRNL) project lead, Pacific Northwest National Lab (PNNL), United Technologies Research Center (UTRC), Jet Propulsion Lab (JPL), Ford, General Motors (GM), Los Alamos National Lab (LANL), Oregon State University (OSU), University of Michigan (UM), and the DOE Vehicle Technologies Office.

Hydrogen Storage Engineering
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Relevance

Support the HSECoE with system design, analysis, modeling, and media engineering properties for materials-based hydrogen storage systems

- Manage Hydrogen Storage Engineering Center of Excellence (HSECoE) vehicle performance, cost, and energy analysis technology area.
- Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance trade-offs at the vehicle system level.
- Energy Analysis: Coordinate hydrogen storage system well-to-wheels (WTW) energy analysis to evaluate off-board energy impacts with a focus on storage system parameters, vehicle performance, and refueling interface sensitivities.
- Media Engineering Properties: Assist center in the identification and characterization of adsorbent materials that have the potential for meeting U.S. Department of Energy (DOE) technical targets for onboard systems.
- Lead effort to make select HSECoE wide models available for use by other researchers via Web-based portal.

Relevance: Vehicle Performance

- Develop and apply a model for evaluating hydrogen storage requirements, performance and cost trade-offs at the vehicle system level (e.g., range, fuel economy, cost, efficiency, mass, volume, on-board efficiency)
- Provide high level evaluation (on a common basis) of the performance of materials based systems:
  - Relative to DOE technical targets
  - Relative in class and across class for materials systems
  - Relative to physical storage systems
  - Relative to conventional vehicles

Relevance: HSECoE Model Web Access

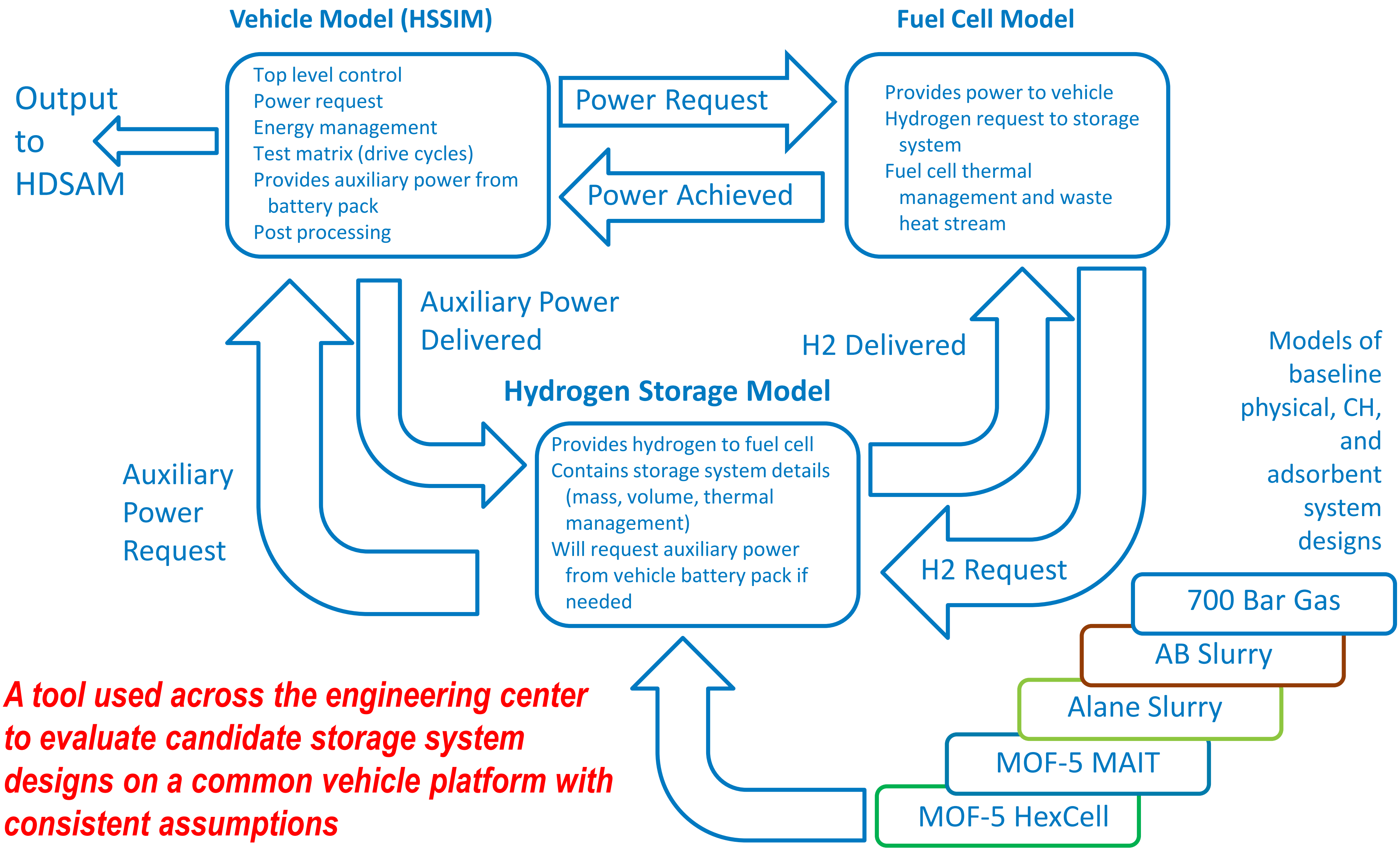
Coordinate across the HSECoE to make select models developed under this effort available to other researchers and research organizations through Web-based access

- Assist with model selection
- Coordinate model validation
- Coordinate model documentation
- Manage website and model posting
- Track and record Web activity
- Track and record model downloads

Approach: Milestones

Date	Milestone	Status
10/14	Attend, participate in, and present a Web model posting status at face-to-face meeting in Lincoln, Nebraska.	100%
3/15	Lead the coordination of the immigration into the modeling framework and Web posting of two validated chemical hydrogen storage and two validated adsorbent storage system models and exercise the models to assess the phase III systems designs.	100%
6/15	Draft final report section for vehicle modeling and center Web model access and submit to SRNL.	50%
9/15	Complete final report section for vehicle modeling and center Web model access and submit to SRNL.	0%

Approach: Modeling Framework



A tool used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent assumptions

Accomplishments: Framework Enhancements

Framework Updates

- Better user documentation related to compiler and software versions
- Added system diagrams
- Simulation speed improvements and bug fixes
- Troubleshooting of compiler and software versions
- Improved graphical user interface (GUI) with more clarity on reported results and input requirements

