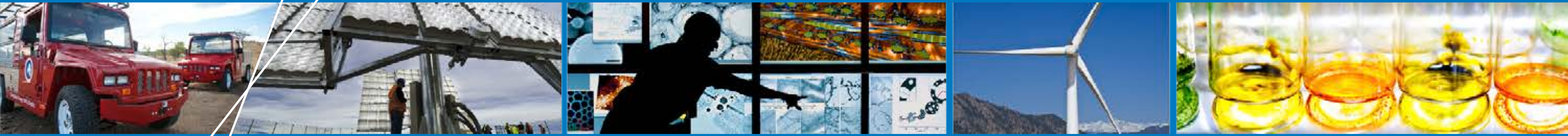
System Design, Analysis, and Modeling for Hydrogen Storage Systems



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National Renewable Energy Laboratory (NREL)

June 18, 2014

Project ID # ST008

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NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Overview

Timeline

Project start date: FY09
Project end date: FY15
Percent complete: 85%

Budget

FY13 DOE funding: $100K

Planned FY14 DOE funding: $125K

Total project value: $1.8M

Cost share percentage: 0%

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

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/Objectives

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 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.

Objective: 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

Objective: 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.

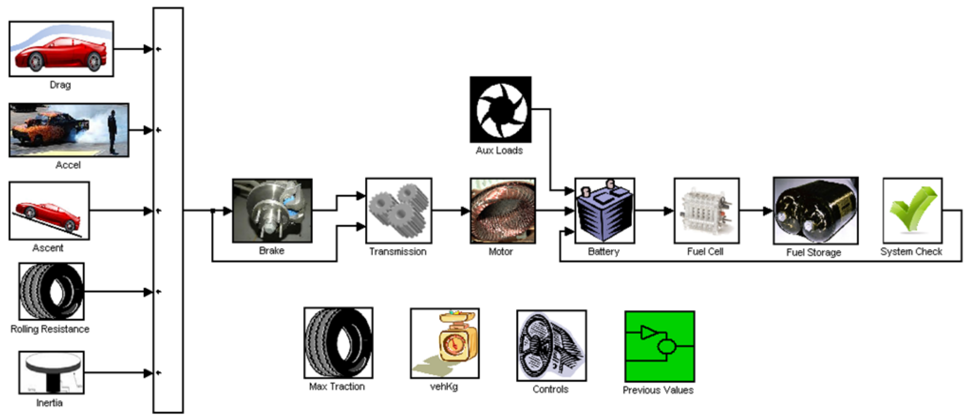
- Assist with model selection
- Coordinate model validation
- Coordinate model documentation
- Manage website and model posting
- Track and record Web activity
- Track and record model downloads

Approach/Milestones

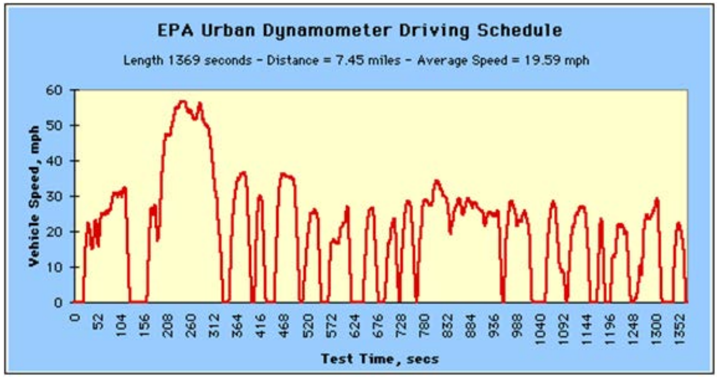
Date	Milestone	Status
10/13	Participate in the HSECoE face-to-face meeting and present on the status of the modeling efforts and development of GUI interface for the public release of the models.	100%
6/14	Update the chemical system model with Phase II performance data, integrate into the framework; document and release models to the public.	30%
6/14	Present modeling efforts of the HSECoE and the projected status of adsorbent systems to meet the DOE 2017 target of 5.5 wt.%.	50%
8/14	Report on vehicle system modeling of hydrogen storage impacts on vehicle range, acceleration, and fuel economy and associated trade-offs on volume and mass.	50%
8/14	NREL will work with center partners to set up and run vehicle simulations to evaluate the key volumetric, gravimetric, and onboard efficiency trade-offs over three test cases (drive cycles) and progress toward 2017 targets for two chemical hydrogen and two to three adsorbent system designs in support of final design selection for each material class for Phase III work.	25%
9/14	Report on progress of public release of HSECoE models.	0%
9/14	NREL will work with center partners to make enhanced and updated versions of the HSECoE "modeling framework", with four new storage system options, available for public access via the current Web portal.	0%

Approach: Develop HSSIM (Vehicle Model)

Structure



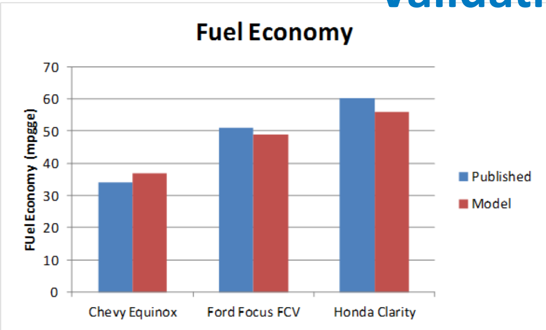
Drive Cycles

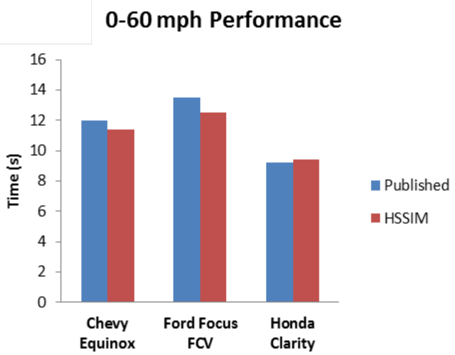


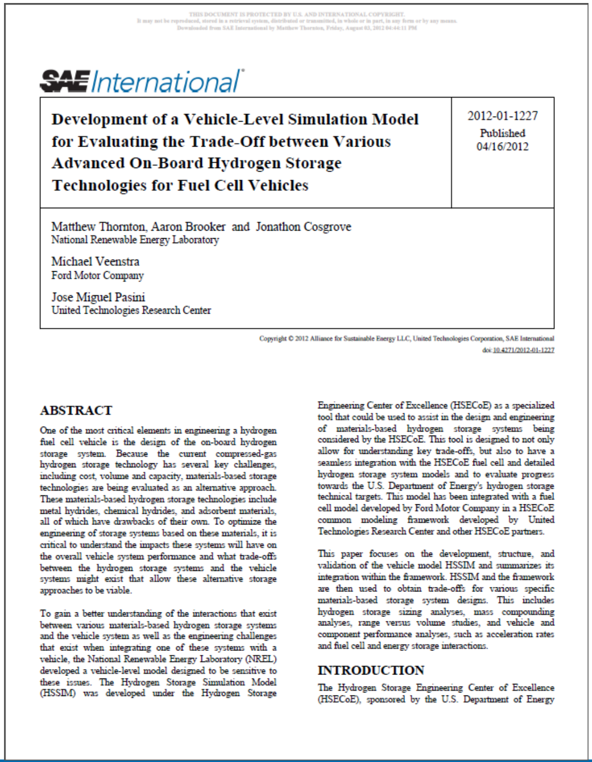
Output

- Fuel economy (mpgge) based on EPA-adjusted five cycle estimate
- Range (miles) from adjusted mpgge
- Onboard efficiency (%)
- Hydrogen flow (moles/s)
- Vehicle performance

Validation







SAE International

Development of a Vehicle-Level Simulation Model for Evaluating the Trade-Off between Various Advanced On-Board Hydrogen Storage Technologies for Fuel Cell Vehicles

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doi:10.4271/2012-01-1227

ABSTRACT

One of the most critical elements in engineering a hydrogen fuel cell vehicle is the design of the on-board hydrogen storage system. Because the current compressed-gas hydrogen storage technology has several key challenges, including cost, volume and capacity, materials-based storage technologies are being evaluated as an alternative approach. These materials-based hydrogen storage technologies include metal hydrides, chemical hydrides, and adsorbent materials, all of which have drawbacks of their own. To optimize the engineering of storage systems based on these materials, it is critical to understand the impacts these systems will have on the overall vehicle system performance and what trade-offs between the hydrogen storage systems and the vehicle systems might exist that allow these alternative storage approaches to be viable.

