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Hydrogen Storage System Modeling:

Public Access, Maintenance, and Enhancements

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Team: Matthew Thornton, Sam Sprik, and Kriston Brooks

NREL National Renewable Energy Laboratory

Pacific Northwest National Laboratory

June 15, 2018

ST008

Hydrogen Storage Engineering Center of Excellence

Savannah River Nuclear Solutions

FLUOR • NEWPORT NEWS NUCLEAR • HONEYWELL

Overview

Timeline

- Start: October 1, 2015
- End: September 30, 2018
- 80% Complete (as of 5/1/18)
  - $950,000 Spent (as of 5/1/18)

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

Relevance

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

- Transfer engineering development **knowledge from HSECoE on to future materials research**.
- Manage the **HSECoE model dissemination** web page.
- Manage, update, and enhance the **modeling framework and the specific storage system models** developed by the HSECoE.
- Develop models that will **accept direct materials property inputs** and can be measured by materials researchers.
- **Ultimate Goal**: **Provide modeling tools that will be used by researchers to evaluate the performance their new materials in engineered systems relative to the DOE Technical Targets**.

Relevance – Barriers Addressed with Models

Barriers	Model Addressing Barrier
A. System Weight and Volume	System Estimator
B. System Cost	Tank Volume/Cost Model
C. Efficiency	Framework Model - On-Board Efficiency - Fuel Economy
E. Charging/Discharging Rates	Framework Model - Drive cycles
I. Dispensing Technology	Framework Model - Initial and Final System Conditions
K. System Life-Cycle Assessment	All Models

Relevance – Challenge to Materials Researchers: Evaluating Materials Relative to the DOE Technical Targets

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Use Material Properties to Estimate DOE Technical Targets

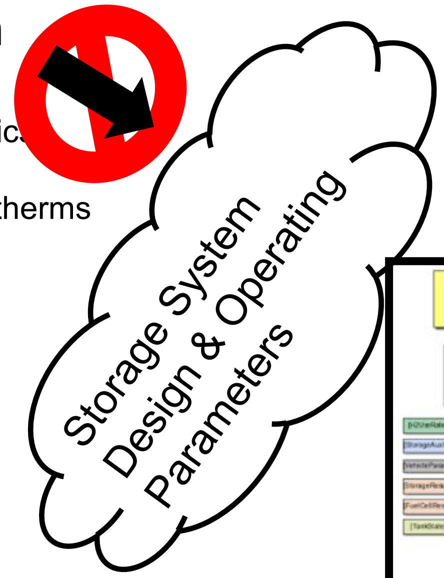
DOE Technical Targets

- Gravimetric & Volumetric Capacity
- Durability & Operability
  - Operating Temperature and Pressure
  - On-Board Efficiency
- Charging/Discharging Rates
  - Startup
  - Refueling

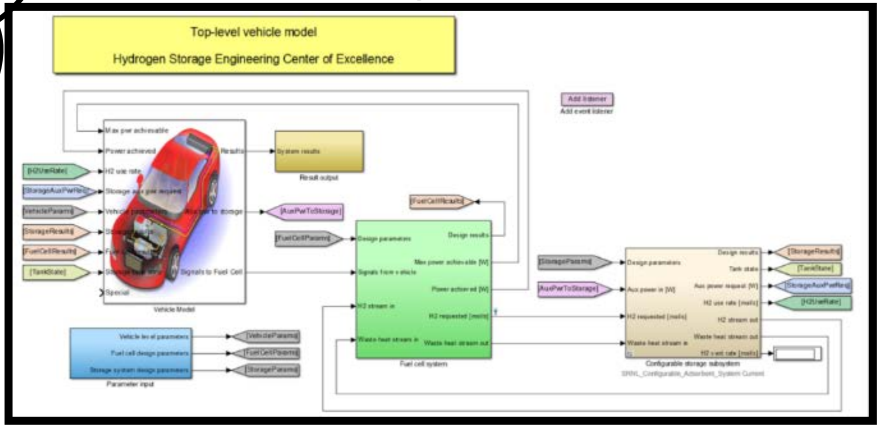
Relevance – Original Framework Does Not Provide Entire Solution

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms



Modeling Framework



DOE Technical Targets

Gravimetric & Volumetric Capacity
Durability & Operability
- Operating Temperature and Pressure
- On-Board Efficiency

Charging/Discharging Rates
- Startup
- Refueling

Relevance – Focus: Improve Model Utilities for Materials Researchers

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Isotherm Fitting Tool

DA Parameters

Improved Website

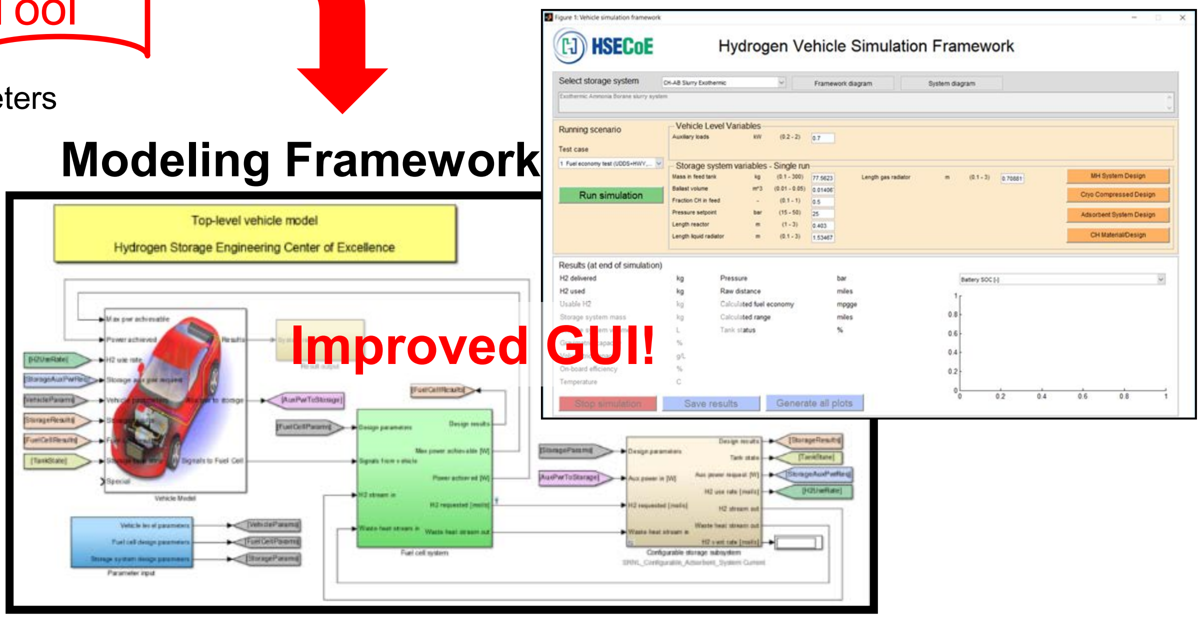
Stand Alone System Design Tools

Component and System Mass & Volume

Stand-Alone Values

Estimated Gravimetric & Volumetric Capacity

Modeling Framework



Improved GUI!