Ongoing Activities

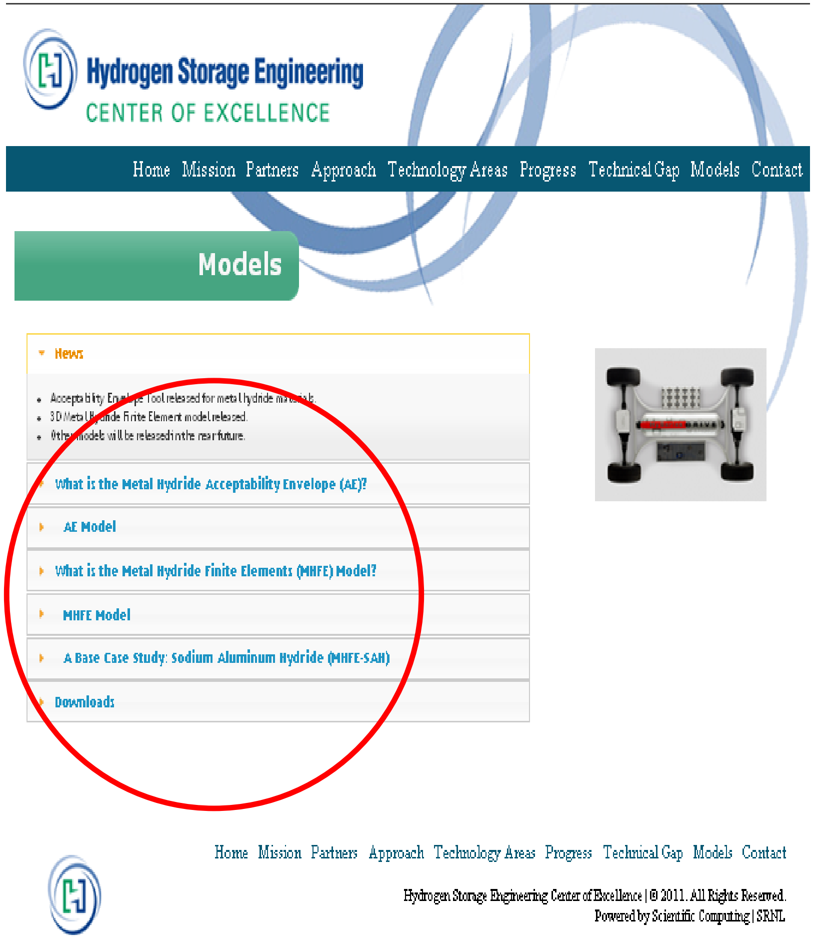
- Web support for publicly available model
- Model validation based on insights from National Fuel Cell Technology Evaluation Center
- Tracking and monitoring Web activity and downloads
- Automated tank sizing for adsorbent and chemical storage systems

