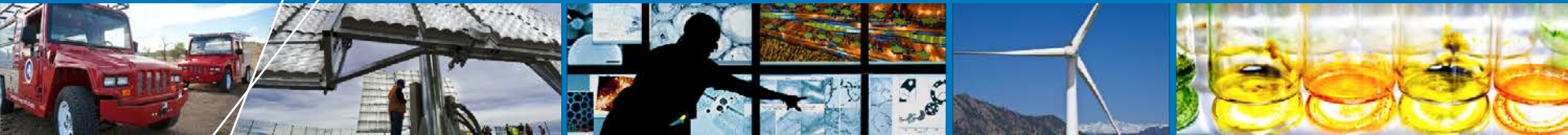


System Design, Analysis, and Modeling for Hydrogen Storage Systems



Matthew Thornton
Jon Cosgrove and Jeff Gonder
National Renewable Energy Laboratory (NREL)
June 9, 2015

Project ID # ST008

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

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.

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



Hydrogen Storage Engineering CENTER OF EXCELLENCE

Home Mission Partners Approach Technology Areas Progress Technical Gap Models Contact

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, materials-based, hydrogen storage systems for hydrogen fuel cell and internal combustion engine light-duty vehicles.

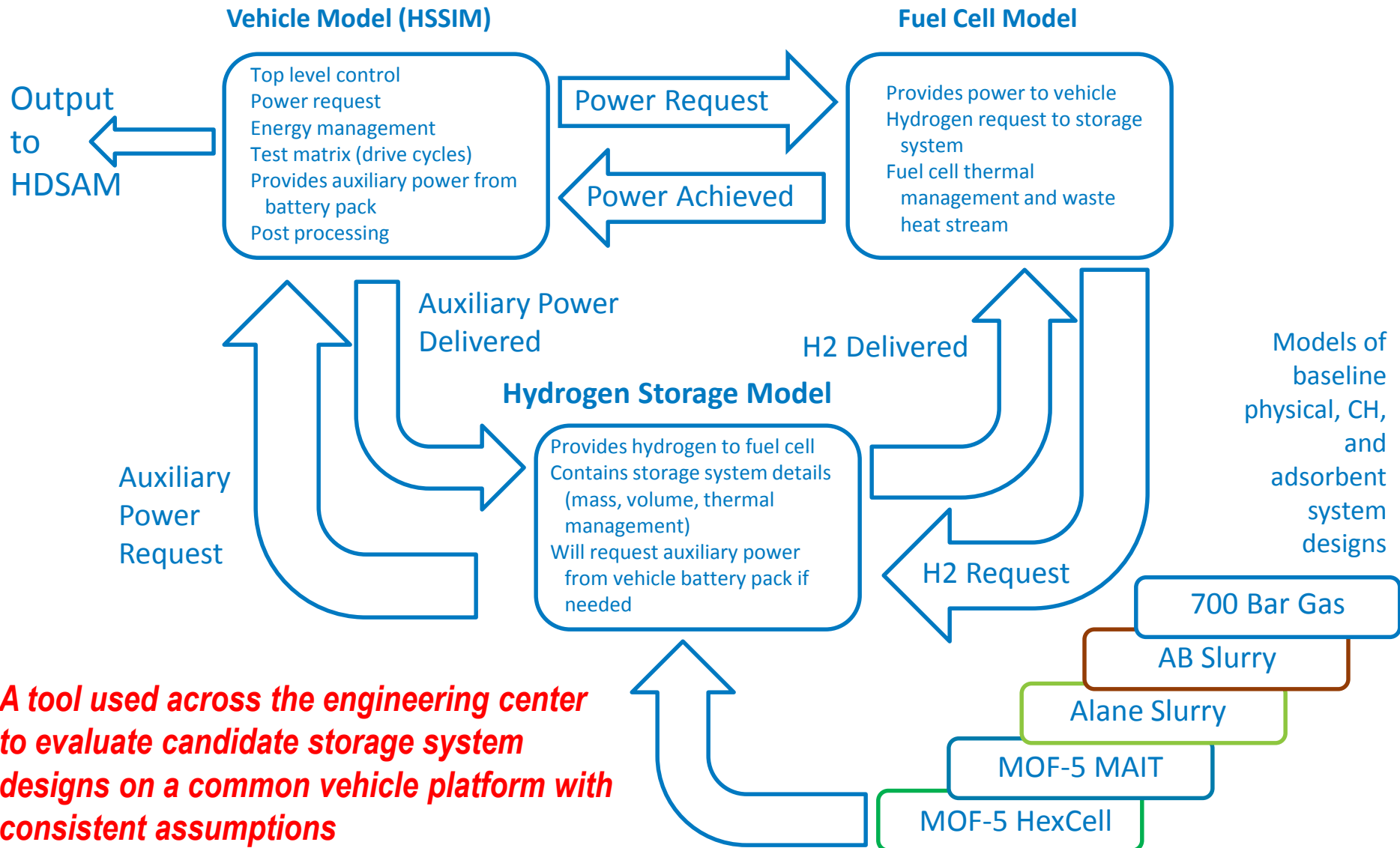
This project is incorporated into the DOE's Fuel Cell Technology Program, which consists of applied research and development activities, conducted through Center of Excellence materials and engineering teams, and independent projects focusing on materials and concepts, testing, and system analysis.

U.S. DEPARTMENT OF ENERGY

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



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



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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, and system analysis.