DOE Technical Targets

Gravimetric & Volumetric Capacity
Durability & Operability
- Operating Temperature and Pressure
- On-Board Efficiency

Charging/Discharging Rates
- Startup
- Refueling

Approach – Modeling Tools Available / In Progress

Finite Element Models:

Metal Hydride (MH)	SRNL	Tank Heat and Mass Transfer Models
Adsorbent (AD) – HexCell	SRNL	Tank Heat and Mass Transfer Models
Adsorbent (AD) – MATI	SRNL	Completed

Framework Model with:

Physical Storage	UTRC/NREL	Estimate performance of light-duty vehicles with four drive cycles for each storage system
Metal Hydride (MH)	UTRC/SRNL/NREL	Estimate performance of light-duty vehicles with four drive cycles for each storage system
Chemical Hydrogen (CH)	PNNL/NREL	Estimate performance of light-duty vehicles with four drive cycles for each storage system
Adsorbent (AD)	SRNL/NREL	Estimate performance of light-duty vehicles with four drive cycles for each storage system
Compressed/Cryo-Compressed H_2	SRNL/NREL	In Progress

Stand-alone System Design Tool:

Adsorbent (AD)	SRNL	Updated
Chemical Hydrogen (CH)	PNNL	Updated
Metal Hydride (MH)	PNNL	Completed
Compressed/Cryo-Compressed H_2	SRNL	In Progress

Additional Tool / Models:

MH Acceptability Envelope	SRNL	Evaluate Material Properties
Tank Volume/Cost Model	PNNL	Estimate tank material, design and cost
AD Isotherm Fitting Tool	SRNL	Completed, working on Version 2

Accomplishments and Progress – Improved Website Access and Support

HSECoE website:
http://hsecoe.org/

Model Support and Feedback:
HSECoE@nrel.gov

Improved model access/description

Estimate All Input Parameters Needed for the Framework

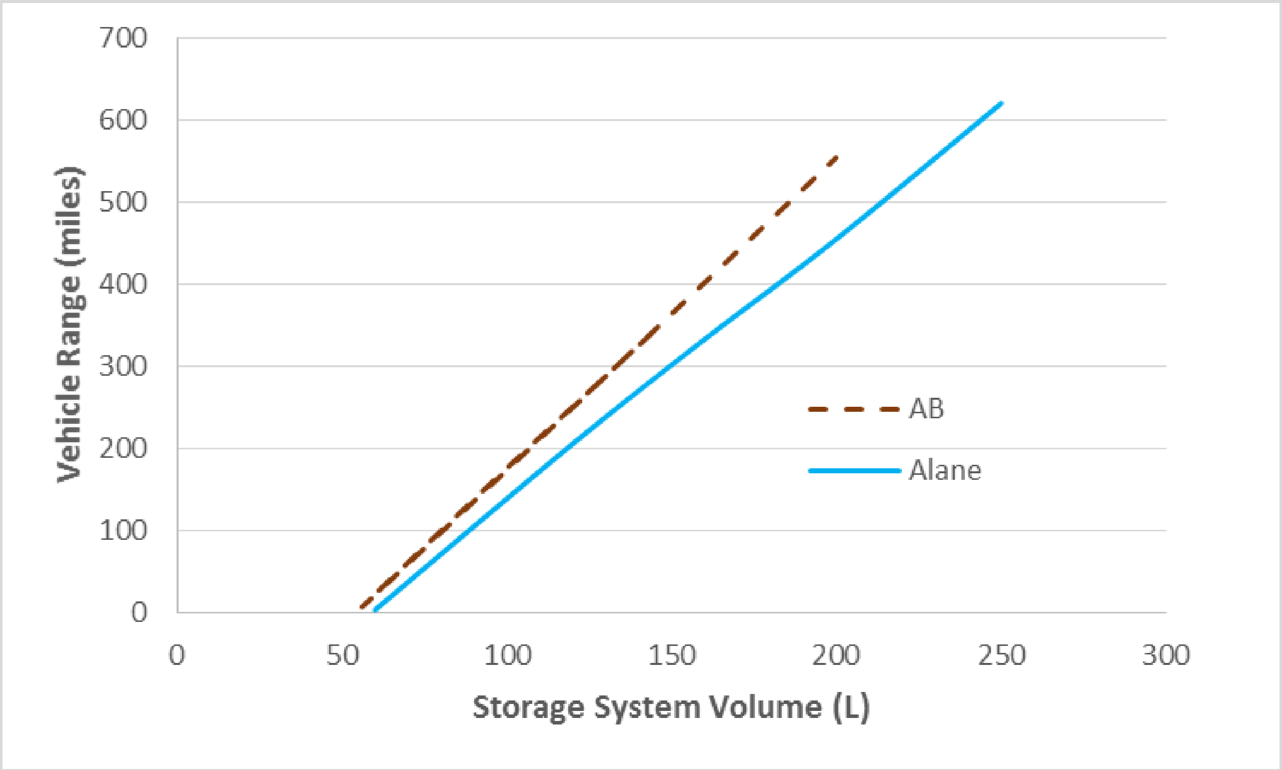
Design Tool Benefits:

- **Availability (No Simulink license required)**
- **Uses inputs measured by materials researchers to calculate Framework parameters**
- **Estimates system mass and volume for preliminary comparison to the DOE Technical Targets**
- **Can be run separate or can be run as a GUI within the framework**

Accomplishments and Progress – Chemical Hydrogen (CH) Stand-Alone System Design Tool

Additional capability this year

- Volume-based vs. Original useable H_2-based estimate
- Use calculated useable H_2 in Framework to estimate vehicle range



Accomplishments and Progress – Adsorbent (AD) Stand-Alone System Design Tool

Updates and Additional Capability this year

- Extended system design options to room temperature and cold-gas temperature system design options
  - With original cryogenic temperature system operation
- UNILAN-based system design formulation (In Progress)
  - With original Dubinin-Astakhov (D-A) system design formulation
- Total H_2 storage system volume-based system design
  - With original useable H2-based system designs
- Use estimate system design parameters within the Framework to estimate vehicle performance

Accomplishments and Progress – Representative Results for ADS

Adsorbent Material	Gravimetric Capacity [g_{H2}/g_{sys}]	Volumetric Capacity [g_{H2}/L_{sys}]	Source
MOF-5 Powder [130 kg/m^3]	0.0338 g_{H2}/g_{sys}	18.6 g_{H2}/L_{sys}	SRNL / HSECoE
MOF-5 Compact [406 kg/m^3]	0.0314 g_{H2}/g_{sys}	21.3 g_{H2}/L_{sys}	SRNL / HSECoE
MOF-5 Powder [200 kg/m^3]	0.0332 g_{H2}/g_{sys}	19.6 g_{H2}/L_{sys}	SRNL / HSECoE
UMCM-9 Powder* [200 kg/m^3]	**0.0345 g_{H2}/g_{sys}**	20.5 g_{H2}/L_{sys}	Ford / U. of Michigan
MOF-177 Powder* [200 kg/m^3]	0.0340 g_{H2}/g_{sys}	20.2 g_{H2}/L_{sys}	Ford / U. of Michigan
SNU-70 Powder* [200 kg/m^3]	0.0341 g_{H2}/g_{sys}	20.2 g_{H2}/L_{sys}	Ford / U. of Michigan
DUT-23 (Co) Powder* [200 kg/m^3]	0.0340 g_{H2}/g_{sys}	20.2 g_{H2}/L_{sys}	Ford / U. of Michigan
IRMOF-20 Powder* [200 kg/m^3]	0.0336 g_{H2}/g_{sys}	19.9 g_{H2}/L_{sys}	Ford / U. of Michigan