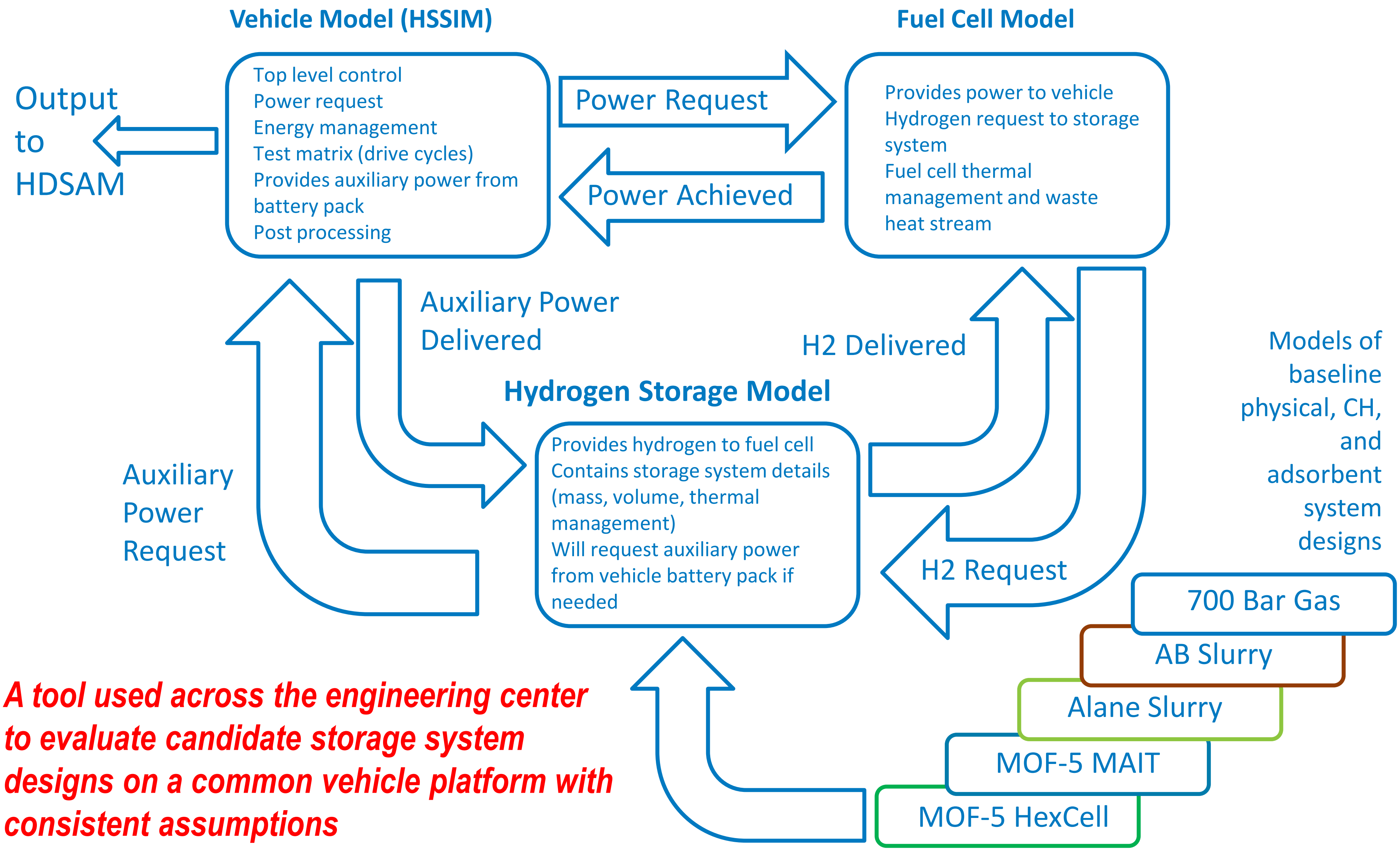
To gain a better understanding of the interactions that exist between various materials-based hydrogen storage systems and the vehicle system as well as the engineering challenges that exist when integrating one of these systems with a vehicle, the National Renewable Energy Laboratory (NREL) developed a vehicle-level model designed to be sensitive to these issues. The Hydrogen Storage Simulation Model (HSSIM) was developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE) as a specialized tool that could be used to assist in the design and engineering of materials-based hydrogen storage systems being considered by the HSECoE. This tool is designed to not only allow for understanding key trade-offs, but also to have a seamless integration with the HSECoE fuel cell and detailed hydrogen storage system models and to evaluate progress towards the U.S. Department of Energy's hydrogen storage technical targets. This model has been integrated with a fuel cell model developed by Ford Motor Company in a HSECoE common modeling framework developed by United Technologies Research Center and other HSECoE partners.

This paper focuses on the development, structure, and validation of the vehicle model HSSIM and summarizes its integration within the framework. HSSIM and the framework are then used to obtain trade-offs for various specific materials-based storage system designs. This includes hydrogen storage sizing analyses, mass compounding analyses, range versus volume studies, and vehicle and component performance analyses, such as acceleration rates and fuel cell and energy storage interactions.

INTRODUCTION

The Hydrogen Storage Engineering Center of Excellence (HSECoE), sponsored by the U.S. Department of Energy