Model access/description sub-page



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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: Model Access Website

Model documentation and downloads



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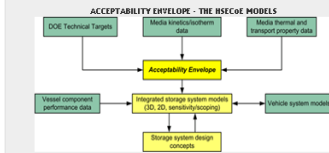
Models

What is the Metal Hydride Acceptability Envelope (AE)?

The design of a katalonit media based hydrogen storage system requires the user to define numerous design parameters (media, adsorption isotherm, etc.) and material properties. The user is required to define a set of performance targets and storage system concepts capable of achieving selected performance targets.

Dr. Joseph E. Buehler, as leader of the DOE HSECC, has developed such a tool, called the Acceptability Envelope.

The Acceptability Envelope tool can be used by researchers and designers to determine which properties the system needs to have to achieve determined targets and compare different materials to each other. The code has been developed for metal hydrides and provides a preliminary, but precise idea on which materials can meet desired objectives (such as DOE targets). The results obtained can be used as inputs to more sophisticated models to develop a strategy to design and predict the full-scale storage system behavior.



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



Home Mission Partners Approach Technology Areas Progress Technical Gap Models Contact

Models

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 tool 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 MHFECC refers to the rectangular coordinate model, while MHFECC refers to the cylindrical coordinate model.

Metal Hydride Finite Element - Sodium Aluminum Hydride (MHFE-SAH) MHFE-SAH is a 3D model, developed under COMSOL 4.3a, 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 UTC prototype.

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

Email



User's manual

H₂ 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

THIS SOFTWARE IS PROVIDED "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE EXPRESSLY DISCLAIMED. THE USERS MUST APPLY THEIR OWN ENGINEERING JUDGEMENT WHILE USING THE MODELS, AND ACCEPT SOLE LIABILITY FOR ANY OUTCOMES RESULTING FROM THEIR USE OF THE MODELS.

CONTENTS

Model description	2
Drive cycles	2
Vehicle model	3
Fuel cell system	5
Hydrogen storage systems	6

H₂ Vehicle Simulation Framework

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... To understand the ...
 ... The user must ...
 ... The user must ...
 ... The user must ...

Accomplishments: GUI Update—Framework and System Diagrams

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

Hydrogen Vehicle Simulation Framework

Select storage system: CH-AB Slurry Exothermic
Exothermic Ammonia Borane slurry system.

Running scenario: Test case: 3 Cold cycle (FTP-75, -20C)
t = 27605.3 s

Storage system variables - Single run				
Auxiliary loads	kW	(0.2 - 2)	0.7	Pressure setpoint atm (15 - 50) 25
Ballast volume	m³	(0.01 - 0.05)	0.02	
Fraction CH in feed	-	(0.1 - 1)	0.5	
Length gas radiator	m	(0.1 - 3)	1.25	
Length liquid radiator	m	(0.1 - 1)	1.33	

System Results

Results (at end of): H2 delivered, H2 used, Usable H2, Storage system max, Storage system vol, Gravimetric capacity, Volumetric capacity, On-board efficiency, Temperature

Buttons: Stop simulation, Save results, Generate all plots

System Diagram: Shows the interaction between the Vehicle-Level Model, Fuel Cell System, and H2 Storage System. The Fuel Cell System includes the Anode, Cathode, and Coolant. The H2 Storage System includes the Hydride bed and a Regulator. A Pump circulates coolant through a Radiator. Air is also supplied to the Fuel Cell System.

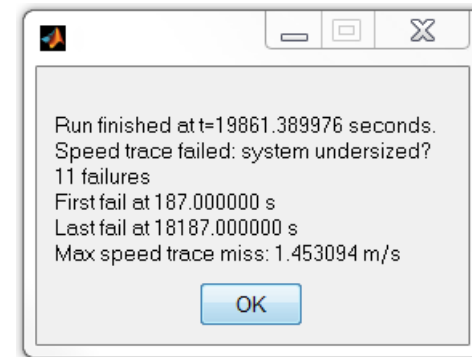
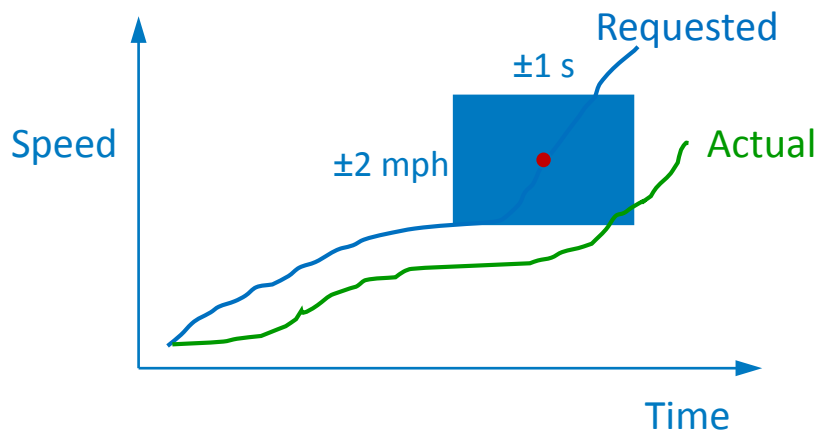
Accomplishments: Overall Simulation Performance Checks

Power failure due to storage system

- Fuel cell can deliver power, but H₂ flow rate is not enough: empty tank or slow kinetics