Accomplishments: Model Access Website

HSECoE website: http://hsecoe.org/

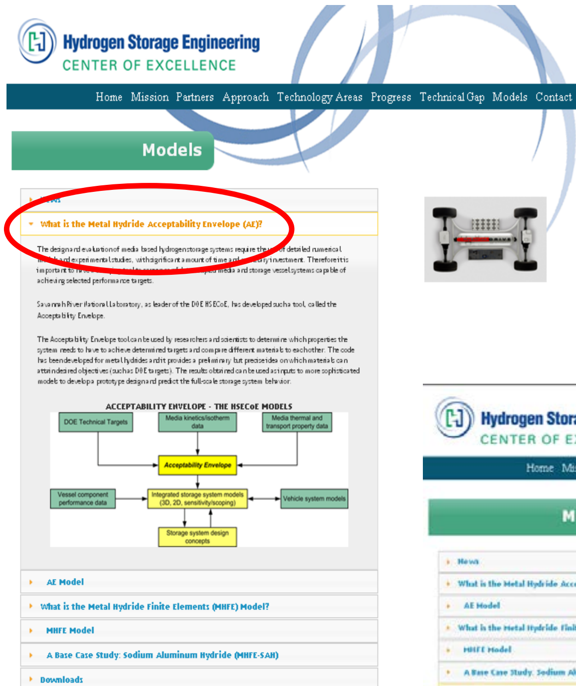
Model support: HSECoE@nrel.gov

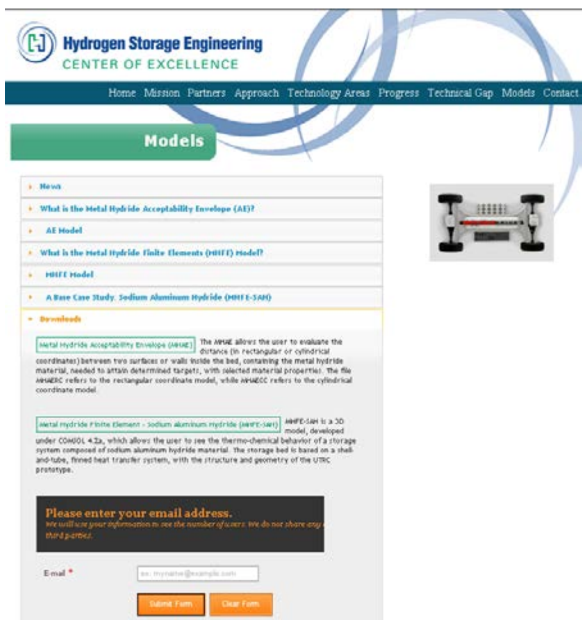
Model access/description sub-page



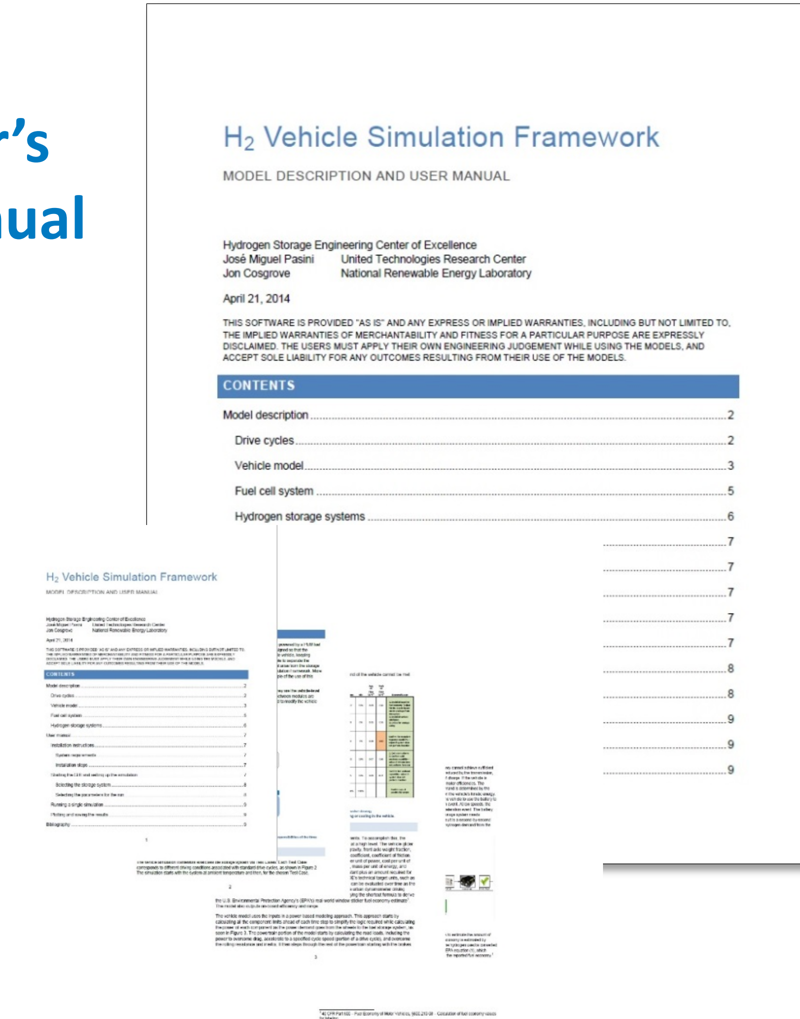
Accomplishments: Model Access Website

Model documentation and downloads



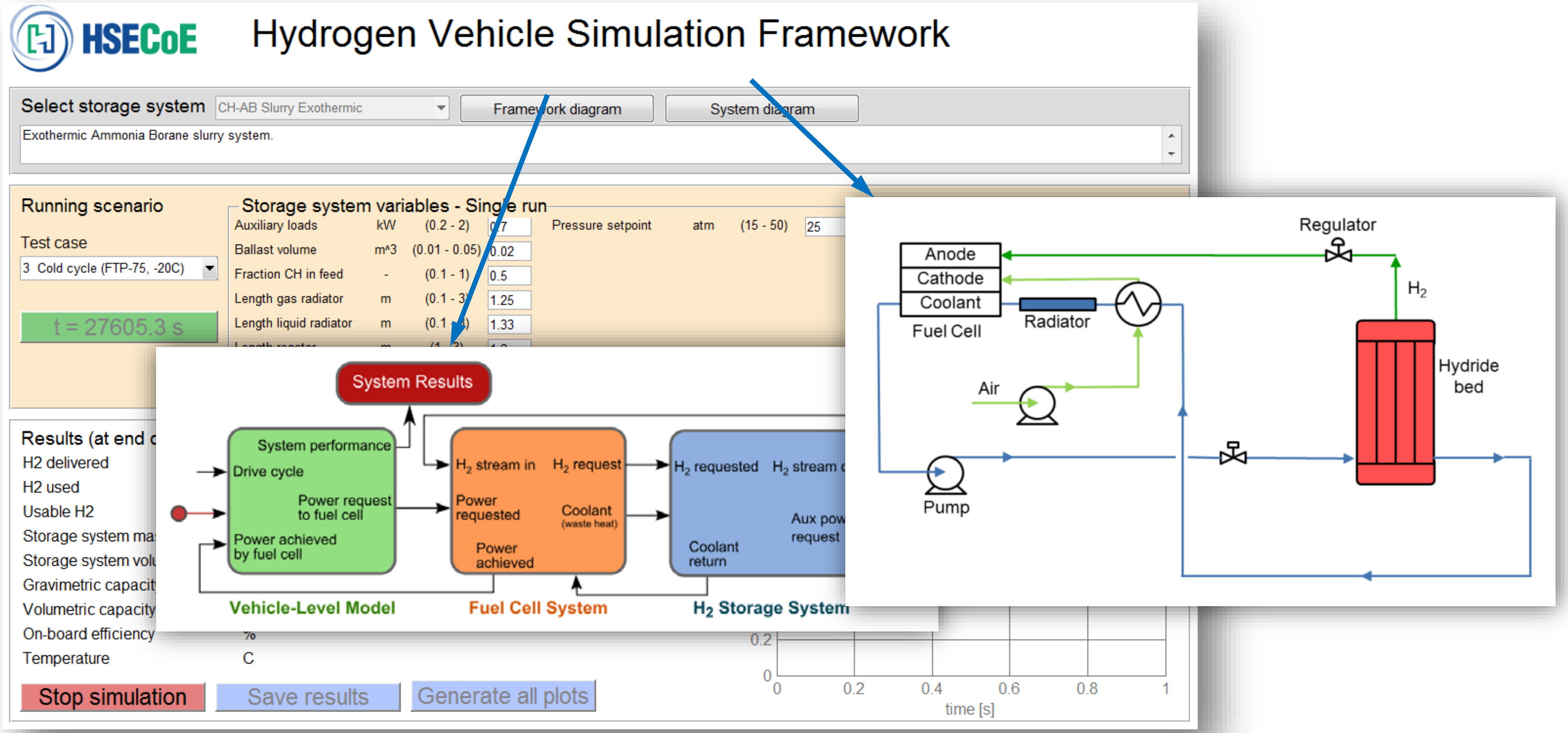


User's manual



Accomplishments: GUI Update—Framework and System Diagrams

Based on feedback from beta testers, framework and system diagrams have been added



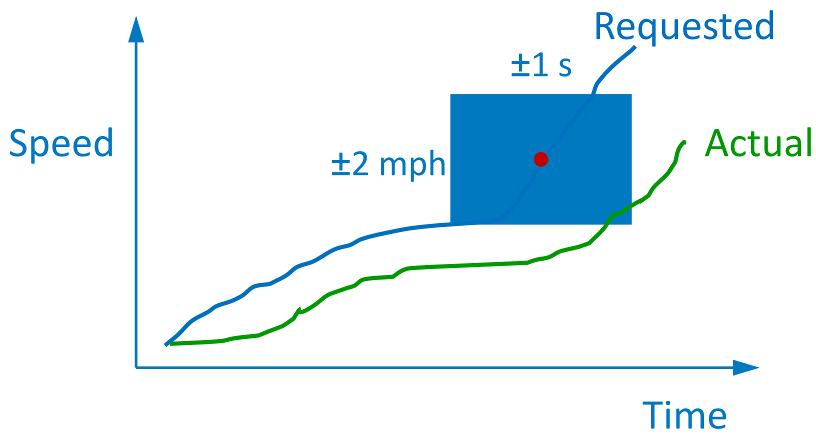
Accomplishments: Overall Simulation Performance Checks

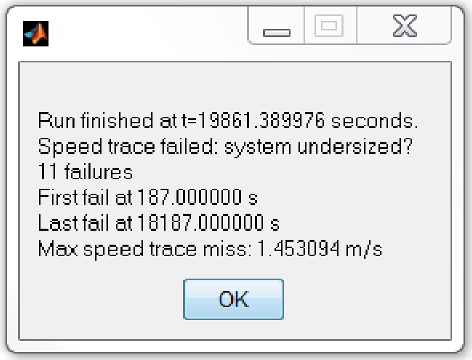
Power failure due to storage system

- Fuel cell can deliver power, but H_2 flow rate is not enough: empty tank or slow kinetics

Speed trace miss due to undersized vehicle components (fuel cell, power train)

- Aligned with standard speed trace miss criteria: ±2 mph in a ±1 s window
- Check performed as post-process: a speed trace miss does not stop the simulation