Approach: Modeling Framework

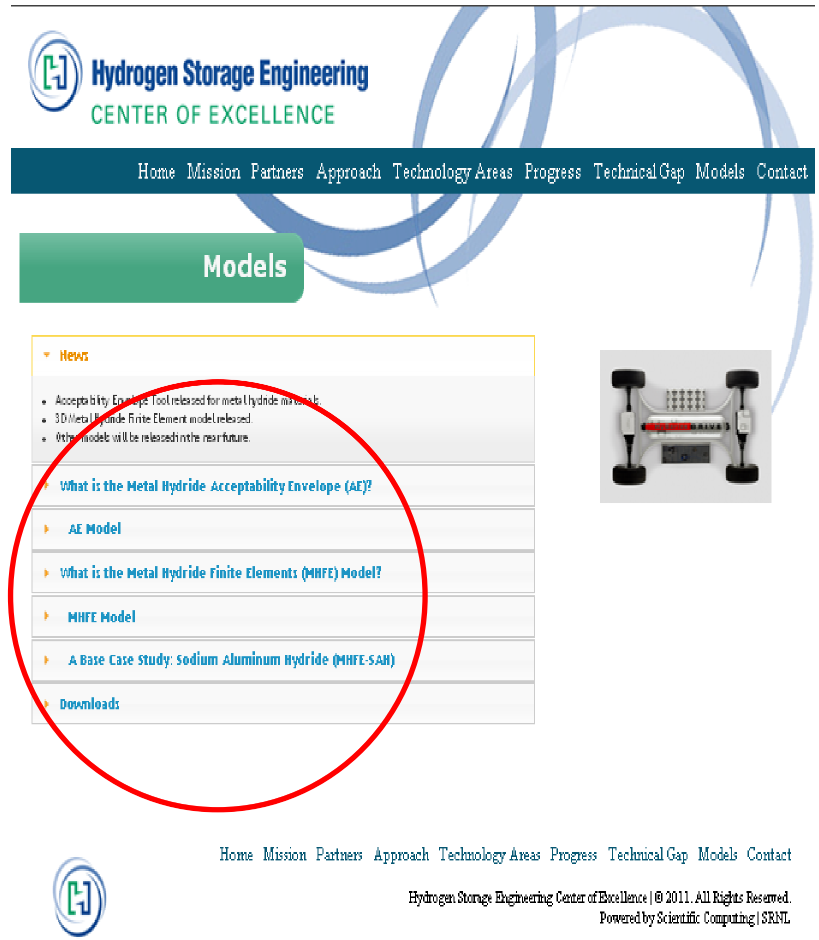


A tool used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent assumptions

Approach: Model Access Website

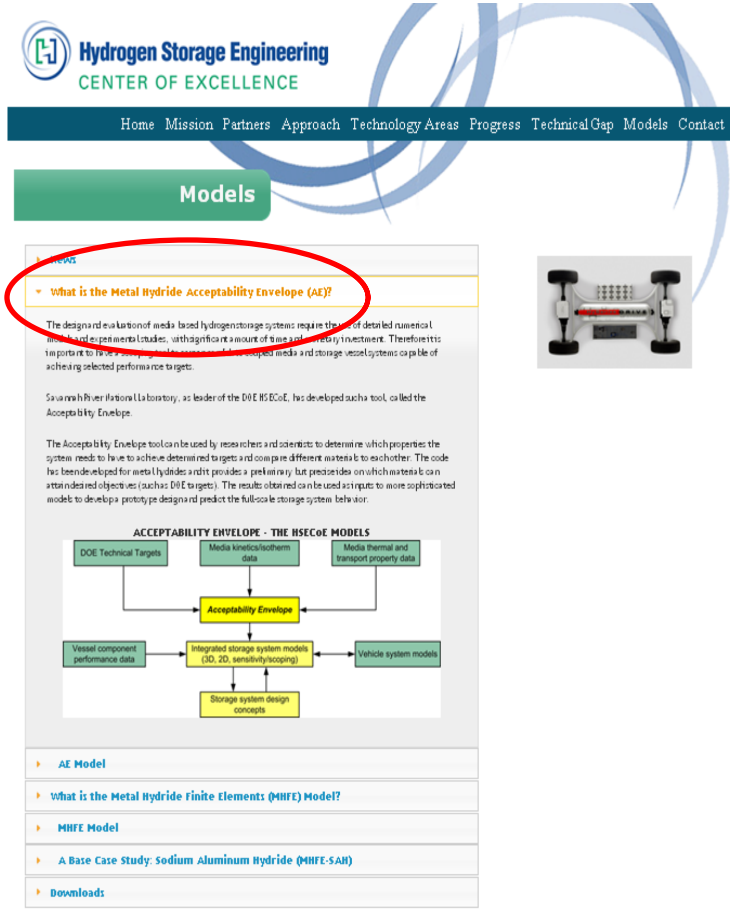
http://hsecoe.org

Model Access/Description Sub-Page



Approach: Model Access Website

Model Documentation and Downloads



Accomplishment: 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	6/2014
• AD Framework Model	UTRC/SRNL/NREL	9/2014
• AD Finite Element Model	SRNL	3/2015

Tanks/Volume Cost Model

Type 3 Tank sizing code	units	
Notes on Calculation Strategy		
Input parameters		
Operating Temperature	C	na
Operating Pressure	Bar	250
Tank Material	-	Carbon Fiber
Liner Material		Aluminum
Fiber Translation Efficiency	%	80%
Primary Geometry Specification: Internal		
Tank Length (Internal) [L_0]	cm	0
Tank Radius (Internal) [R_0]	cm	22.5
Tank Volume Goal (Internal) [V_0]	ccm	105,000
Tank Geometry Calculation		
Tank Internal Length (cm) [L]	cm	81.0
Tank Internal Radius (cm) [R]	cm	22.5
Tank Internal Volume Actual (ccm) [V]	ccm	105,000
Volume goal attainment	%	100.0%
Tank Liner estimate		
total burst pressure load	bar	562.5
liner burst load factor	%	21.0%
liner burst load	bar	118.1
Liner ultimate strength (Room Temp.)	Bar	3103.0
Liner Thickness [t]	cm	0.86
Upper Bound Wall Thickness Calculation		
Carbon Fiber Composite Material strength	Bar	15306
Safety Factor	-	2.25
Wall Radius = R+t	cm	23.4
Tank Wall thickness (ideal)	cm	1.072949179
Layer thickness increment	cm	0.09144
# layers		12
Rounded up thickness	cm	1.09728
Minimum layer thickness	cm	0.27432
Final wall thickness	cm	1.09728

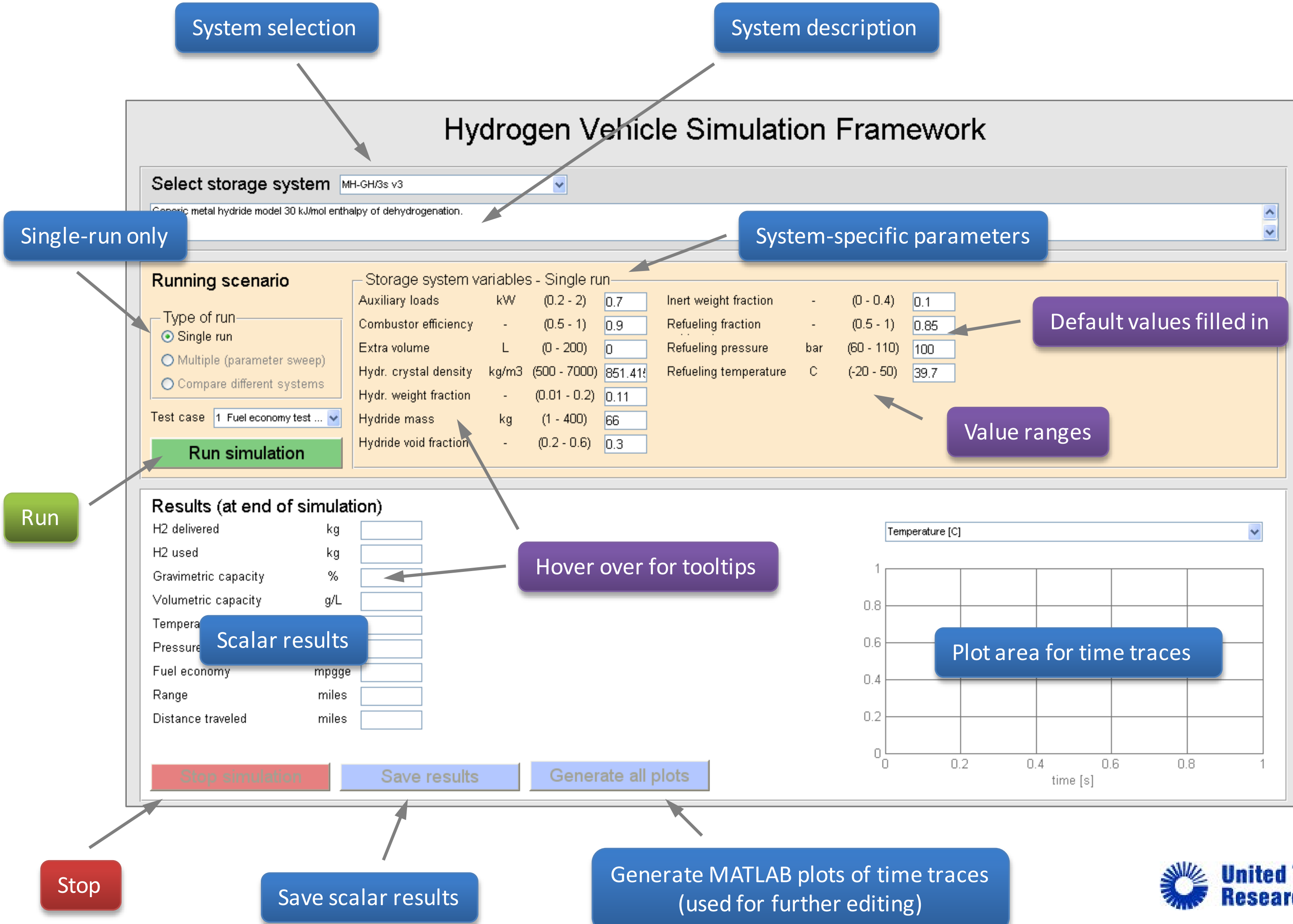
Final safety factor		2.30
Estimated burst pressure	Bar	575.3
Lower Bound Wall Thickness Calculation		
Liner ultimate strength (RT)	Bar	3103
Liner can support	Bar	118.125
Adjusted Burst Pressure on Composite	Bar	444.375
Tank Wall thickness (ideal)	cm	0.847629852
Layer thickness increment	cm	0.09144
# layers		10
Rounded up thickness	cm	0.9144
Minimum layer thickness	cm	0.27432
Final wall thickness	cm	0.9144
Load share estimate	%CF	79%