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

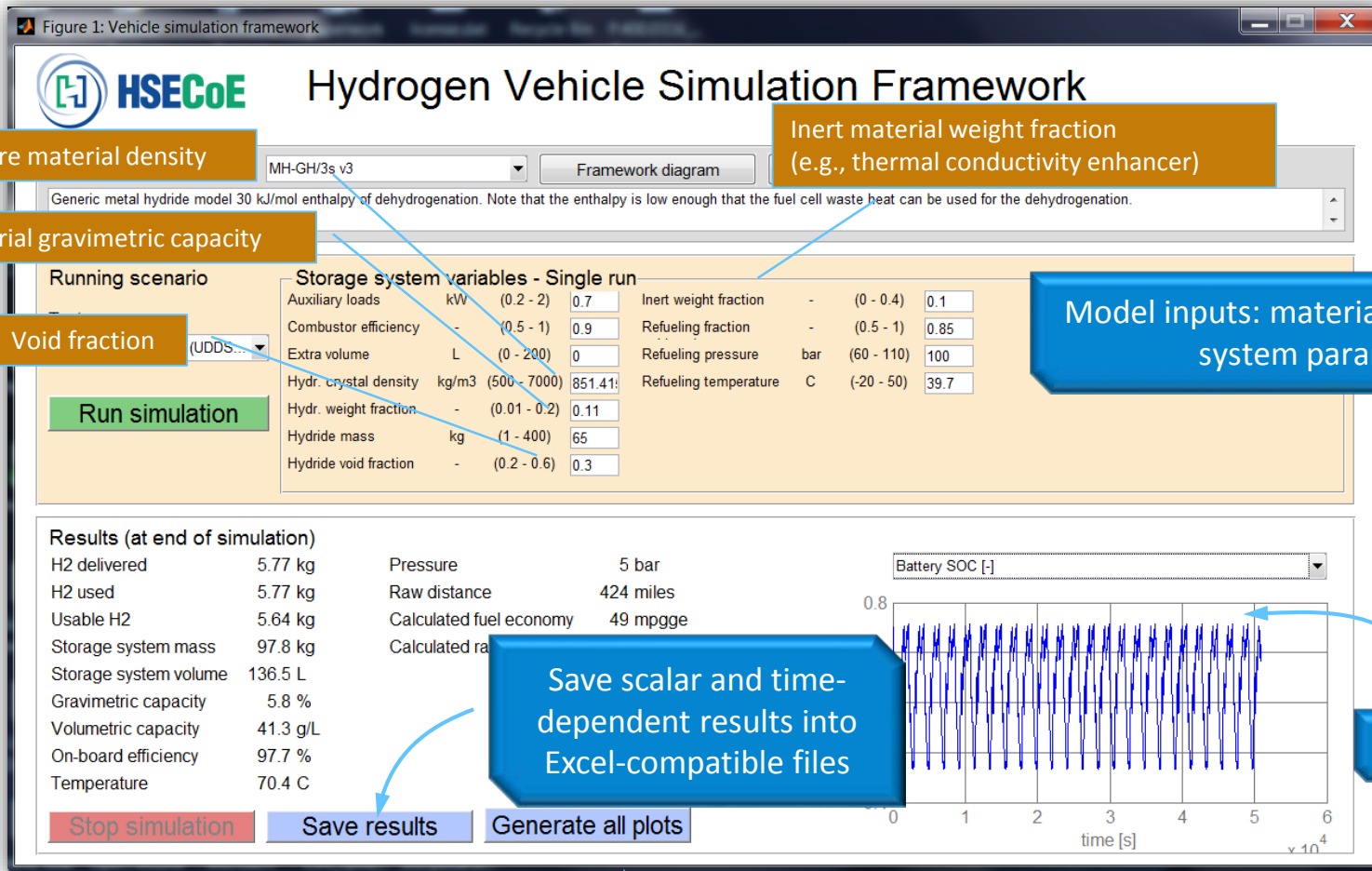
- Aligned with standard speed trace miss criteria: ± 2 mph in a ± 1 s window
- Check performed as post-process: a speed trace miss does not stop the simulation