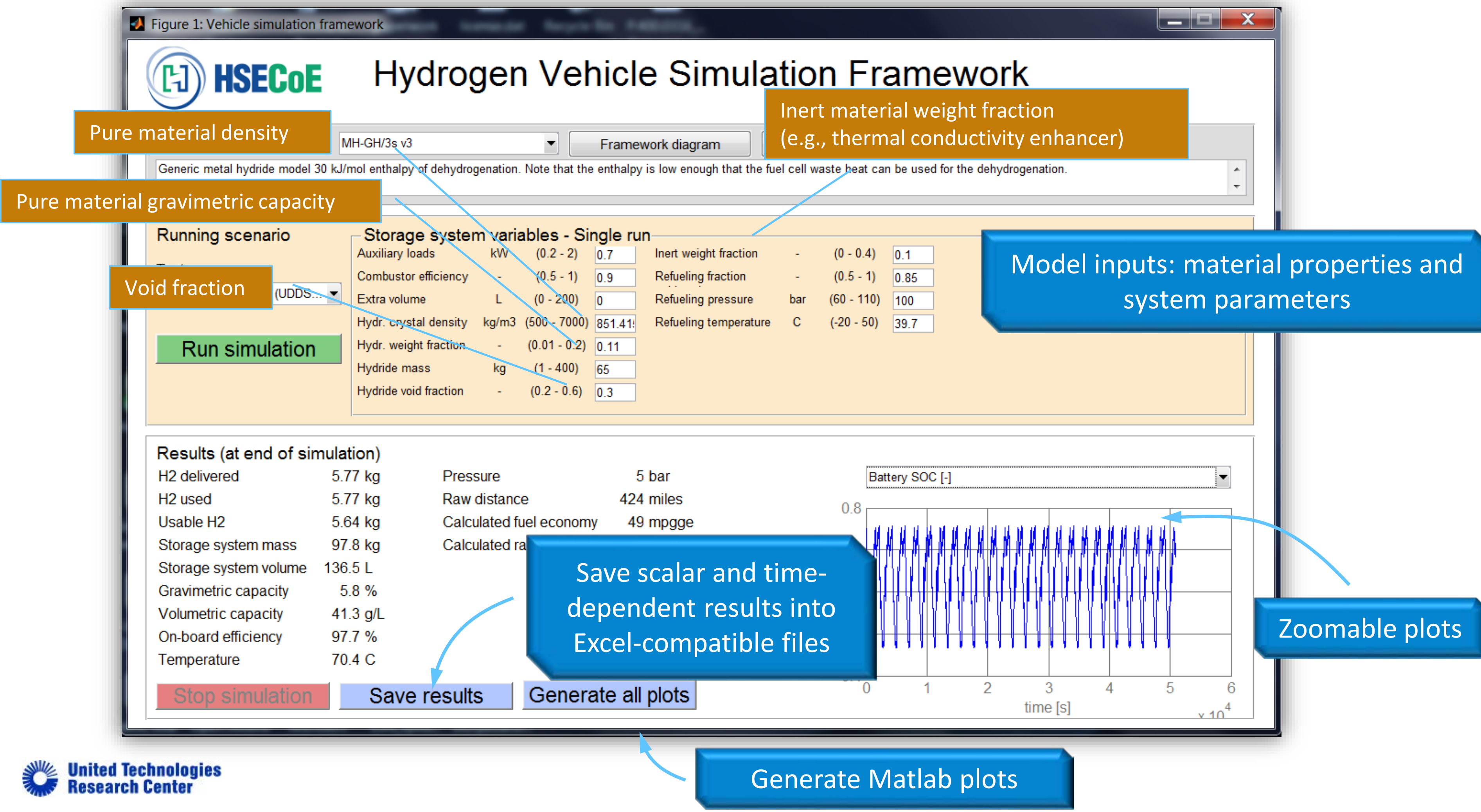




Sample error message if speed trace miss detected

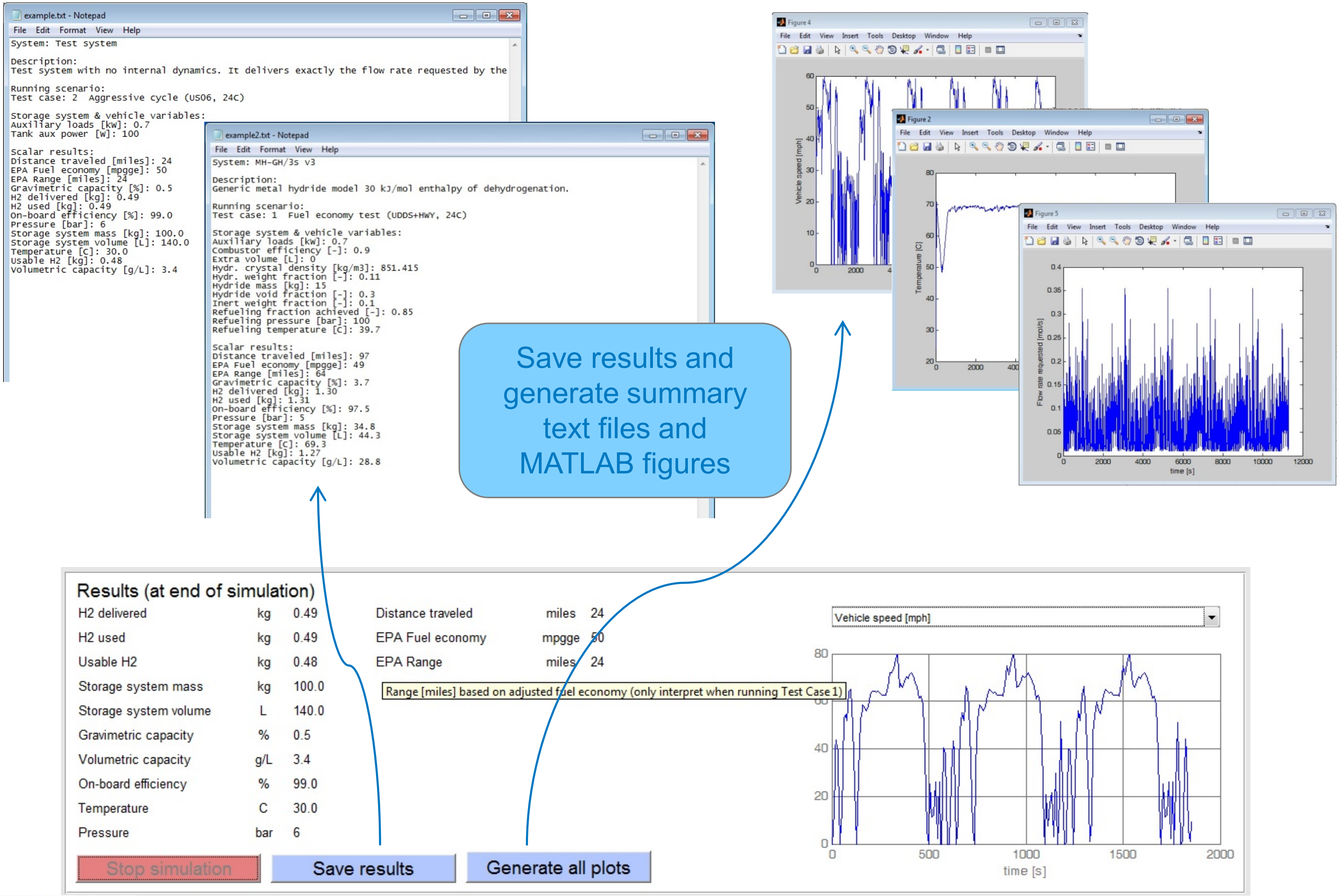
Accomplishments: Graphical User Interface

Metal hydride storage system model example in Simulink framework



United Technologies Research Center

Accomplishments: Framework—Model Results



United Technologies Research Center

Accomplishments: Model Posting

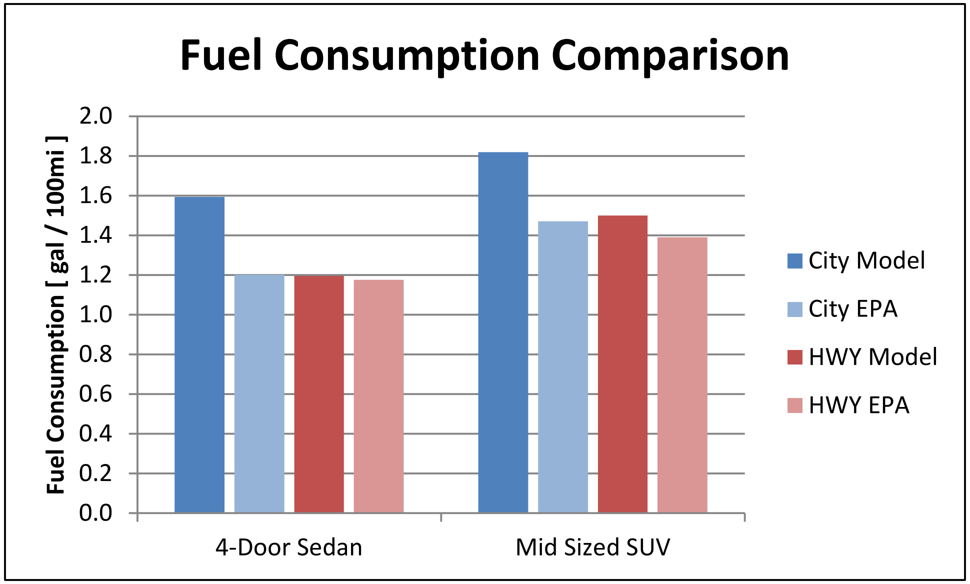
MH Acceptability Envelope	SRNL	complete
MH Finite Element Model	SRNL	complete
Physical H2 Framework Modes	UTRC/NREL	complete
MH Framework Model	UTRC/SRNL/NREL	complete
Tank Volume/Cost Model	PNNL	complete
CH Framework Model	UTRC/PNNL/NREL	complete
AD Framework Model	UTRC/SRNL/NREL	complete
AD Finite Element Model	SRNL	7/2015