***Special thanks to Ford and the University of Michigan for sharing their data.**

<u>System Design Assumptions</u>:

- Operating Conditions: 80 K, 100 bar to 160 K, 5 bar
- 5.6 kg of usable hydrogen (~5.71 kg of actual hydrogen storage)
- Type 1 aluminum pressure vessel
- LN_2 pressure vessel chiller channel thickness of 9.525 mm
- Uniform insulation thickness of 23 mm, with a 2 mm outer aluminum shell

Accomplishments and Progress – Metal Hydride (MH) Stand-Alone System Design Tool

Predict the mass and volume of a MH-based H_2 storage system for light duty vehicles

- Developed in MATLAB and converted to an executable file.
- Microsoft Excel Input and Output
  - Input parameters: H2 capacity, Cp, density, ΔH, ΔS, k
  - Results: System mass and volume, tank length and volume
- Design Tool Steps:
  - van't Hoff equation determines if fuel cell waste heat can be used (~85°C) or hydrogen combustor is required for > 5 atm equilibrium pressure requirement
  - MATLAB MHAE estimates cooling tube spacing required during refueling (5 minute refueling)
  - Calculate total mass and volume of tank interior (MT + tubes)
  - Tank Cost/Volume Model (estimates thickness and mass of tank)
  - Include mass and volume of BOP (with/without combustor)

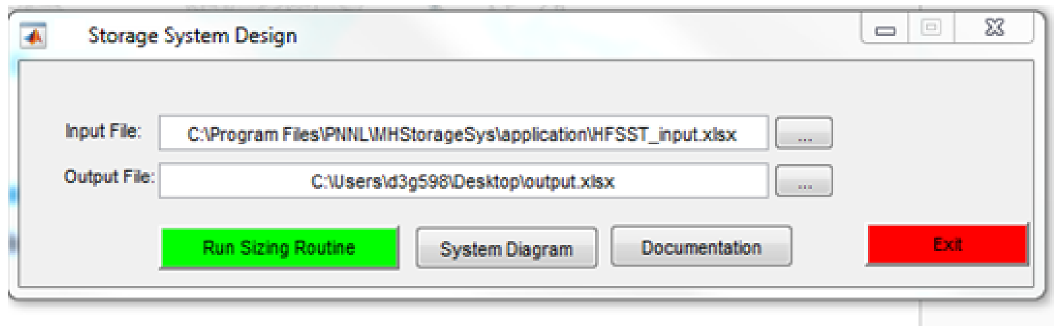
Accomplishments and Progress – Input Information for MH Stand-Alone System Design Tool

Material Properties			
Name	**Value**	**Units**	**Description**
hydcap	0.08	decimal fraction	Hydride Carrying capacity
kbed	6	W/m-K	Thermal Conductivty of Hydride Bed
rhobed	600	kg/m^3	Density of Hydride Bed
dH	-30000	J/mol	Enthalpy per mole H2
dS	-110	J/mol-K	Entropy
dHcombust	241950	J/mol	Enthalpy of Combustion H2
WH2	0.002	kg/mol	Molar Mass H2
Rgas	8.314	J/mol-K	Universal Gas Constant

System Parameters			
Name	**Value**	**Units**	**Description**
dmH2	5.6	kg	mass of hydride to add to tank
d_tube	0.01	m	Coolant tube external radius
th_tube	0.00089	m	Coolant tube thickness
dT	45	K	Acceptable hydride temperature rise during refueling
PH2hi	100	atm	Upper Hydrogen Operating Pressure
PH2lo	5	atm	Lower Hydrogen Operating Pressure
HemObl	1	option	Hemispherical endcap option
Type	1	option	Material Option 1 = 6061-T6 2 = 316 SS 3 = Composite Type III (AL liner) 4 = Composite Type IV (plastic liner)
L/d	4	decimal fraction	Desired Ltank over dtank Enter Zero to Calculate
Ltube	0	m	Desired tank length Enter 0 to calculate
dtank	0	m	Desired tank inner diameter Enter 0 to Calculate
dt	300	seconds	Target Refueling time (300 s = DOE 2020 target)
Vessel	0	option	design only tank = 0, no insulation
th_Ins	0	m	Insulation thickness
eff	0.7	decimal fraction	Combustion Efficiency if required

Accomplishments and Progress – Output Results for MH Stand-Alone System Design Tool