Sample error message if speed trace miss detected

Accomplishments: Graphical User Interface

Metal hydride storage system model example in Simulink framework



Accomplishments: Framework—Model Results

```

example2.tbt - Notepad
File Edit Format View Help
System: Test system

Description:
Test system with no internal dynamics. It delivers exactly the flow rate requested by the

Running scenario:
Test case: 2 Aggressive cycle (us06, 24C)

Storage system & vehicle variables:
Auxiliary loads [kw]: 0.7
Tank aux power [w]: 100
    
```

```

example2.tbt - Notepad
File Edit Format View Help
System: MH-GH/3s v3

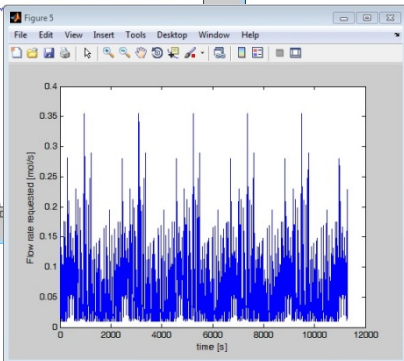
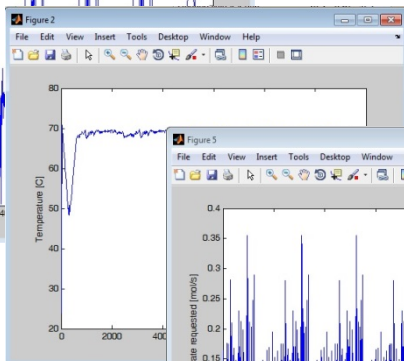
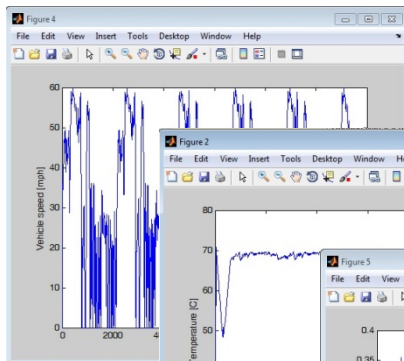
Description:
Generic metal hydride model 30 kJ/mol enthalpy of dehydrogenation.

Running scenario:
Test case: 1 Fuel economy test (UDDS+Hwy, 24C)

Storage system & vehicle variables:
Auxiliary loads [kw]: 0.7
Combustor efficiency [-]: 0.9
Extra volume [L]: 0
Hydr. crystal density [kg/m3]: 851.415
Hydr. weight fraction [-]: 0.11
Hydride mass [kg]: 15
Hydride void fraction [-]: 0.3
Inert weight fraction [-]: 0.1
Refueling fraction achieved [-]: 0.85
Refueling pressure [bar]: 100
Refueling temperature [C]: 39.7

Scalar results:
Distance traveled [miles]: 97
EPA Fuel economy [mpgge]: 49
EPA Range [miles]: 64
Gravimetric capacity [%]: 3.7
H2 delivered [kg]: 1.30
H2 used [kg]: 1.31
On-board efficiency [%]: 97.5
Pressure [bar]: 5
Storage system mass [kg]: 34.8
Storage system volume [L]: 44.3
Temperature [C]: 69.3
Usable H2 [kg]: 1.27
Volumetric capacity [g/L]: 28.8
    
```

Save results and generate summary text files and MATLAB figures



Results (at end of simulation)

H2 delivered	kg	0.49	Distance traveled	miles	24
H2 used	kg	0.49	EPA Fuel economy	mpgge	50
Usable H2	kg	0.48	EPA Range	miles	24
Storage system mass	kg	100.0			
Storage system volume	L	140.0			
Gravimetric capacity	%	0.5			
Volumetric capacity	g/L	3.4			
On-board efficiency	%	99.0			
Temperature	C	30.0			
Pressure	bar	6			

Range [miles] based on adjusted fuel economy (only interpret when running Test Case 1)

Vehicle speed [mph]

Stop simulation Save results Generate all plots

Accomplishments: Model Posting

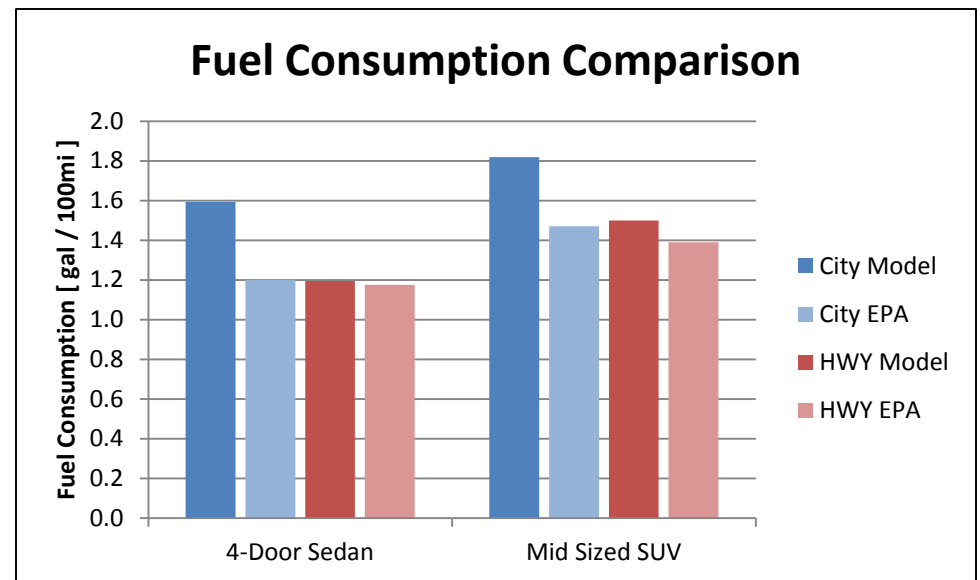
- **MH Acceptability Envelope** **SRNL** **complete**
- **MH Finite Element Model** **SRNL** **complete**
- **Physical H2 Framework Modes** **UTRC/NREL** **complete**
- **MH Framework Model** **UTRC/SRNL/NREL** **complete**
- **Tank Volume/Cost Model** **PNNL** **complete**
- **CH Framework Model** **UTRC/PNNL/NREL**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