Mass Calculations	**Low Bound**	**High Bound**
Internal Radius (cm)	22.5	22.5
Internal Length (cm)	81.0	81.0
liner thickness (cm)	0.9	0.856529971
wall thickness (cm)	0.9144	1.09728
liner density (kg/ccm)	0.002663	0.002663
wall density (kg/ccm)	0.001611	0.001611
Ext Radius (cm)	24.27092997	24.45380997
Ext Length (cm)	84.56168819	84.92744819
Liner Ext Radius (cm)	23.35652997	23.35652997
Liner Ext Length (cm)	82.73288819	82.73288819
exterior volume (L)	126.5489622	128.9213116
Liner ext volume (L)	115.1036997	115.1036997
internal volume (L)	105	105
wall volume (ccm)	11445.26251	13817.61194
liner volume (ccm)	10103.69967	10103.69967
Carbon Fiber Composite mass (kg)	18.44	22.26
Aluminum liner mass (kg)	26.91	26.91
total mass (kg)	45.34	49.17
exterior L:D	1.742036426	1.73648704
Layers of composite (minimum is 3)	10	12
Tank Efficiency		
Gravimetric (L/kg)	2.32	2.14
Tank Material Cost		
aluminim material cost ($/kg)	4.45	4.45
Carbon fiber composite cost ($/kg)	30.65	30.65
aluminum line cost ($)	119.73	119.73
Carbon fiber composite cost ($)	565.13	682.27
Tank Wall total material cost ($)	684.87	802.01

Pacific Northwest NATIONAL LABORATORY

Framework Model GUI

Initial screen



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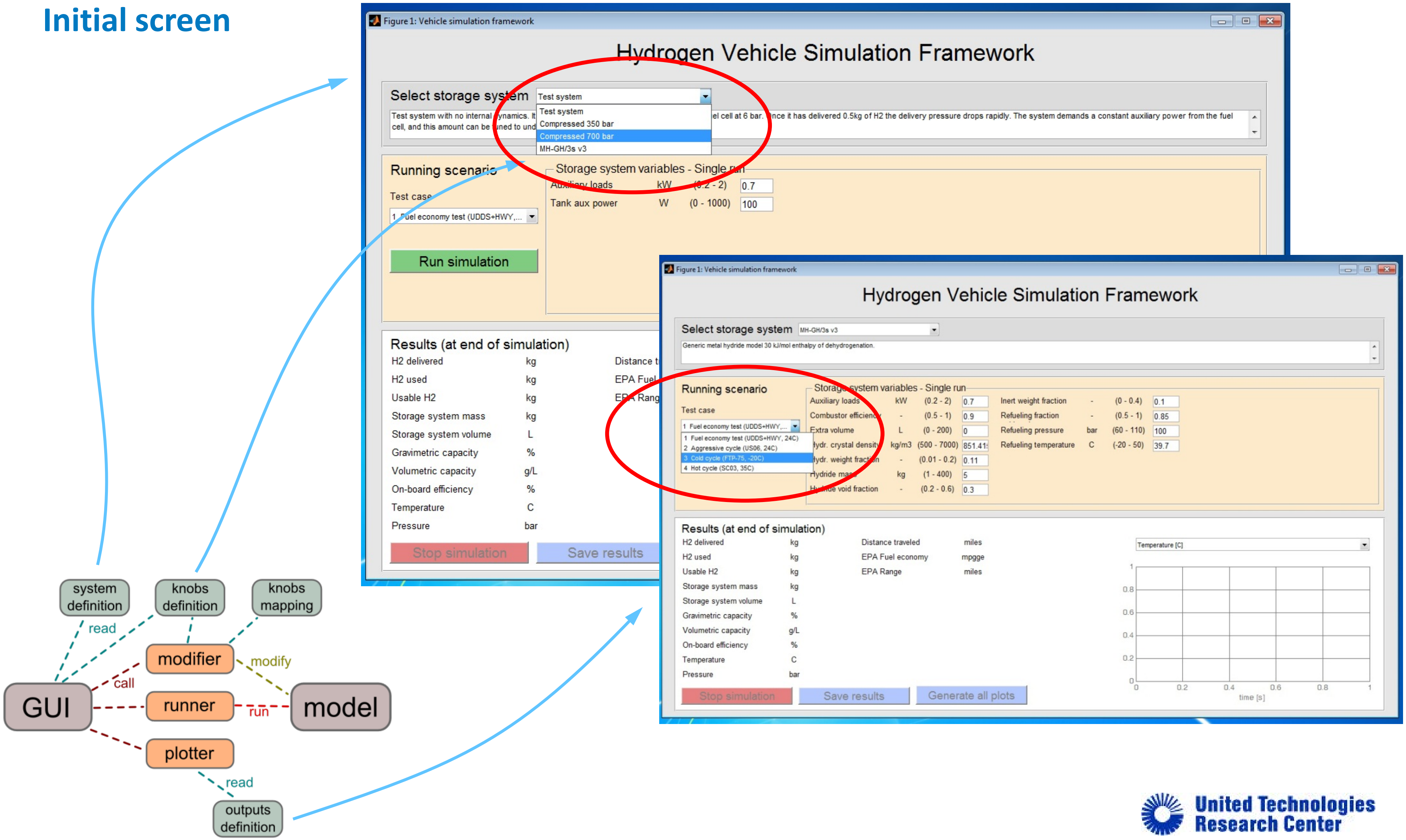
United Technologies Research Center