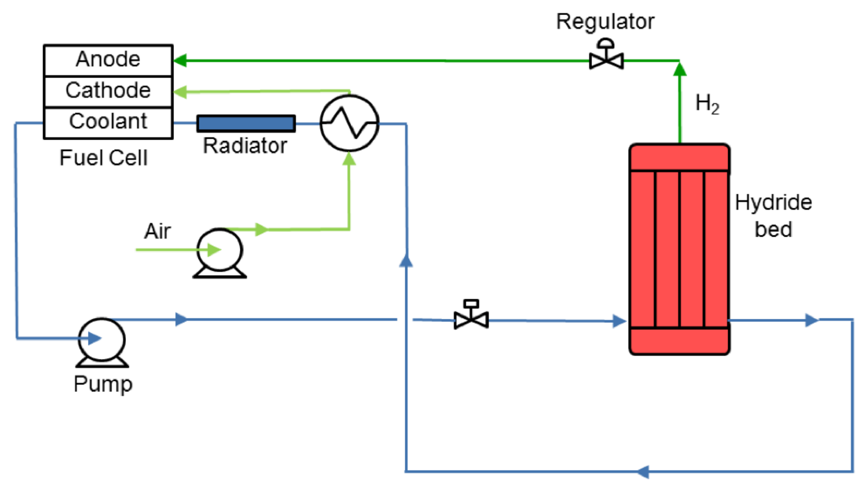
Model Operator Interface



Results Excel Table

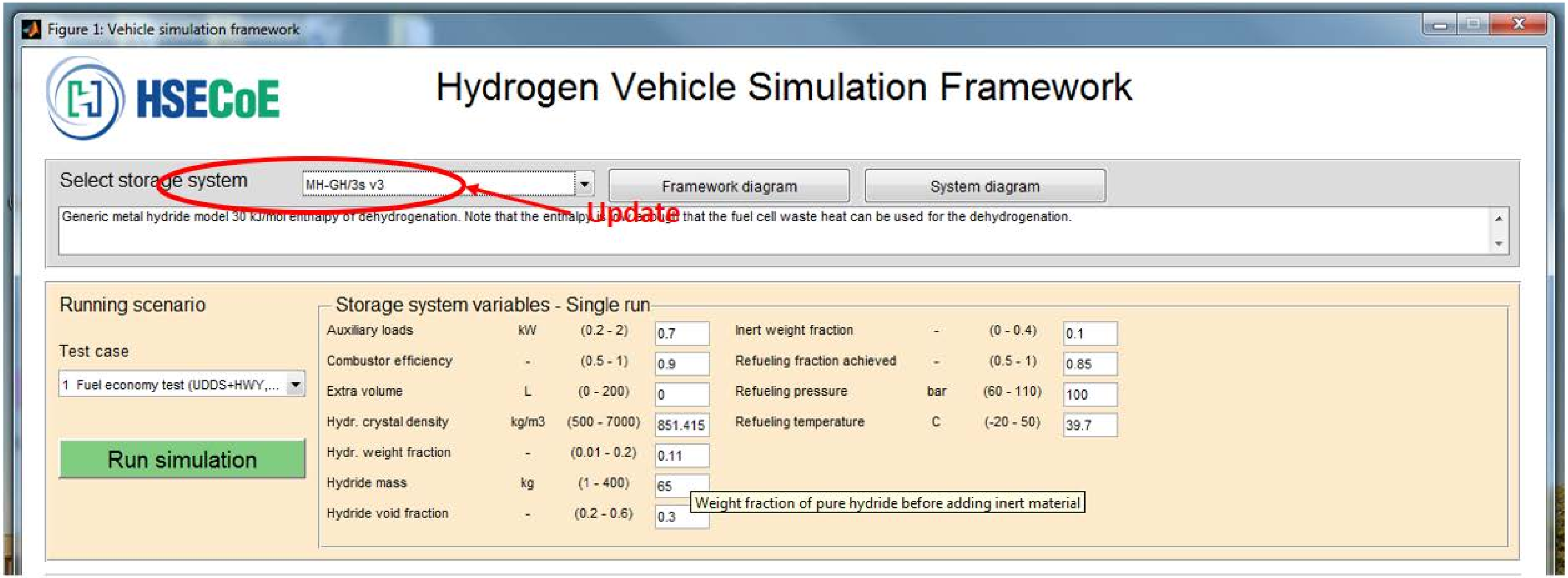
System mass (kg)	192
System volume (m3)	0.249
Combustor y=1/n=0	0
Mass H2 Burned (kg)	0
Tank Outer Diameter (m)	0.413
Tank Length (m)	1.96
Number of coolant Tubes	56
Total Hydride Mass (kg)	70
Percentage of DOE 2020 Gravimetric Target (%)	64
Percentage of DOE 2020 Volumetric Target (%)	75

System Diagram

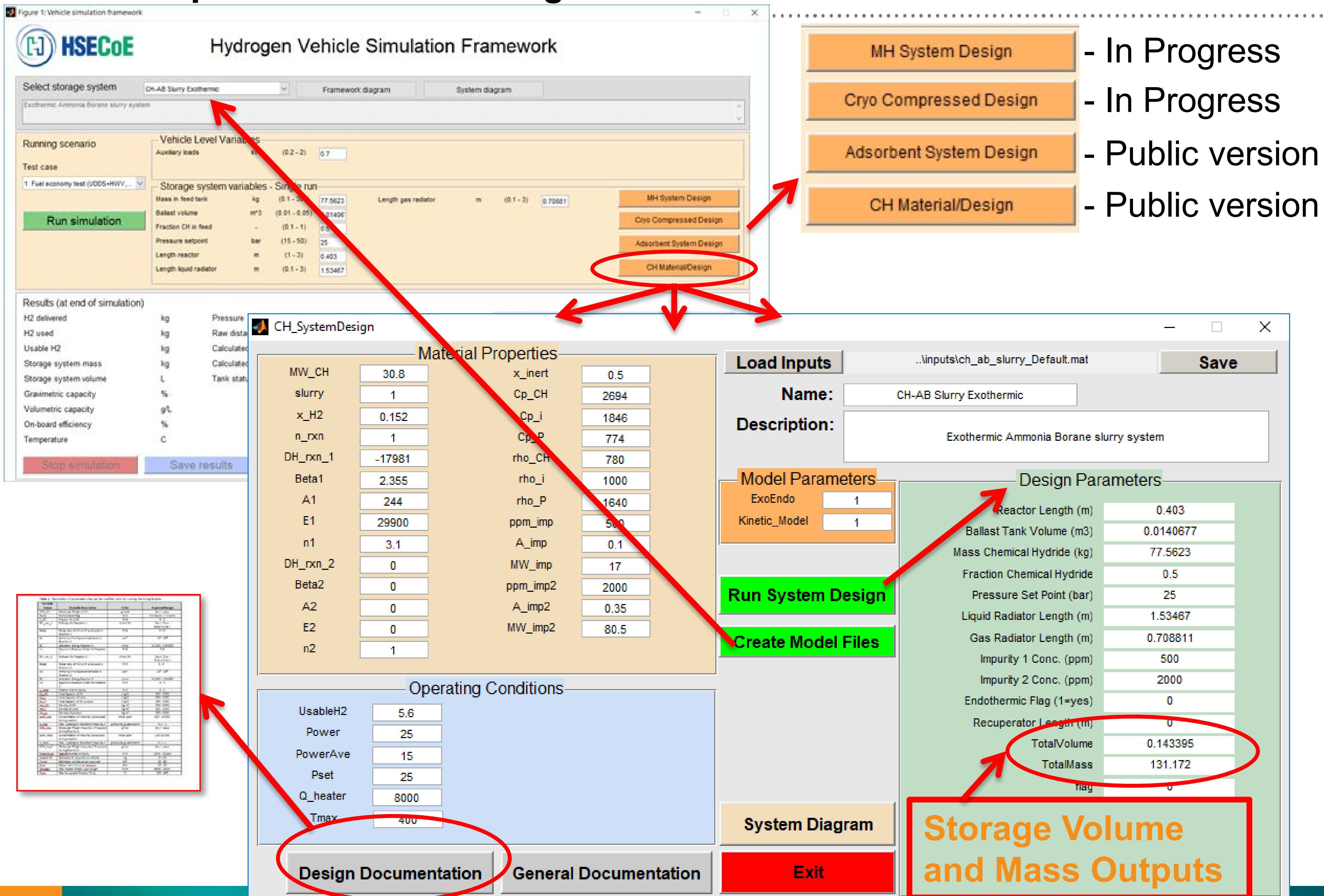


Accomplishments and Progress – Integration of the Updated MH Model into the Full Vehicle Framework

- **Perform beta testing of the MH design tool, produce an executable file, and upload onto the HSECoE website with appropriate documentation**
- **Update MH storage system in framework to allow alternative material evaluation**
    - Currently a generic model with 30 kJ/mol enthalpy and only fuel cell waste heat required for dehydrogenation



Accomplishments and Progress – Vehicle Framework GUI



Accomplishments and Progress – Chemical Hydrogen Storage

Variables/Settings Stored in the Matlab files

Example filename: **ch_ab_slurry_sys.mat**

Stores Matlab structure variable, HS, with info needed to run in Vehicle Framework