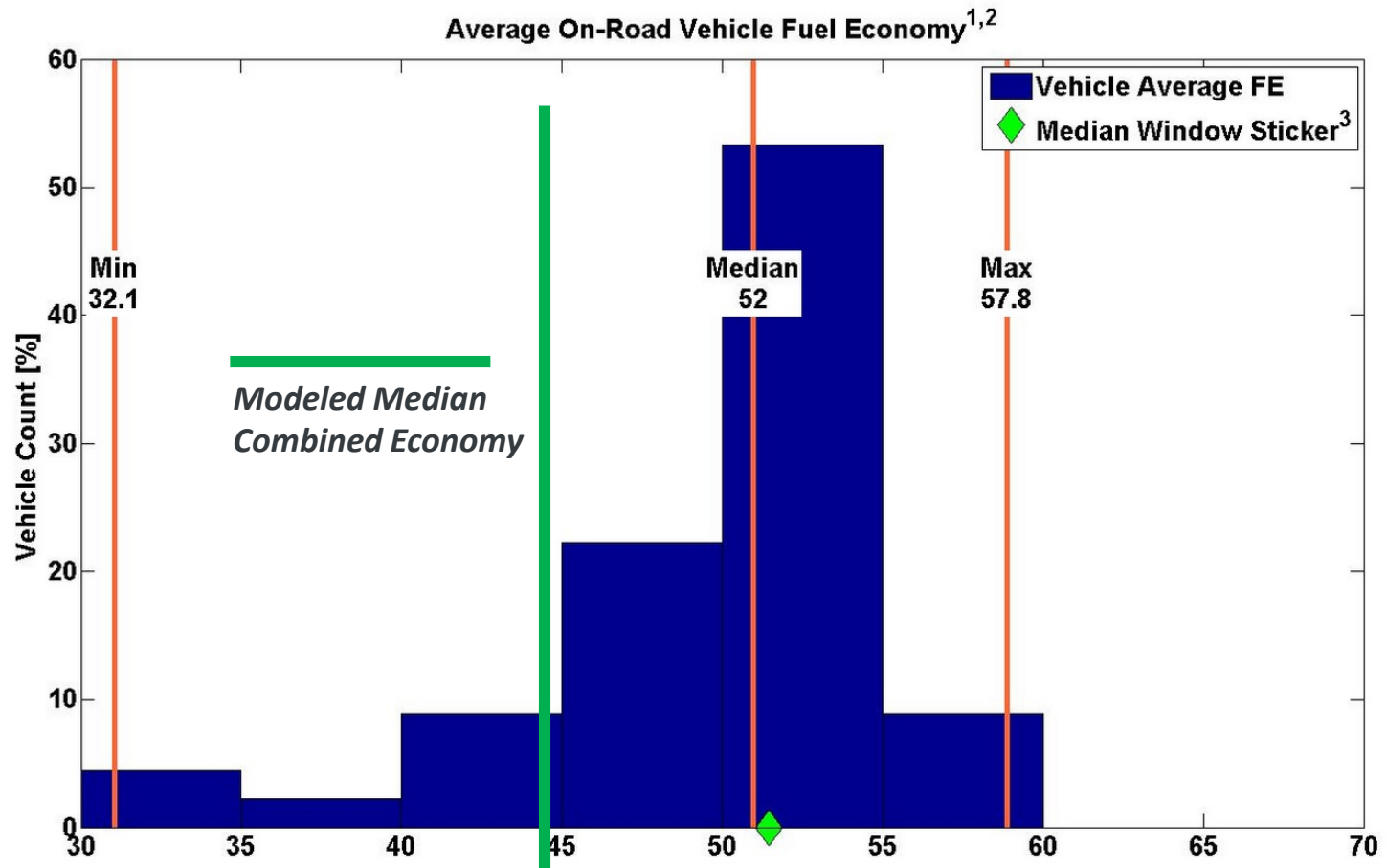
Fuel consumption validation


- 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

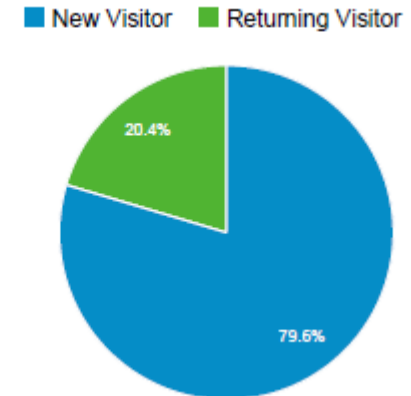
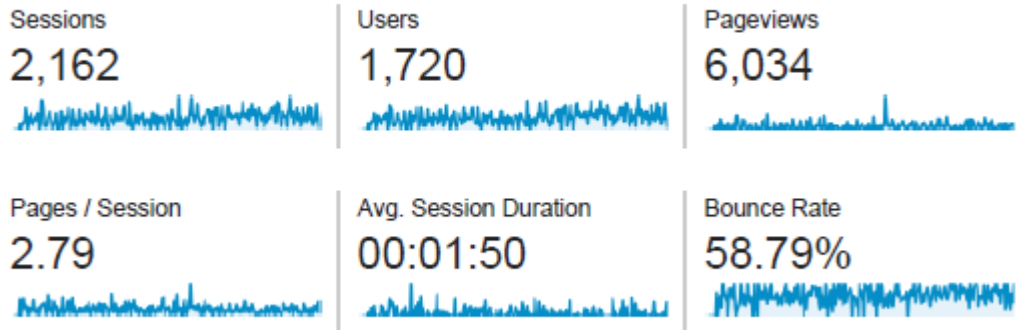
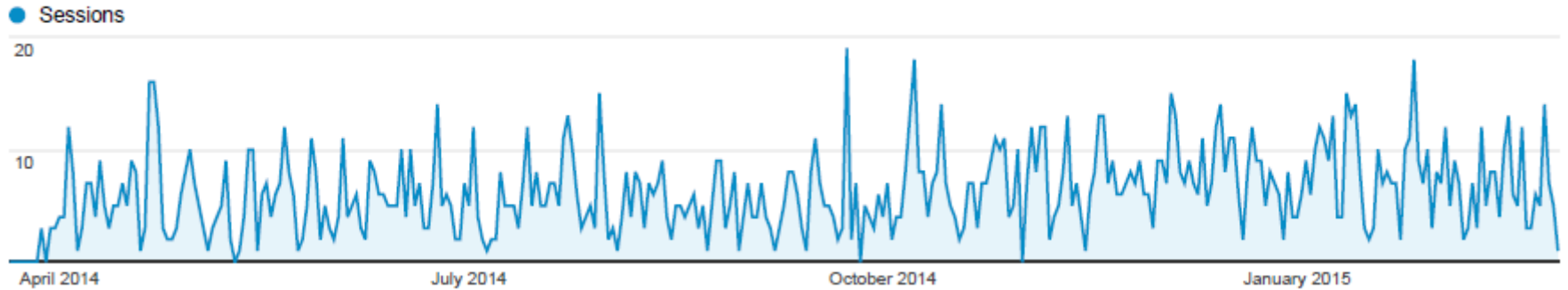