Model	Platform	Description
MHAE	Excel	Metal Hydride Acceptability Envelope: Tank internal HX sizing based on steady-state thermal model during refueling
MHFE-SAH	Comsol 4.2a	Finite Element Sodium Aluminum Hydride Model: 3D model of SAH bed with shell-and-tube, finned HX based on UTRC prototype.
Vehicle Framework	Matlab/Simulink 2011b or newer	Hydrogen Vehicle Simulation Framework: Dynamic model of Fuel Cell light-duty vehicle. 4 hydrogen discharge scenarios
Tankinator	Excel	Tank Mass & Cost Estimation Model

Accomplishments: Vehicle Model Validation

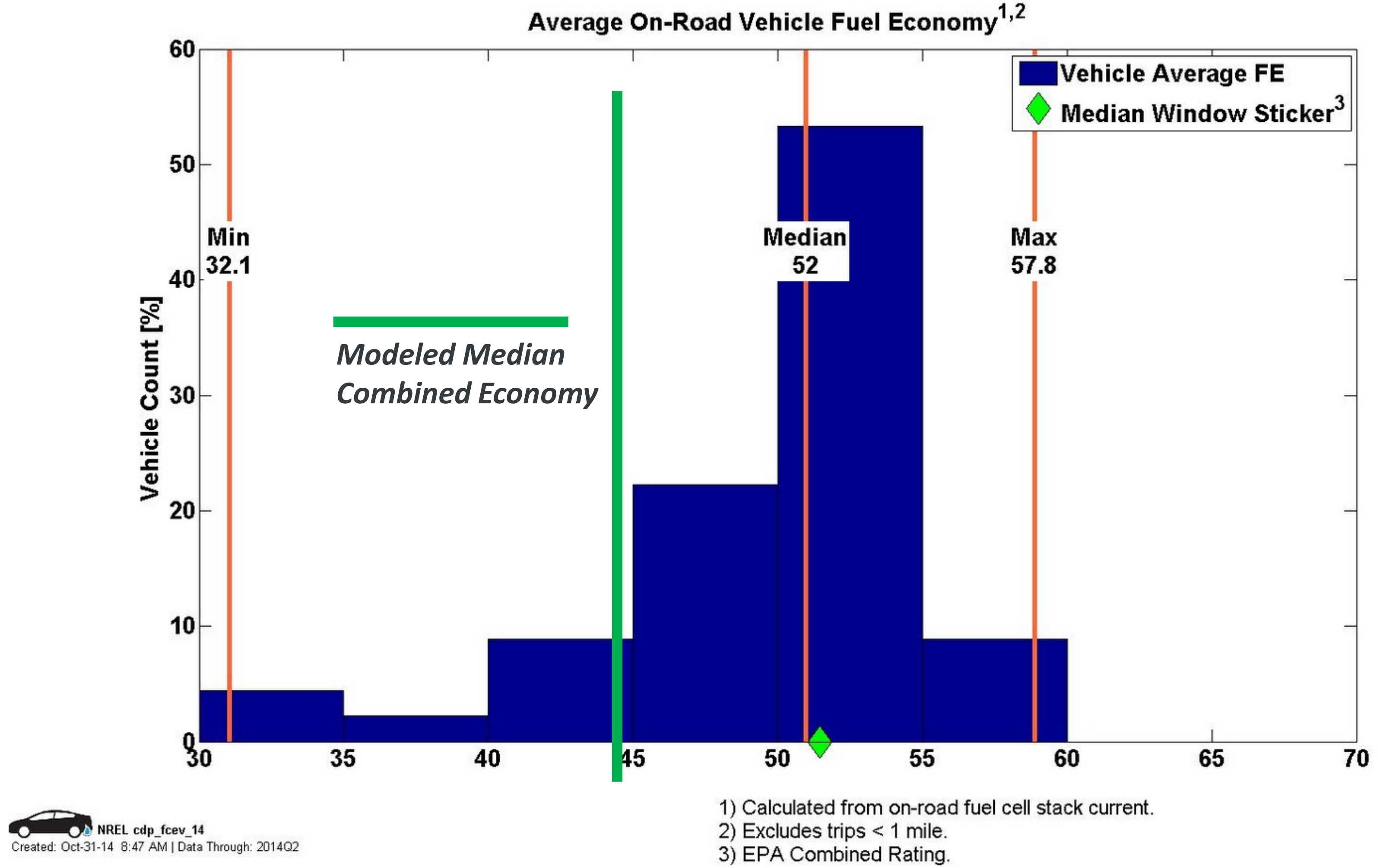
Fuel consumption validation

- **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



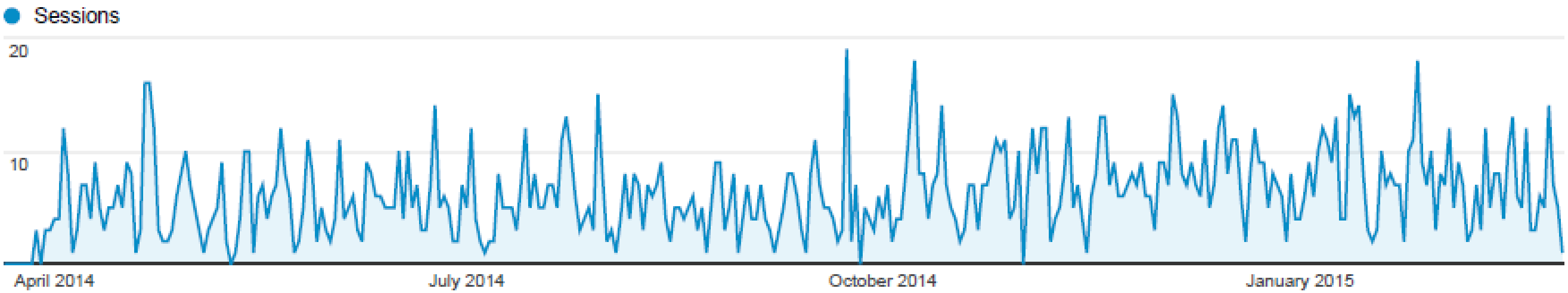
Accomplishments: Vehicle Model Validation

Vehicle model results compared with technology validation results



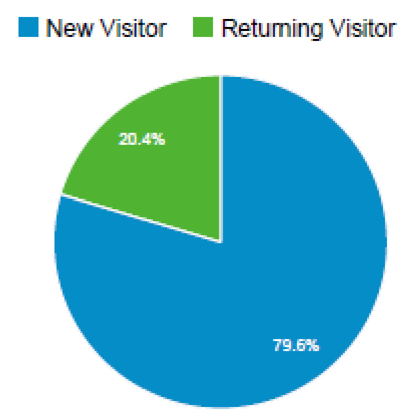
**Note composite data product (CDP) contains data for many vehicles through Q2 of 2014. Modeled results for 2014 and 2015 vehicles.