Variables - HS

1x1 struct with 12 fields

Field	Value
Name	'CH-AB Slurry Exothermic'
BlockChoice	'PNNL Exothermic AB Slurry'
DiagramFile	'ch_ab_and_alane_slurry_diagram.png'
Description	'Exothermic Ammonia Borane slurry system'
InitScriptFile	'CH_RunInputFile.m'
MatProps	1x27 struct
OpCond	1x6 struct
ModelParams	1x2 struct
Sized	1x1 struct
DesignParams	1x14 struct
Vars	1x7 struct
OutVars	1x3 struct

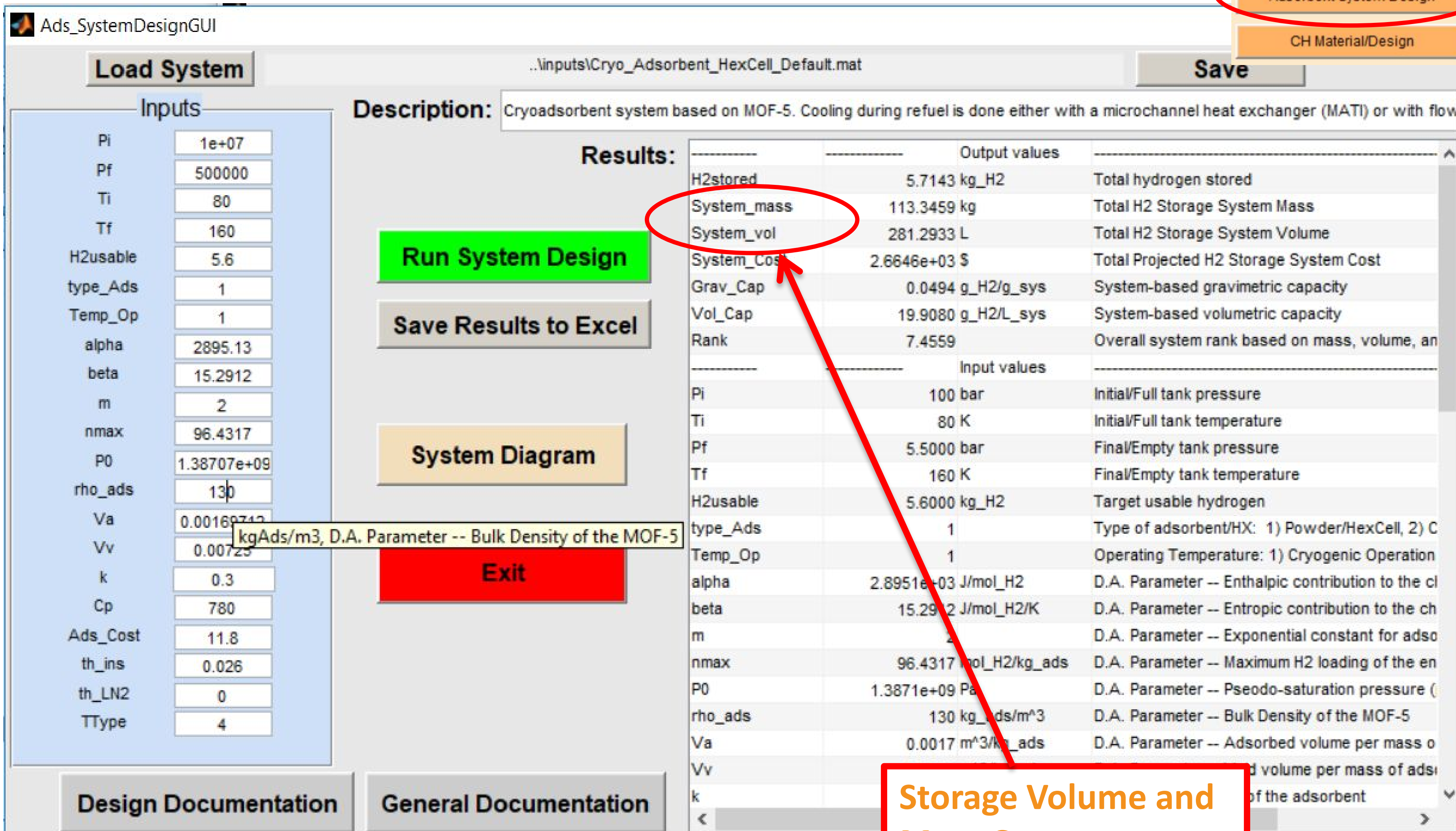
Variables - HS.DesignParams

1x14 struct with 3 fields

Fields	Name	Value	Description
1	'Reactor Length (m)'	0.4030	'Reactor Length (m)'
2	'Ballast Tank Volume (m3)'	0.0141	'Ballast Tank Volume (m3)'
3	'Mass Chemical Hydride (kg)'	77.5623	'Mass Chemical Hydride (kg)'
4	'Fraction Chemical Hydride'	0.5000	'Fraction Chemical Hydride'
5	'Pressure Set Point (bar)'	25	'Pressure Set Point (bar)'
6	'Liquid Radiator Length (m)'	1.5347	'Liquid Radiator Length (m)'
7	'Gas Radiator Length (m)'	0.7088	'Gas Radiator Length (m)'
8	'Impurity 1 Conc. (ppm)'	500	'Impurity 1 Conc. (ppm)'
9	'Impurity 2 Conc. (ppm)'	2000	'Impurity 2 Conc. (ppm)'
10	'Endothermic Flag (1=yes)'	0	'Endothermic Flag (1=yes)'
11	'Recuperator Length (m)'	0	'Recuperator Length (m)'
12	'TotalVolume'	0.1434	'Total Volume (m^3)'
13	'TotalMass'	131.1720	'Total Mass (kg)'
14	'flag'	0	'1=too hot, 2=reactor too long'

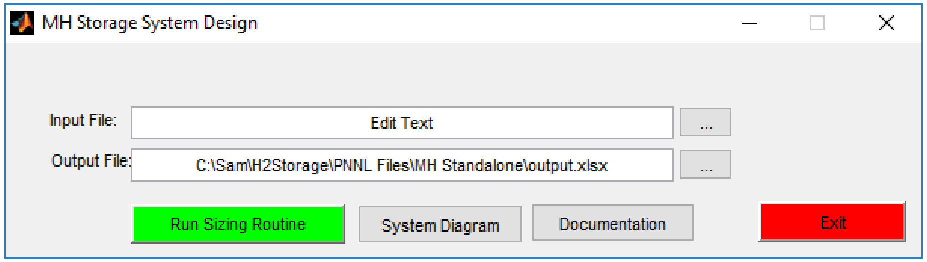
Accomplishments and Progress – Adsorbent System Design Tool in the Framework

MH System Design
Cryo Compressed Design
Adsorbent System Design
CH Material/Design



Storage Volume and Mass Outputs

Accomplishments and Progress – Metal Hydride Tool Integration with the Vehicle Framework