 NREL cdp_fcev_14
Created: Oct-31-14 8:47 AM | Data Through: 2014Q2

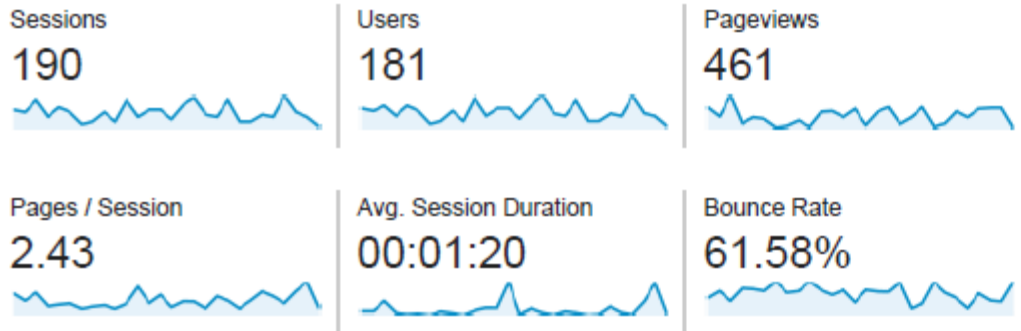
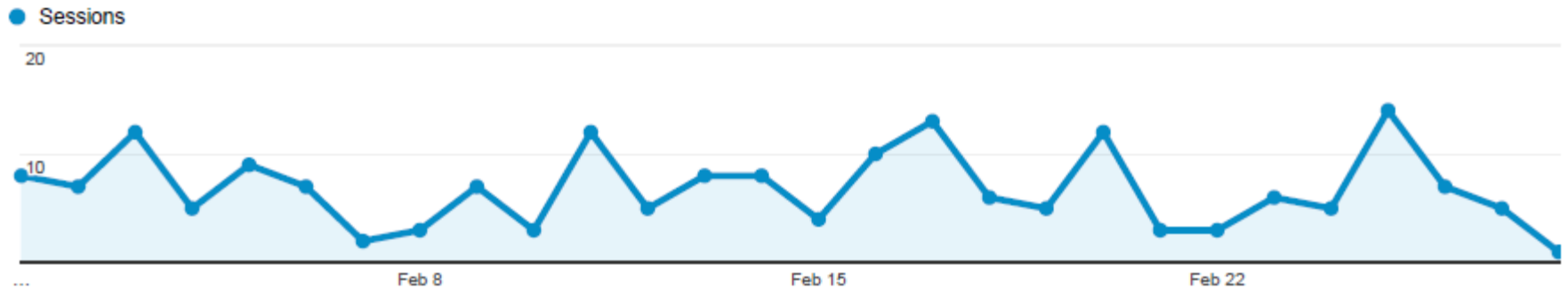
- 1) Calculated from on-road fuel cell stack current.
- 2) Excludes trips < 1 mile.
- 3) EPA Combined Rating.