Accomplishments: Model Website Analytics

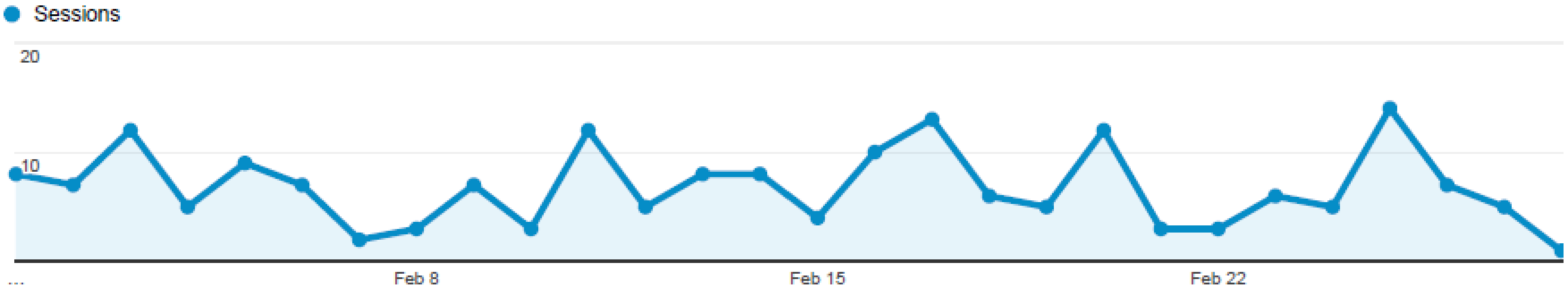


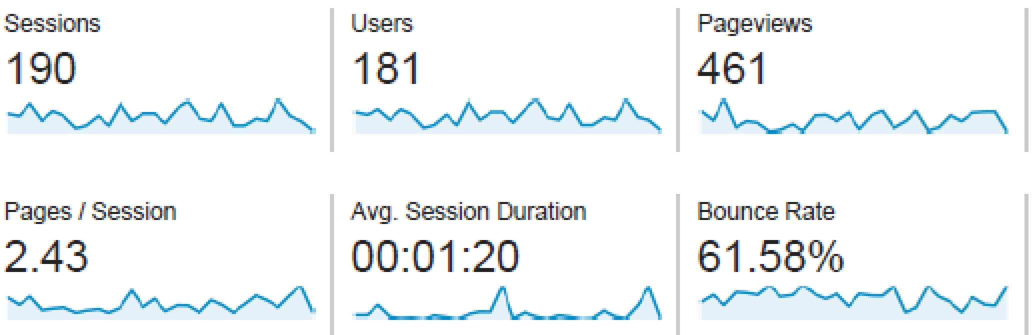
Sessions	Users	Pageviews
2,162	1,720	6,034

Pages / Session	Avg. Session Duration	Bounce Rate
2.79	00:01:50	58.79%



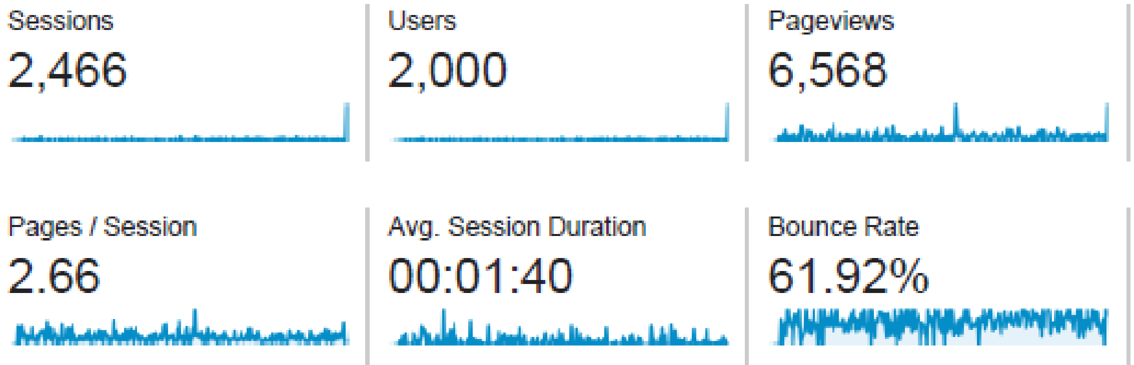
Accomplishments: Model Website Analytics