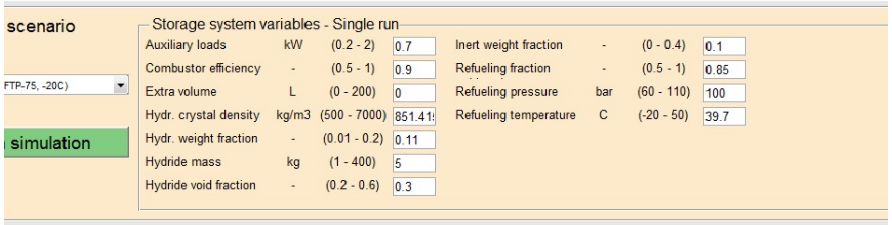
Framework Model GUI

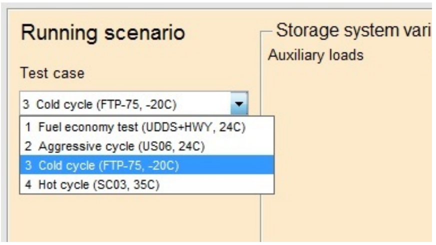
Initial screen



United Technologies Research Center

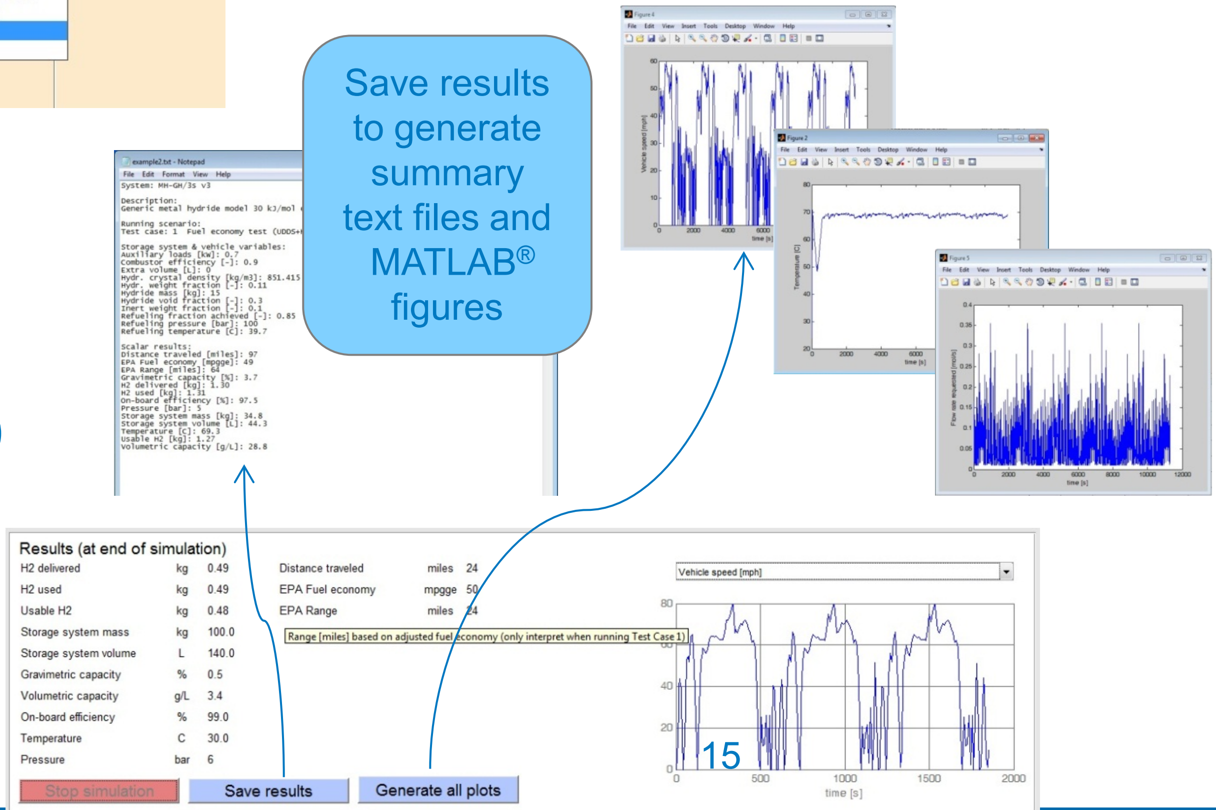
Framework Model GUI—Inputs





Key Results
- Volumetric and gravimetric capacity
- Fuel economy and range (case 1)
- Onboard efficiency
- H2 flow rate

Key Parameters
- Storage system
- Test case / drive cycle
- Auxiliary loads
- System specific
  - Hydride mass (MH sys)
  - Tank aux power (test sys)



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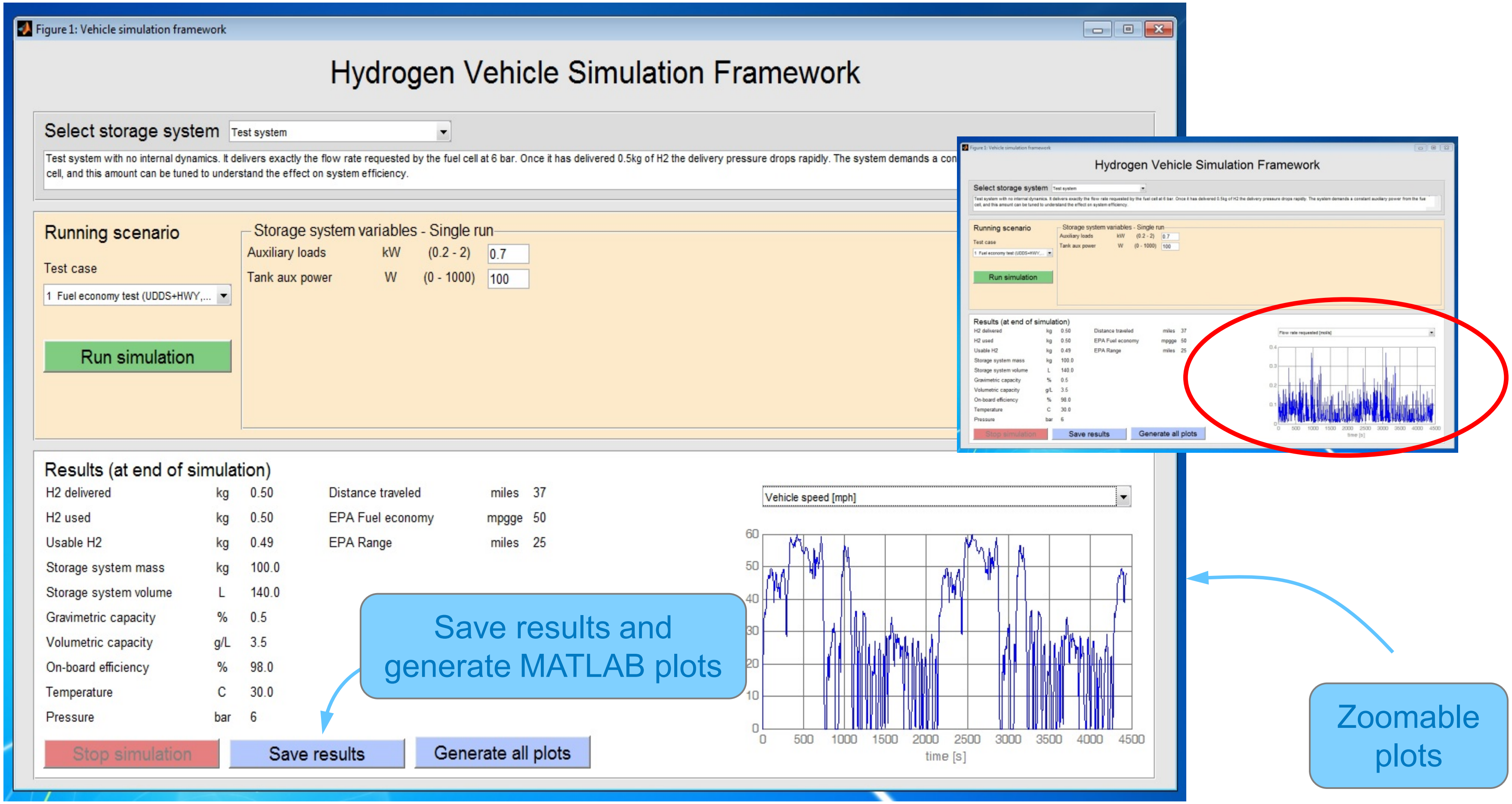
Framework Model GUI—Model Results