**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

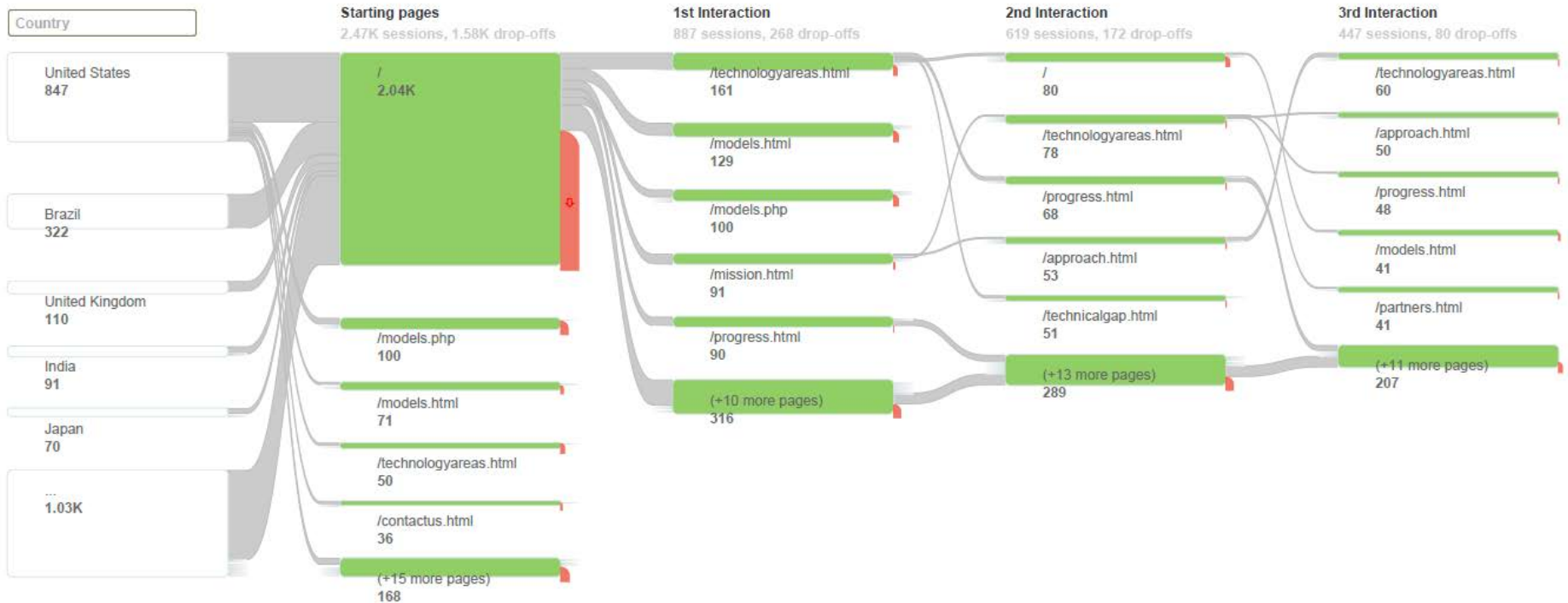
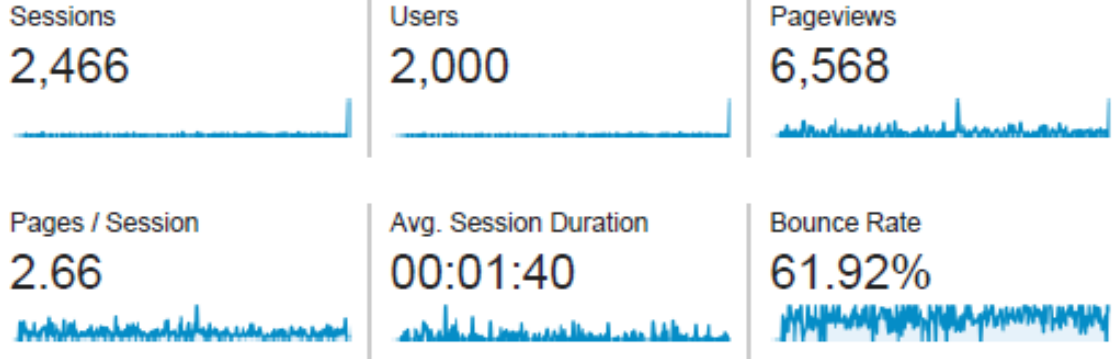