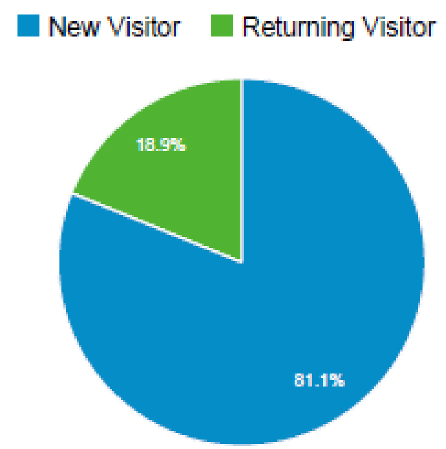


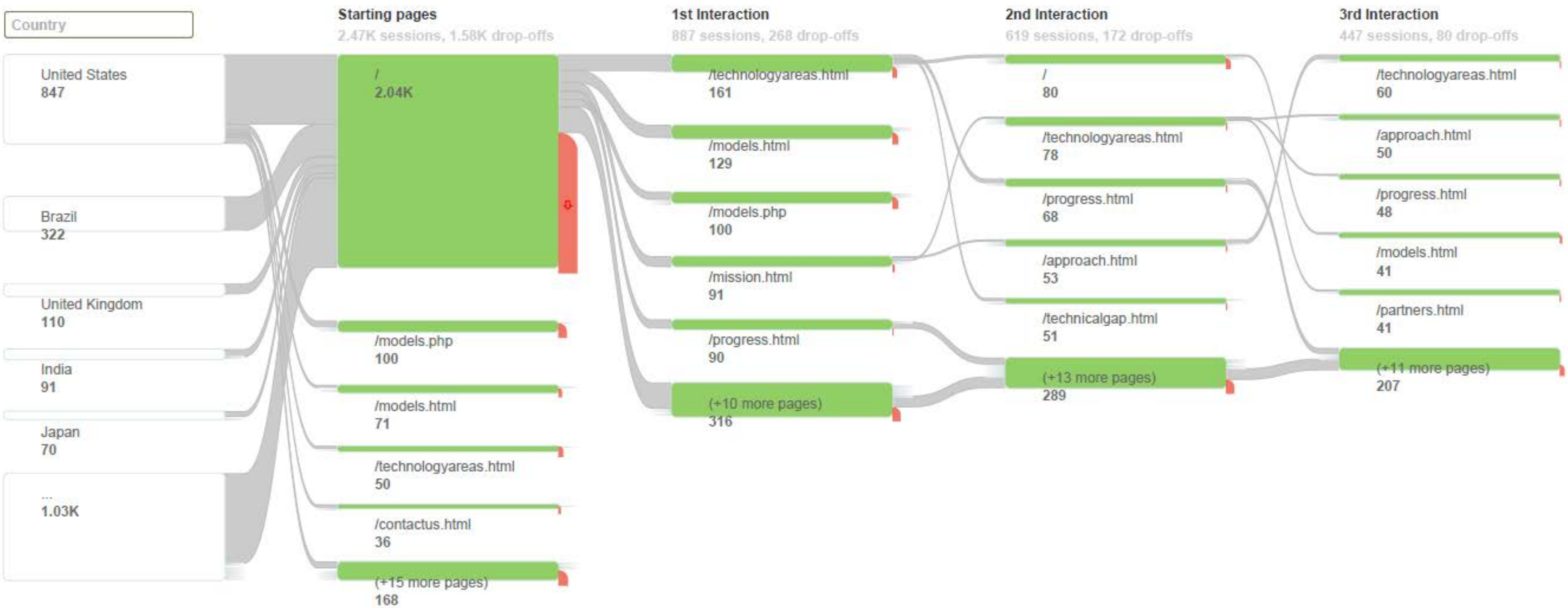


One month user data

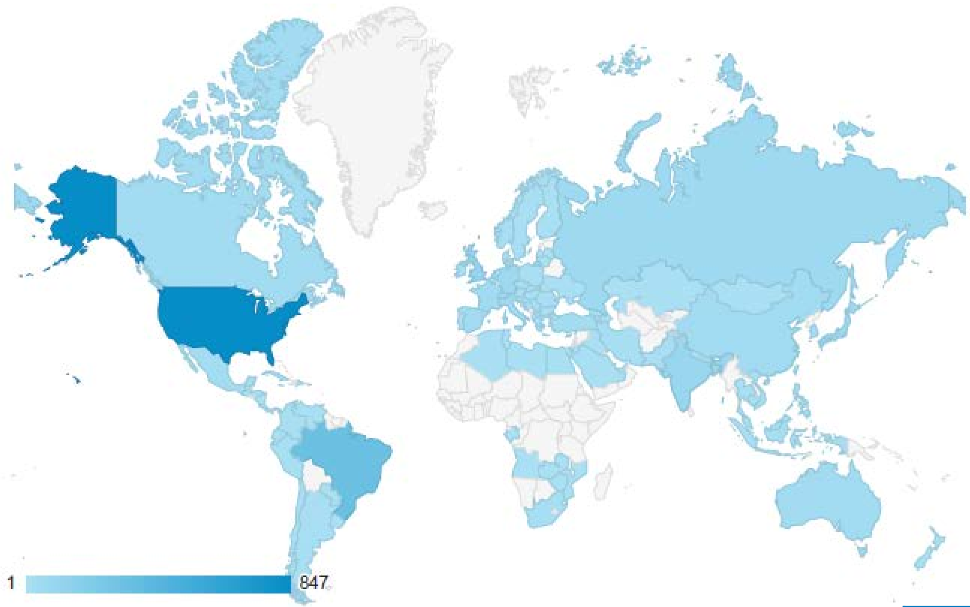
Accomplishments: Model Website Analytics

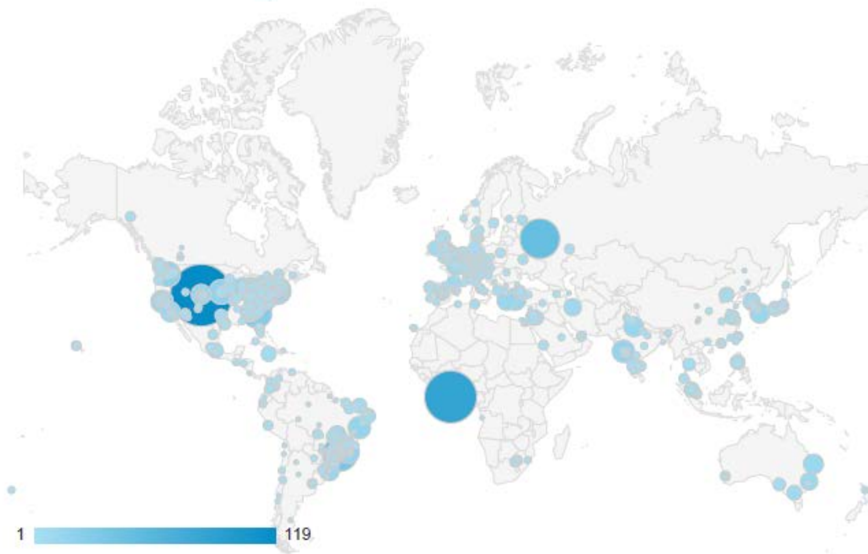






Accomplishments: Model Website Analytics





25 downloads of the Vehicle Simulator Model

MODEL	DOWNLOAD COUNT
Hydrogen Storage Tank Mass and Cost Model	39
MHAE Model	9
MHFE Model	13
Vehicle Simulator Model	25
TOTAL UNIQUE USERS DOWNLOADING	**56**

Accomplishments: Framework Results

Framework results can be used to calculate higher-level attributes

Simulated vehicle performance results for
Phase I and II H_2 storage systems with fixed on-board H_2

Phase I

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi) 5.6kg H2	On-Board Efficiency (%) UDDS/HFET	Gravimetric Density (wt. %)	Volumetric Density (g/l)
Fluid AB	45	254	96	4.6	38.9
Alane	43	239	88	4.6	38.9
AX21 press FCHX	49	273	97	4.3	25.2
MOF5 Cmpct-FCHX	48	271	97	3.5	24.1
MOF5 Press FCHX	49	276	98	4.6	25.3
350 bar Compressed Gas	50	280	100	4.8	17.0
700 bar Compressed Gas	50	279	100	4.7	25.0

Phase II

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi)	On-Board Efficiency (%) UDDS/HFET	Gravimetric Density (wt. %)	Volumetric Density (g/l)	System Mass (kg)
Exothermic AB Slurry	47	264	97	4.2	36.8	137.1
Endothermic Alane Slurry	44	244	93	3.4	34.3	185.1
HexCell Powder MOF-5	49*	274*	92**	3.5	17.5	137.6
MATI Puck MOF-5 (.32g/cc)	48*	269*	97**	3.4	20.7	149.3
700 bar Compressed Gas	50	279	100	4.7	25.0	119.0

Phase III: Case 1 (FTP/HFET) – Results

CASE 1	H_2 Delivered [kg]	Usable H_2 [kg]	System Mass [kg]	System Volume [L]	Gravimetric Capacity [weight %]	Volumetic Capacity [g/L]	On-Board Efficiency [%]	Economy [mpgge]	Calculated Range [mi]
CH - AB Slurry - Exothermic	5.13	4.99	126.1	133.4	4	37.4	97.3	49	251
CH - Alane Slurry - Endothermic	6.17	5.22	172.7	153.4	3	34	84.7	44	270
Compressed 350 Bar	5.63	5.63	117	329	4.8	17.1	100	50	280
Compressed 700 Bar	5.67	5.67	119	224	4.8	25.3	100	50	282
MH-GH/3s v3	5.77	5.64	97.8	136.5	5.8	41.3	97.7	49	285

Accomplishments: Response to Reviewers' Comments

- **Comment: There is a lack of clear and compelling plans for model validation. More attention seems to have been paid to Web based access and evaluation of user analytics than to the crucial task of model validation.**
    - **Response: Slides have been included in this years presentation detailing validation activities and results for both the framework model and individual storage system models.**