Input file

	A	B	C	D
1	**Metal Hydride Storage Design Tool Input Sheet**			
2				**Material Properties**
3	**Name**	**Value**	**Units**	**Description**
4	hydcap	0.08	decimal fraction	Hydride Carrying capacity
5	kbed	6	W/m-K	Thermal Conductivty of Hydride Bed
6	rhobed	600	kg/m^3	Density of Hydride Bed
7	dH	-30000	J/mol	Enthalpy per mole H2
8	dS	-110	J/mol-K	Entropy
9	dHcombust	241950	J/mol	Enthalpy of Combustion H2
10	WH2	0.002	kg/mol	Molar Mass H2
11	Rgas	8.314	J/mol-K	Universal Gas Constant
12				**System Parameters**
13	**Name**	**Value**	**Units**	**Description**
14	dmH2	5.6	kg	mass of hydride to add to tank
15	r	0.01	m	Coolant tube external radius
16	th_tube	0.00089	m	Coolant tube thickness
17	dT	45	K	acceptable hydride temperature rise during refueling
18	PH2hi	100	atm	Upper Hydrogen Operating Pressure
19	PH2lo	5	atm	Lower Hydrogen Operating Pressure
20	HemObl	1	option	Hemispherical endcap option
21	Type	1	option	Material Option 1 = 6061-T6 2 = 316 SS 3 = Composite Type III (AL liner) 4 = Composite Type IV (plastic liner)
22	L/d	4	decimal fraction	Desired Ltank over dtank Enter Zero to Calculate
23	Ltube	0	m	desired tank length Enter 0 to calculate
24	dtank	0	m	desired tank inner diameter Enter 0 to Calculate
25	dt	300	seconds	Target Refueling time (300 s = DOE 2020 target)
26	Vessel	0	option	design only tank = 0, no insulation
27	th_Ins	0	m	Insulation thickness
28	eff	0.7	decimal fraction	Combustion Efficiency if required
29				
30	Options that should be specified			
31	Options that can be left at the default values			

Output file

	A	B
1	System mass (kg)	192.6501
2	System volume (m3)	0.249515
3	Combustor y=1/n=0	0
4	Mass H2 Burned (kg)	0
5	Tank Outer Diameter (m)	0.413082
6	Tank Length (m)	1.963682
7	Number of coolant Tubes	56
8	Total Hydride Mass (kg)	70
9	Percentage of DOE 2020 Gravimetric Target (%)	64.5961
10	Percentage of DOE 2020 Volumetric Target (%)	74.81179

Accomplishments and Progress – Model Website Analytics (through April 2018)

Users
Sessions > 10 sec
422

New Users
Sessions > 10 sec
383

Sessions
Sessions > 10 sec
567

Number of Sessions per User
Sessions > 10 sec
1.34

Pageviews
Sessions > 10 sec
3,304

Pages / Session
Sessions > 10 sec
5.83

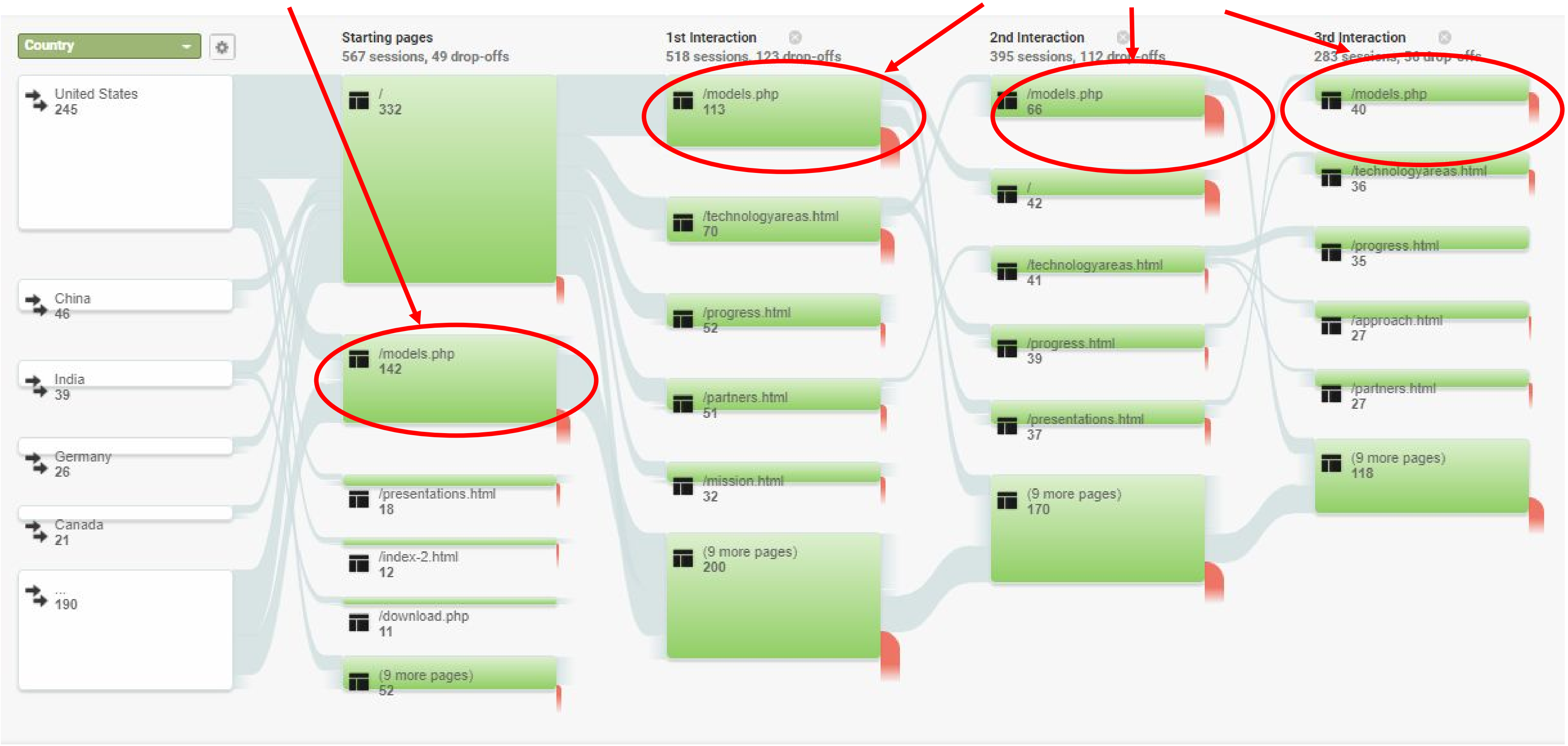
Avg. Session Duration
Sessions > 10 sec
00:06:41