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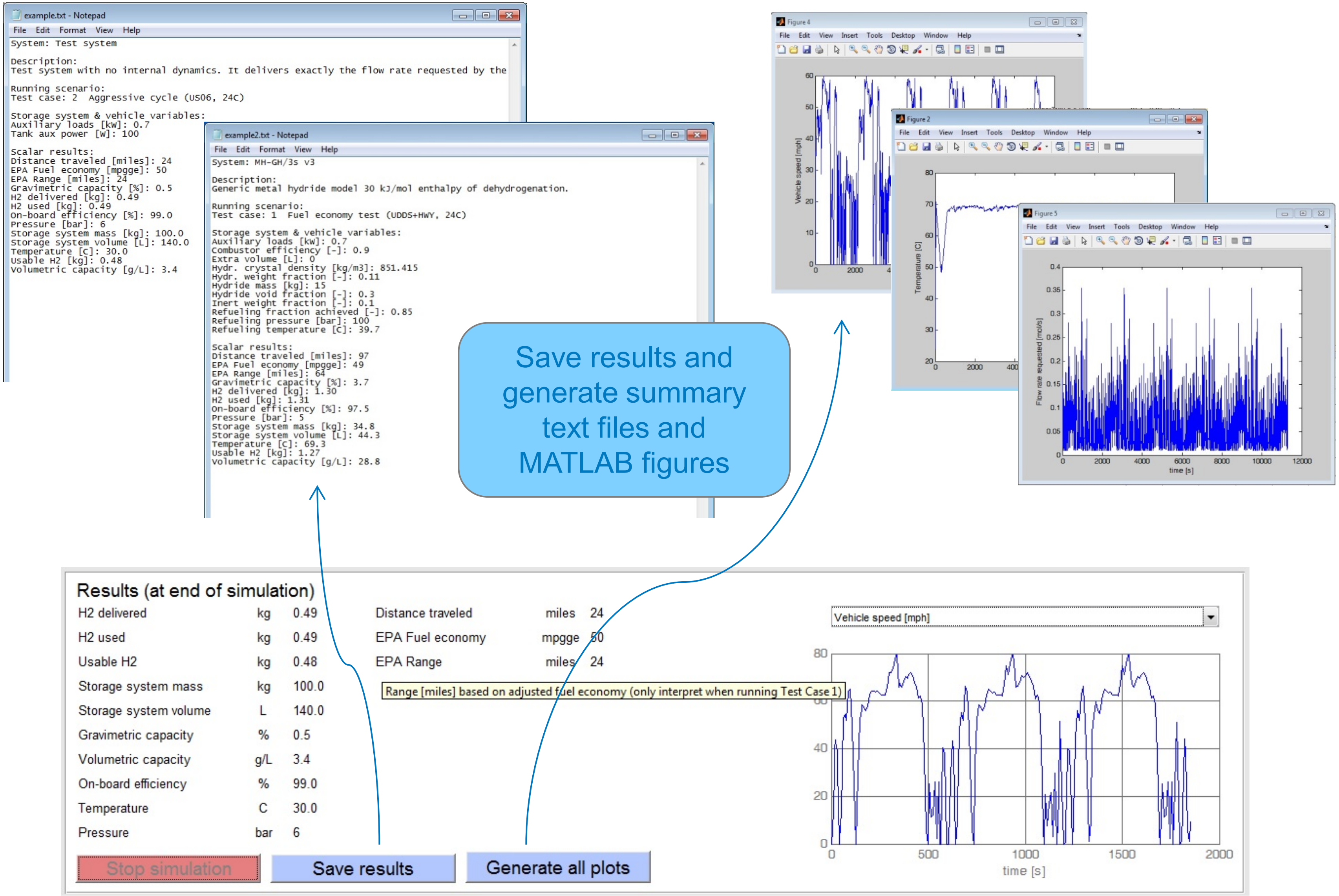
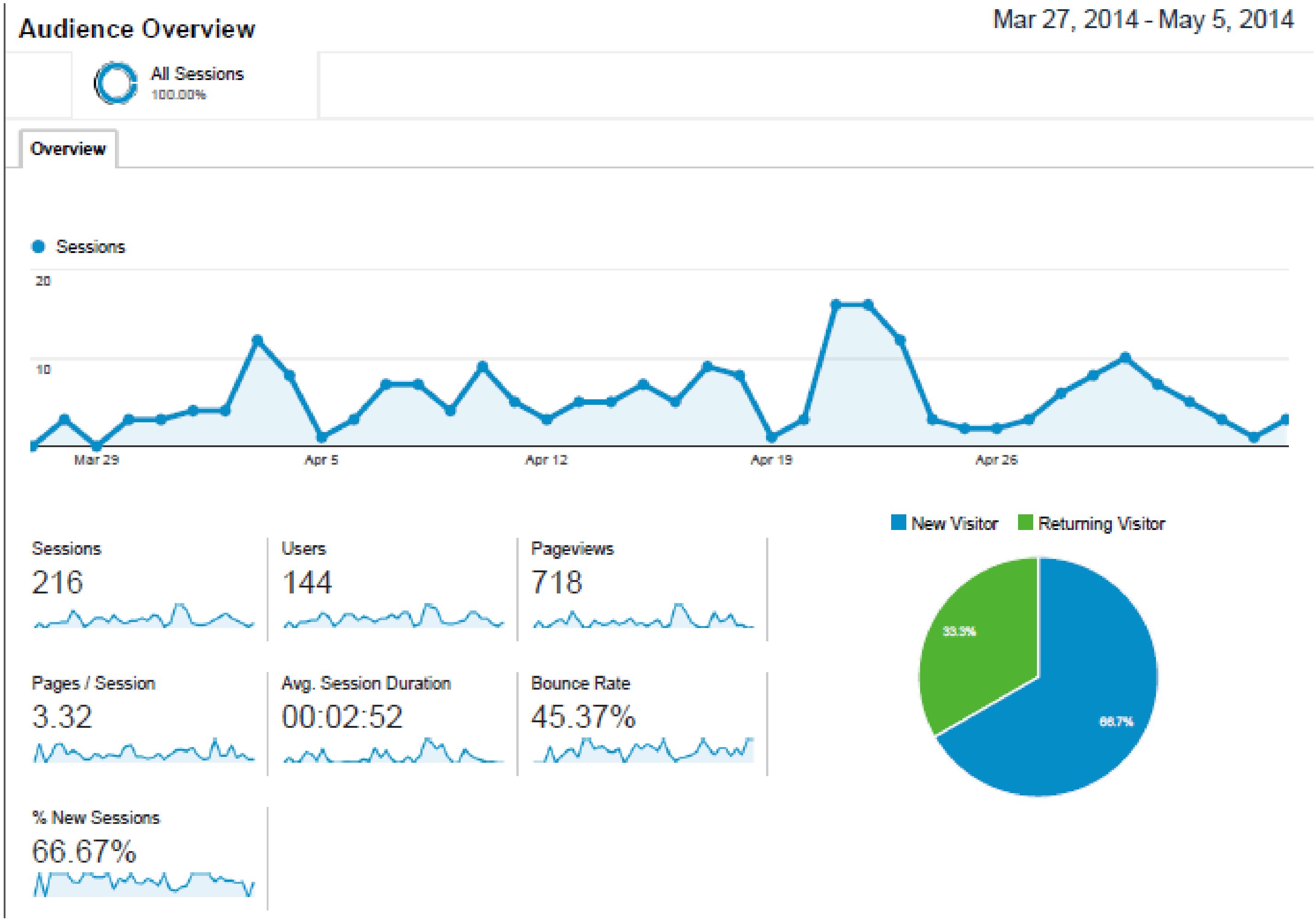
Framework—Model Results