Collaboration and Coordination: Web Model Team Roles and Responsibilities

- Storage system model development, coding, and documentation—convert models to appropriate format for use in framework (Simulink). PNNL and SRNL
- Framework management—GUI development and storage system model integration. UTRC
- Vehicle model development and validation—framework output management and validation. Storage system model integration and framework update posting. NREL
- Fuel cell model development and validation. Ford
- Framework model and standalone model posting and Web portal management. NREL
- Model documentation. NREL, PNNL, Ford, SRNL, UTRC

Management of collaboration efforts across organizations is done through monthly and on-demand modeling team telecons, bi-annual face-to face-meetings, and through SharePoint

Proposed Future Work

- **Focus on model validation and model Web access**
  - Add Adsorbent models to Framework (September)
- **Vehicle simulations**
  - Work complete
- **Energy analysis**
  - Work complete
- **Media engineering properties**
  - Work complete

Technology Transfer Activities

- **None**

Summary

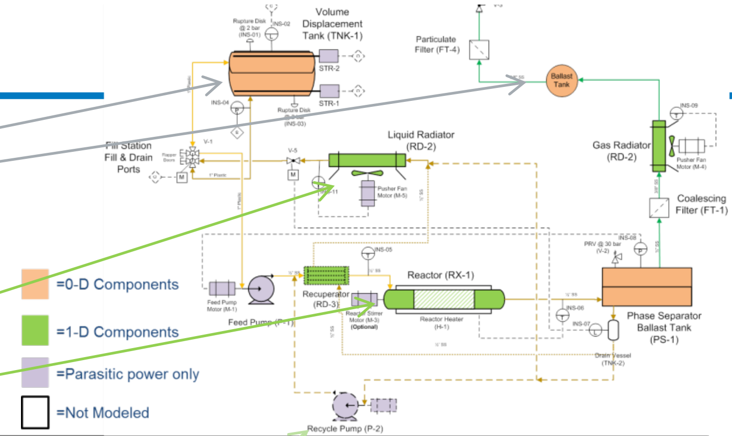
- **Manage HSECoE vehicle performance, cost, and energy analysis technology area.**
- **Lead effort to make models developed by HSECoE available to other researchers via Web-based portal.**
- **Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance trade-offs at the vehicle system level.**

Technical Back-Up Slides

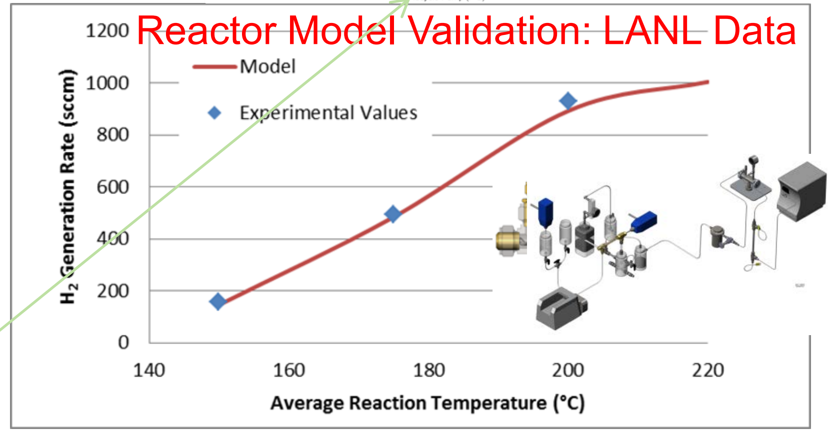
Accomplishment: Chemical Hydrogen Storage Model Validation

- **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 and mass transfer and reaction
    - Reactor, radiators, recuperator
    - Approach 1: compare to 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 hydride in vs. hydrogen out

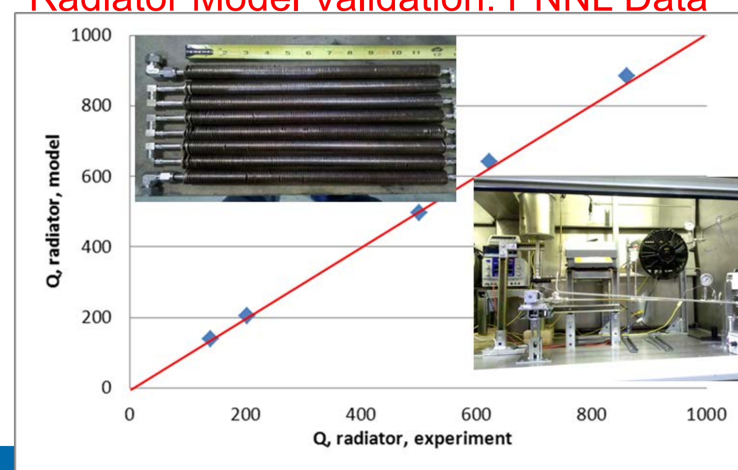
Flowsheet with Model Validation Approach



Reactor Model Validation: LANL Data



Radiator Model Validation: PNNL Data



Pacific Northwest NATIONAL LABORATORY

Accomplishments: Framework Results

Phase III: Case 2 (US06) – Results

CASE 2	H_2 Delivered [kg]	Usable H_2 [kg]	System Mass [kg]	System Volume [L]	Gravimetric Capacity [weight %]	Volumetic Capacity [g/L]	On-Board Efficiency [%]	Economy [mpgge]
CH - AB Slurry - Exothermic	5.11	5.01	126.1	133.4	4	37.6	98.2	[51]
CH - Alane Slurry - Endothermic	5.78	4.93	172.7	153.4	2.9	32.1	85.4	[44]
Compressed 350 Bar	5.61	5.61	117	329	4.8	17.1	100	[52]
Compressed 700 Bar	5.66	5.66	119	224	4.8	25.3	100	[52]
MH-GH/3s v3	5.75	5.68	97.8	136.5	5.8	41.6	98.8	[52]

Phase III Case 3 (Cold FTP) – Results

CASE 3	H_2 Delivered [kg]	Usable H_2 [kg]	System Mass [kg]	System Volume [L]	Gravimetric Capacity [weight %]	Volumetic Capacity [g/L]	On-Board Efficiency [%]	Economy [mpgge]
CH - AB Slurry - Exothermic	5.03	4.57	126.1	133.4	3.6	34.3	90.9	[63]
CH - Alane Slurry - Endothermic	6	4.31	172.7	153.4	2.5	28.1	71.8	[55]
Compressed 350 Bar	5.63	5.63	117	329	4.8	17.1	100	[65]
Compressed 700 Bar	5.67	5.67	119	224	4.8	25.3	100	[65]
MH-GH/3s v3	5.71	5.35	97.8	136.5	5.8	41.3	92.9	[64]

Accomplishments: Framework Results

Phase III: Case 4 (SC03) – Results

CASE 4	H_2 Delivered [kg]	Usable H_2 [kg]	System Mass [kg]	System Volume [L]	Gravimetric Capacity [weight %]	Volumetic Capacity [g/L]	On-Board Efficiency [%]	Economy [mpgge]
CH - AB Slurry - Exothermic	5.1	4.91	126.1	133.4	3.9	36.8	96.3	[61]
CH - Alane Slurry - Endothermic	5.97	4.83	172.7	153.4	2.8	31.5	80.9	[54]
Compressed 350 Bar	5.63	5.63	117	329	4.8	17.1	100	[63]
Compressed 700 Bar	5.67	5.67	119	224	4.8	25.3	100	[63]
MH-GH/3s v3	5.77	5.58	97.8	136.5	5.8	41.3	96.8	[62]