Bounce Rate
Sessions > 10 sec
0.00%

Accomplishments and Progress – Model Website Analytics Web Flow

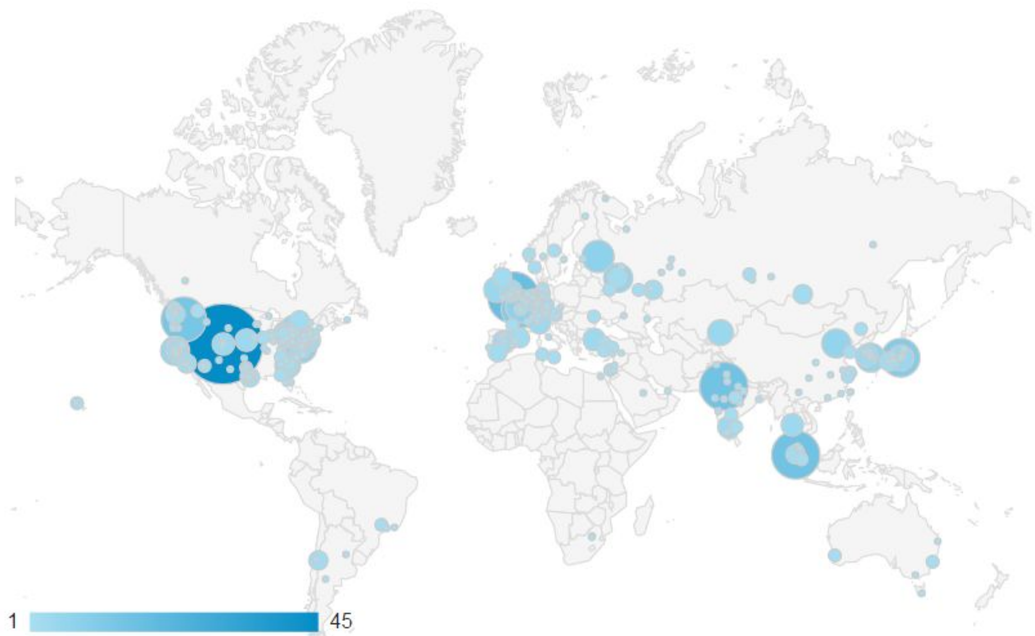
25% of users go directly to modeling webpage

Largest fraction of subsequent interactions are to the modeling webpage



Website users are going to the model webpage

Accomplishments and Progress – Model Website Analytics



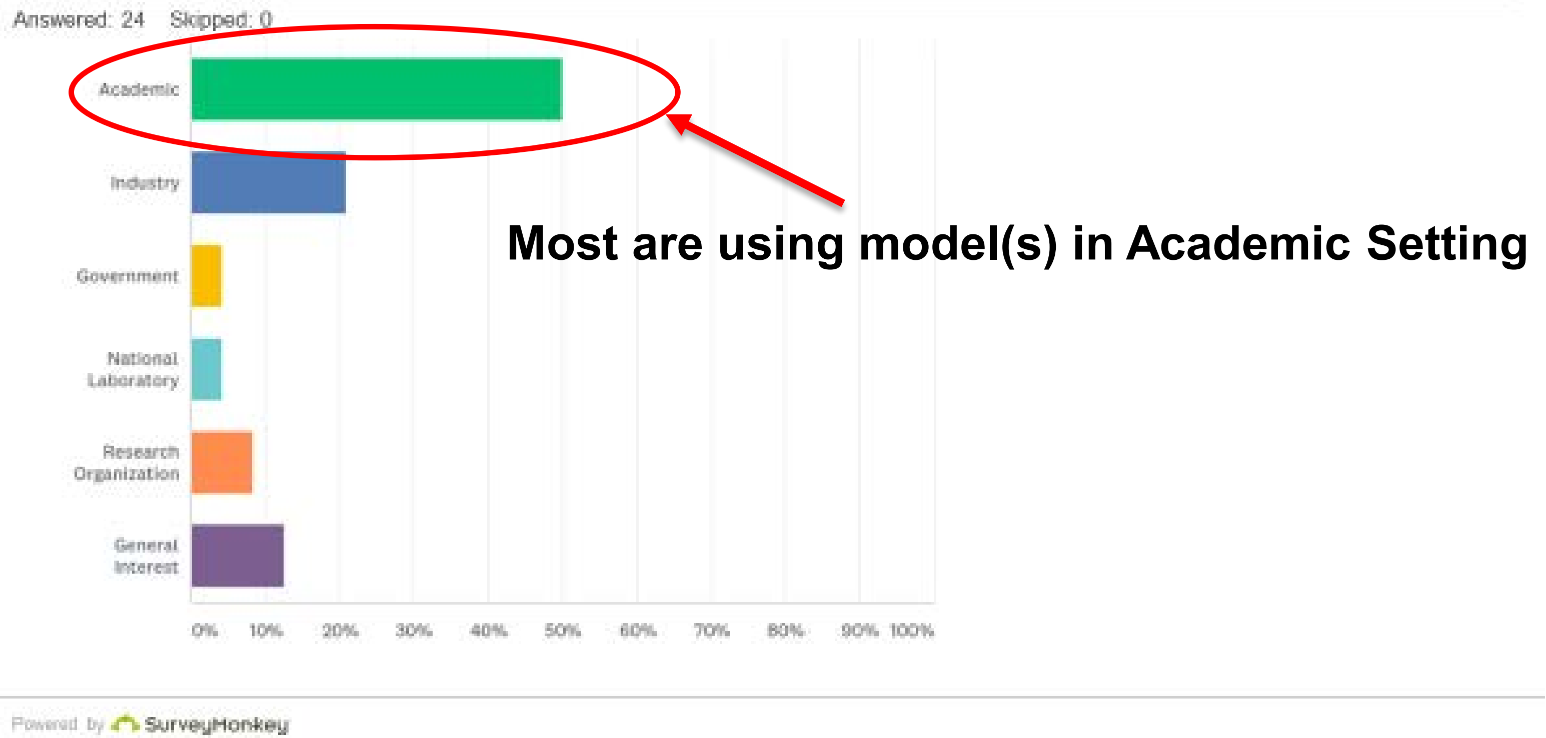
MODEL	DOWNLOADS (Since AMR17)
H_2 Storage Tank Mass and Cost Model	194 (44)
MHAE Model	60 (14)
MHFE Model	92 (18)
Vehicle Simulator Framework Model	138 (31)
CH System Design Standalone	18 (18)
Adsorbent System Design Standalone	18 (18)
MH System Design Standalone	New

44 new downloads of the H2 Storage Tank Mass and Cost Model since April, 2017.

Accomplishments and Progress – Survey on H_2 Storage Models (December 2017)

- **For each model: questions on usage frequency, value, issues**
- **Sent to email list compiled through hsecoe.org model downloads**
  - 229 unique recipients, 11 bounced, 24 responses
  - 4 outside responders willing to work/share material data with us

Q1: In what type of setting are you using the hydrogen storage model(s)?