Accomplishments: Model Website Analytics

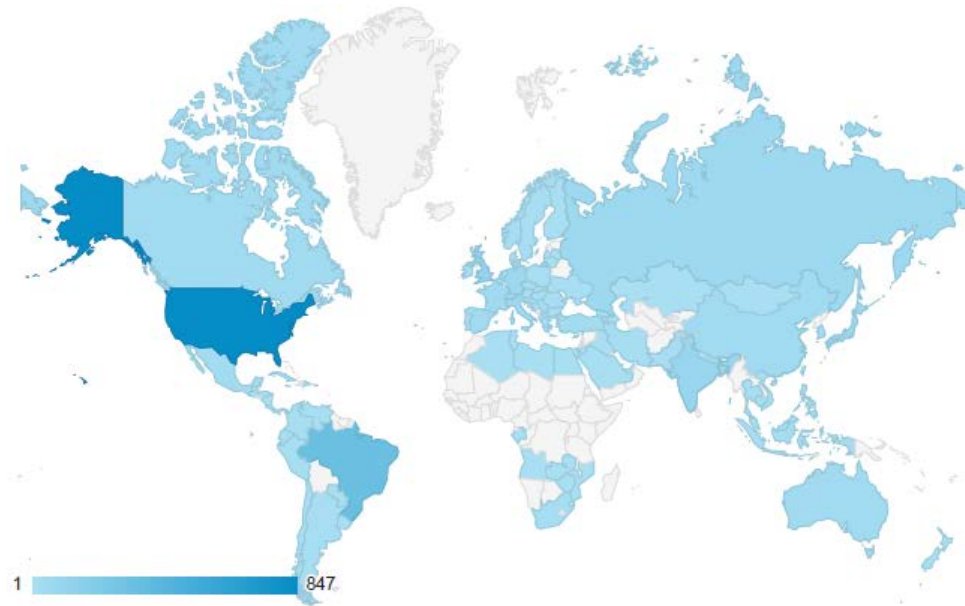


One month user data

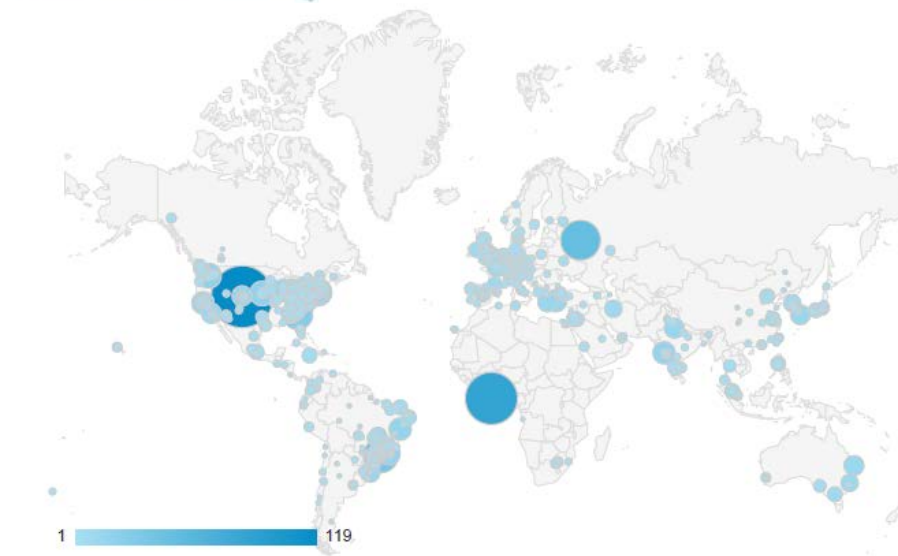
Accomplishments: Model Website Analytics



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 H₂ storage systems with fixed on-board H₂

Phase I

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi) 5.6kg H ₂	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/HFE T	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

Accomplishments: Framework Results

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 %]	Volumetric 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.**

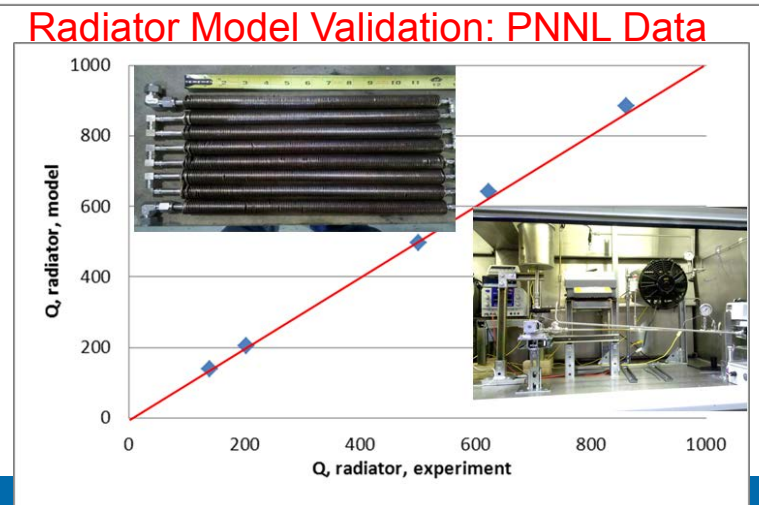
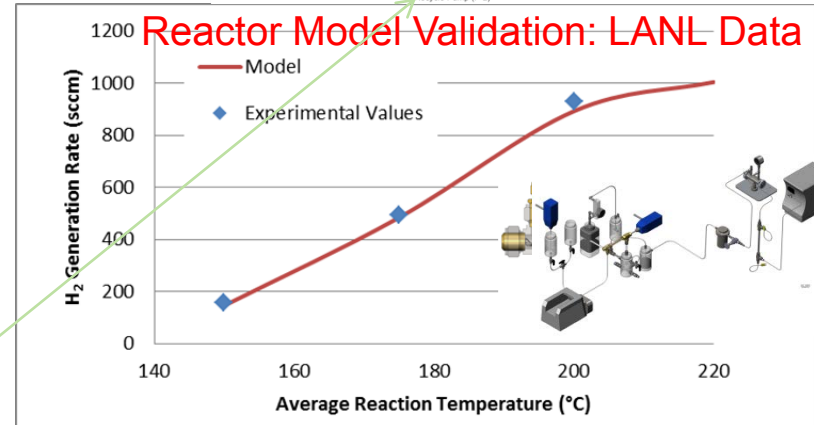
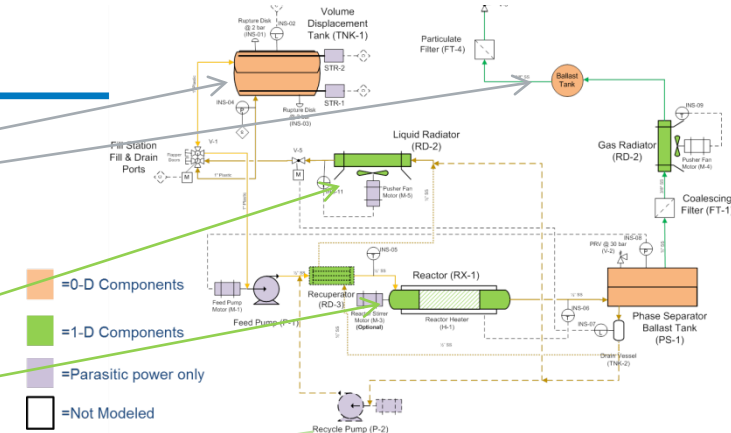
Technical Back-Up Slides

Accomplishment: Chemical Hydrogen Storage Model Validation

Flowsheet with Model Validation Approach

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



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 %]	Volumetric 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]

Accomplishments: Framework Results

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 %]	Volumetric 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 %]	Volumetric 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]