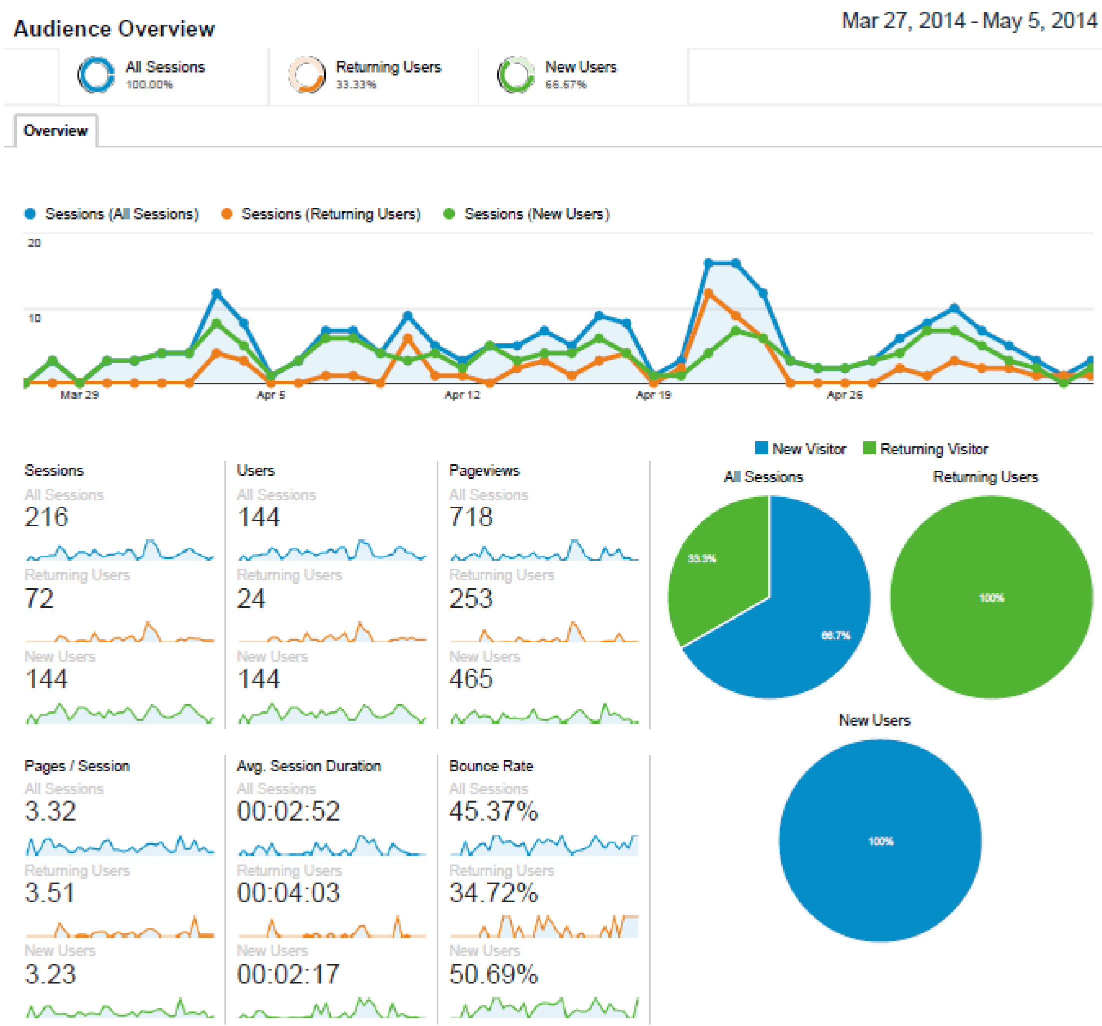
Accomplishments: Model Website Analytics

Site Visits



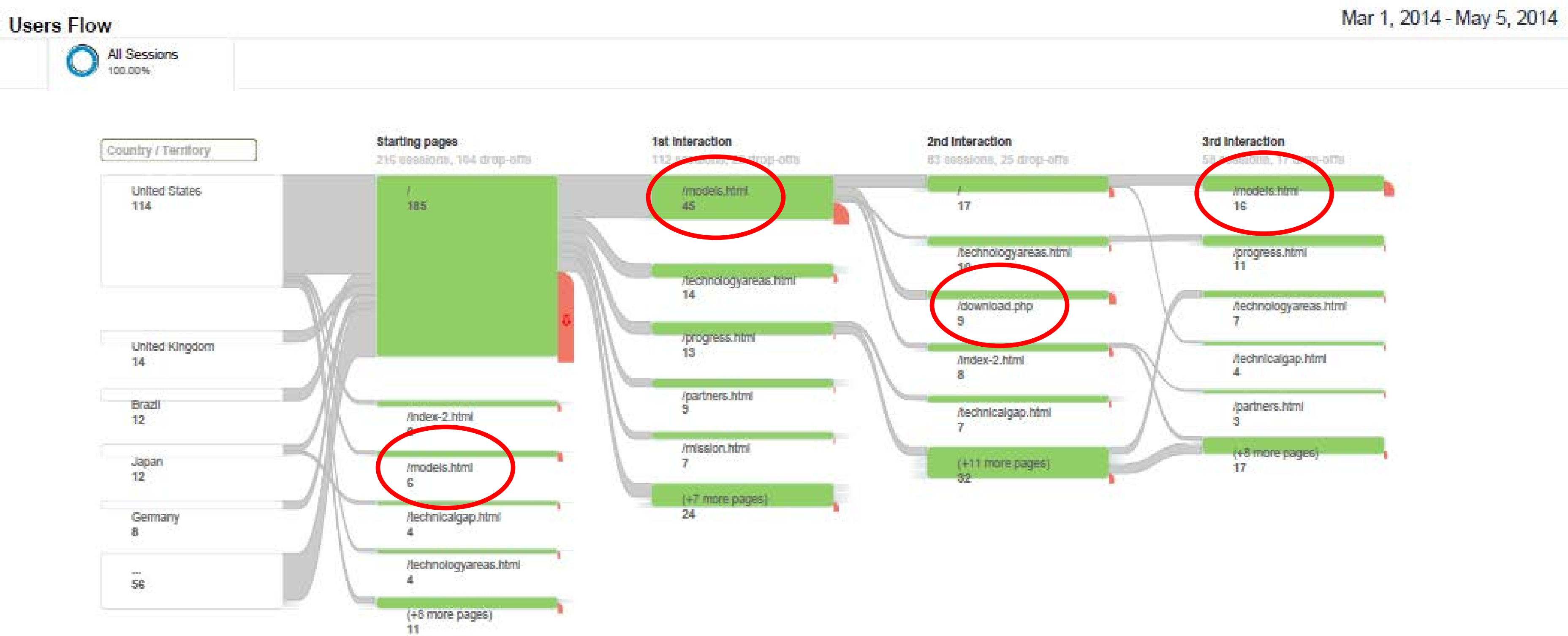
Accomplishments: Model Website Analytics