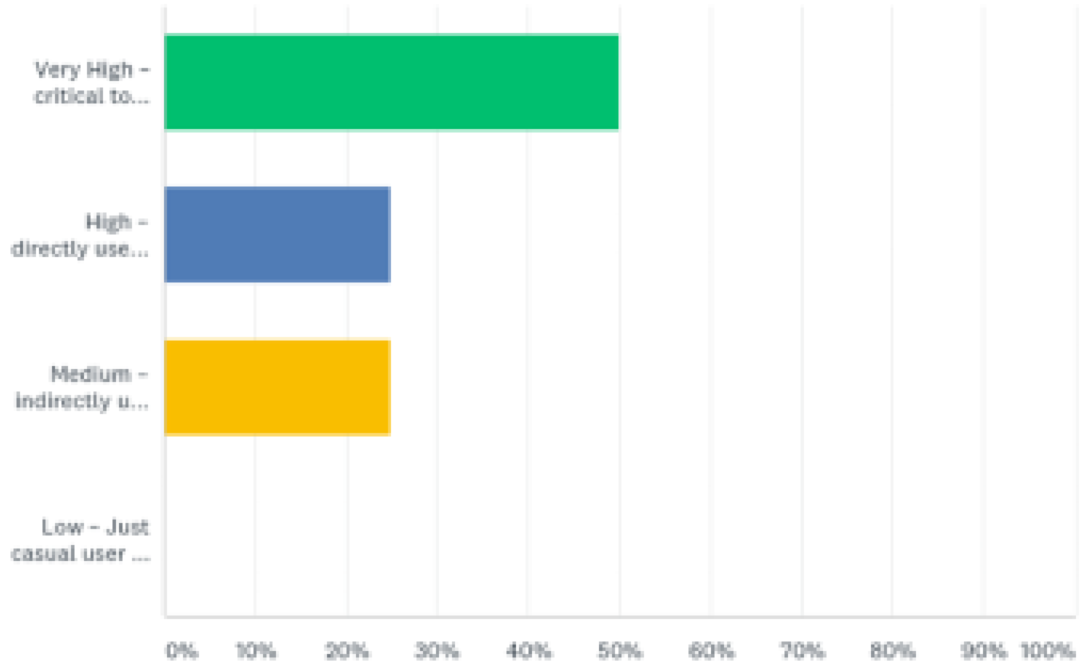
Most are using model(s) in Academic Setting

Accomplishments and Progress – Survey Example Results for Vehicle Framework

H2 Vehicle Simulation Framework

Q4: How would you rate the value of the model results?

Answered: 4 Skipped: 20



Powered by SurveyMonkey

AMR Comments

2017 AMR Comment	2018 Response/Approach
The investigators should recognize other team members of the HSECoE that have contributed significantly to the development of these models. New model should be vetted with the HSECoE team members.	Acknowledgments will be added to the web site, presentations and papers. HSECoE team member have been engaged on new model development throughout the term of this project and that will continue as appropriate.
The team should consider including raw test data that have been collected by the HSECoE partners.	Without permission from HSECoE partners, we cannot post their raw test data. Assuming permission can be obtained, a section will be added to www.hsecoe.org where raw test data is made available.
It was not clear where and how different heat removal strategies could be explored within their models.	The current models are written to evaluate hydrogen storage materials. In the vehicle framework, the material's thermal conductivity and specific heat are used to evaluate heat removal strategies in coordination with the internal heat exchanger designs.
The lack of feedback from outside users is a project weakness	Evaluating materials from non-HSECoE members such as HyMARC and other, for example: -- Mike Veenstra, Ford Motor Co. -- Don Siegel, University of Michigan -- Jeff Long, UC Berkeley Have also conducted a user feedback survey this year.

Collaborations

Organization	Relationship	Type	Responsibility
NREL	Team Member	Federal Lab	Update Website and Framework
SRNL	Team Member	Federal Lab	Adsorbent and Compressed Gas Modeling
PNNL	Team Member	Federal Lab	Chemical Hydrogen and Metal Hydride Modeling
Ford	Consultant	Industry	Beta Testing, Fuel Cell Model, Adsorption Data
RCB Hydrides LLC	Consultant	Industry	Beta Testing, H_2 Storage Expertise
University of Michigan	Material Developer	Academia	Adsorption Data
University of California Berkeley	Material Developer	Academia	Adsorption Data
Purdue University	Material Developer	Academia	Chemical Hydrogen Storage Reaction Rate
HyMARC	Material Research	Federal Lab / Collaboration	Material development

Remaining Challenges and Barriers

- Increase the use of the models by material developers
  - *Expand the capability of the models to include other kinetic and thermodynamic expressions*
  - *Simplify the model use for non-modelers*
- Increase the use of the models by systems engineers
  - *Potential expansion of the model capabilities to other vehicle classes*
- Demonstrate the model's utility to other researchers
  - *Applying the models to their applications*
- Find available data to validate the model

Proposed Future Work – Recent Past and Proposed Future Milestones/Deliverables

Deliverable		Date
FY17 Q3	Update web models: Stand-Alone System Design Tools, Isotherm Fitting Tool, GUI/framework.	Complete
FY17 Q4	Develop MH and compressed gas storage system design tools	Complete
FY18 Q1	Provide update on web portal activity—web site hits and time on site, web site use locations and model down loads.	Complete
FY18 Q2	Update Adsorbent and CH models with any newly available data from DOE program and/or the hydrogen storage research community.	Complete
FY18 Q3	**SMART Milestone –** Alternative Storage System Formulations: Update the hydrogen storage equations for additional theoretical formulation(s). (i.e. Unilan or 2-state Langmuir)	In Progress
FY18 Q4	Update models with any newly available data from DOE program and or the hydrogen storage research community.	In Progress

Any proposed future work is subject to change based on funding levels

Proposed Future Work – Next Steps in Model Development

- Include a vehicle-side refueling model within the framework to address the forecourt requirements and their effect on refueling time and energy needs.
- Include dormancy calculations in all adsorbent design tools.
- Convert Stand-alone Design Tools from .exe to Excel VBA tools.
- Continue to develop volume-based design to target specific vehicle volume limitations/designs and/or, potentially, additional vehicle classes
- Expand model to other vehicle platforms (medium and heavy duty trucks, forklifts, buses, etc.)
- Work with Material Based H_2 Storage Developers to apply models to their materials
- Maintain and enhance existing framework models and track web activity and downloads

Any proposed future work is subject to change based on funding levels

Summary

Relevance	• Provide materials based hydrogen storage researchers with models and materials requirements to assess their material's performance in an automotive application.
Approach	• Improve framework utility by bridging the gap between the information generated by the materials researcher and the parameters required for the framework model.
Technical Accomplishments and Progress	• Developed system estimators for MH, CH, and Adsorbents. • System estimator used with framework GUI and as stand-alone executable. • Developed a stand-alone isotherm data fitting routine for D-A parameters. • Performed Survey • Improved website and model accessibility.
Collaborations	• Project team includes NREL, SRNL, and PNNL. • Consultants from industry participate in team meetings and provide input. • Material developers from academia provide new material properties.
Proposed Future Research	• Expand the use of models by demonstrating their utility with other storage materials, theoretical formulations, and vehicle class options.

Questions?

HSECoE Models on the WEB Team:

Matthew Thornton

David Tamburello

Kriston Brooks

Sam Sprik

With support from Bob Bowman and Mike Veenstra

Adsorption data provided by Ford, University of Michigan, and University of California Berkeley

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