New versus Return Visits



Accomplishments: Model Website Analytics

User Flows



Accomplishments: Model Website Analytics

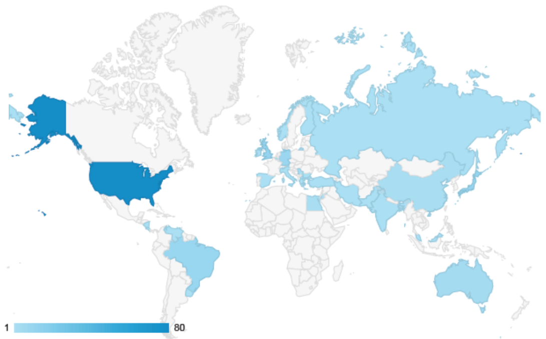
Visitor Locations

Location Mar 23, 2014 - Apr 22, 2014

All Sessions
100.00%

Map Overlay

Summary

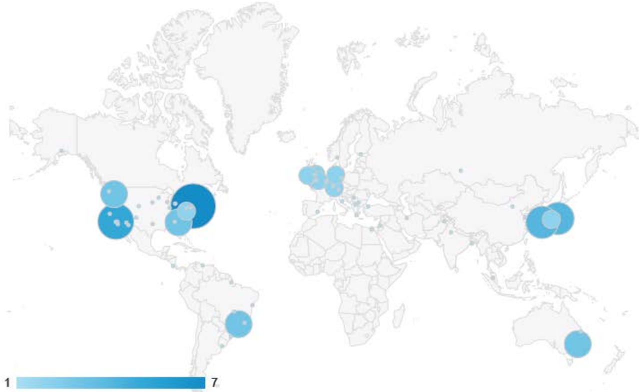


Country / Territory	Acquisition			Behavior			Conversions		
	Sessions	% New Sessions	New Users	Bounce Rate	Pages / Session	Avg. Session Duration	Goal Conversion Rate	Goal Completions	Goal Value
	151 % of Total: 100.00% (151)	64.90% Site Avg: 64.90% (0.00%)	98 % of Total: 100.00% (98)	43.71% Site Avg: 43.71% (0.00%)	3.27 Site Avg: 3.27 (0.00%)	00:03:04 Site Avg: 00:03:04 (0.00%)	0.00% Site Avg: 0.00% (0.00%)	0 % of Total: 0.00% (0)	$0.00 % of Total: 0.00% ($0.00)
1. United States	80 (52.98%)	51.25%	41 (41.84%)	30.00%	3.71	00:03:51	0.00%	0 (0.00%)	$0.00 (0.00%)
2. United Kingdom	11 (7.28%)	72.73%	8 (8.16%)	36.36%	3.55	00:03:20	0.00%	0 (0.00%)	$0.00 (0.00%)
3. Japan	10 (6.62%)	30.00%	3 (3.06%)	50.00%	4.20	00:05:03	0.00%	0 (0.00%)	$0.00 (0.00%)
4. Brazil	9 (5.96%)	100.00%	9 (9.18%)	100.00%	1.00	00:00:00	0.00%	0 (0.00%)	$0.00 (0.00%)
5. Germany	8 (5.30%)	87.50%	7 (7.14%)	12.50%	4.88	00:03:20	0.00%	0 (0.00%)	$0.00 (0.00%)
6. Australia	4 (2.65%)	50.00%	2 (2.04%)	25.00%	4.00	00:01:50	0.00%	0 (0.00%)	$0.00 (0.00%)
7. Bangladesh	2 (1.32%)	100.00%	2 (2.04%)	100.00%	1.00	00:00:00	0.00%	0 (0.00%)	$0.00 (0.00%)
8. Belgium	2 (1.32%)	100.00%	2 (2.04%)	0.00%	6.00	00:13:57	0.00%	0 (0.00%)	$0.00 (0.00%)
9. China	2 (1.32%)	100.00%	2 (2.04%)	100.00%	1.00	00:00:00	0.00%	0 (0.00%)	$0.00 (0.00%)
10. Egypt	2 (1.32%)	100.00%	2 (2.04%)	50.00%	1.50	00:00:18	0.00%	0 (0.00%)	$0.00 (0.00%)

New Custom Report Mar 23, 2014 - Apr 22, 2014

All Sessions
75.50%

Report Tab



City	Sessions
	114 % of Total: 75.50% (151)
1. Stratford	7 (6.14%)
2. Los Angeles	5 (4.39%)
3. (not set)	4 (3.51%)
4. Yokohama	4 (3.51%)
5. Fukuoka	4 (3.51%)
6. Sydney	3 (2.63%)
7. Sao Paulo	3 (2.63%)
8. Aiken	3 (2.63%)
9. Richland	3 (2.63%)
10. Stuttgart	2 (1.75%)

Accomplishments: Response to Reviewers' Comments

- **Comment: There is a lack of variation in powertrain configurations. The project team should add range extender powertrain sensitivity analysis.**
  - Response: The powertrain and vehicle platforms included in the vehicle performance modeling task were limited by design due to project budget and time constraints.
- **Comment: It would be instructive to redo the analyses on a fixed volume basis. FCEVs will have a fixed packaging volume for fitting the storage system on board the vehicle. Greater discrimination between the various storage concepts could result from a fixed-volume analysis.**
  - Response: The focus of the vehicle level analysis for this project was to perform simulations on a fixed usable H2 mass basis. As such, most of the analyses used a 5.6 kg usable H2 assumption and the storage models were designed and coded to be consistent with this assumption. That said, a fixed volume analysis was performed in FY12. A summary table of the results from this study is presented on the following slide.

Results: Fixed Volumetric Effects on Range Analysis

Example simulated volume effects on vehicle range and onboard usable H2 (from framework) for various adsorbent system designs

For three fixed volume scenarios: 140/205/253 liters

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Usable H2 (kg)	Range (mi) Usable H2	Gravimetric Capacity (weight percent)	Volumetric Capacity (g/L)	Volume (L)
Powder MOF-5 60 bar 80k Al	51.11	2.00	102.20	2.80	12.86	140[1]
Powder MOF-5 60 bar 40k CF	51.30	4.20	215.50	6.61	29.84	140
0.52 g/cc MOF-5 200 bar 80k Al	50.47	3.35	169.10	2.68	23.94	140
0.52 g/cc MOF-5 200 bar 40k CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60 bar 80k Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60 bar 40k CF	50.97	6.70	341.50	7.97	32.64	205
0.52 g/cc MOF-5 200 bar 80k Al	49.93	5.35	267.10	2.92	26.11	205
0.52 g/cc MOF-5 200 bar 40k CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60 bar 80k Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60 bar 40k CF	50.89	8.60	437.60	8.68	33.96	253
0.52 g/cc MOF-5 200 bar 80k Al	49.32	6.85	337.90	3.02	27.05	253
0.52 g/cc MOF-5 200 bar 40k CF	49.71	9.30	462.30	4.77	39.56	253

[1] *Actual volume used = 155.56 L, which represents the lowest value in the data set available.*

Response to Reviewers Comments, Cont.

- **Comment: The progress in MOF-5 isotherm measurement appears to be slow, perhaps due to limited funding.**
  - Response: The "material characterization" component of this effort was only involved with sorbents, and leveraged the vast amount of information generated by the Hydrogen Sorption Center of Excellence. This part of the effort provided guidance for identifying potential sorbents for the Engineering Center and providing the specific engineering properties needed to make down-selections and to improve model confidence. Most of this activity in the past focused on non-metal organic framework materials (MOFs), and ultimately, since MOFs were selected for Phase II and Phase III activities, the vast majority of the work and information provided was down selected. At this time, the main focus of the NREL "material characterization" effort is involved with model validation, especially for temperatures below 75 K.

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 CH models to Framework (June)
  - Add Adsorbent models to Framework (September)
  - Post Adsorbent finite element model similar to MH FE Model
- Continue to run vehicle simulations to:
  - Evaluate the impact of changes to Phase III storage system designs and refinements
- Energy analysis
  - Work complete
- Media engineering properties
  - Work complete

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

Results: Fixed Volumetric Effects on Range Analysis

Example simulated volume effects on vehicle range and onboard usable H2 (from framework) for various adsorbent system designs

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0.52 g/cc MOF-5 200 bar 80k Al	50.47	3.35	169.10	2.68	23.94	140
0.52 g/cc MOF-5 200 bar 40k CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60 bar 80k Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60 bar 40k CF	50.97	6.70	341.50	7.97	32.64	205
0.52 g/cc MOF-5 200 bar 80k Al	49.93	5.35	267.10	2.92	26.11	205
0.52 g/cc MOF-5 200 bar 40k CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60 bar 80k Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60 bar 40k CF	50.89	8.60	437.60	8.68	33.96	253
0.52g/cc MOF-5 200 bar 80k Al	49.32	6.85	337.90	3.02	27.05	253
0.52 g/cc MOF-5 200 bar 40k CF	49.71	9.30	462.30	4.77	39.56	253

[1] *Actual volume used = 155.56 L, which represents the lowest value in the data set available.*