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

Presenter: David Tamburello

Team: Matthew Thornton, Sam Sprik, and Kriston Brooks

June 15, 2018

ST008

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

Timeline

• Start: October 1, 2015
• End: September 30, 2018
• 80% Complete (as of 5/1/18)
  o $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
  o FY16 Funding: $336,000
  o FY17 Funding: $389,000
  o FY18 Funding: $375,000

Partners

[Logos of NREL, SRNL, and Pacific Northwest National Laboratory]

Savannah River National Laboratory
Operated by Savannah River Nuclear Solutions
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

<table>
<thead>
<tr>
<th>Barriers</th>
<th>Model Addressing Barrier</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. System Weight and Volume</td>
<td>System Estimator</td>
</tr>
<tr>
<td>B. System Cost</td>
<td>Tank Volume/Cost Model</td>
</tr>
<tr>
<td>C. Efficiency</td>
<td>Framework Model</td>
</tr>
<tr>
<td></td>
<td>- On-Board Efficiency</td>
</tr>
<tr>
<td></td>
<td>- Fuel Economy</td>
</tr>
<tr>
<td>E. Charging/Discharging Rates</td>
<td>Framework Model</td>
</tr>
<tr>
<td></td>
<td>- Drive cycles</td>
</tr>
<tr>
<td>I. Dispensing Technology</td>
<td>Framework Model</td>
</tr>
<tr>
<td></td>
<td>- Initial and Final System Conditions</td>
</tr>
<tr>
<td>K. System Life-Cycle Assessment</td>
<td>All Models</td>
</tr>
</tbody>
</table>
Relevance – **Challenge to Materials Researchers: Evaluating Materials Relative to the DOE Technical Targets**

**Materials Research**

- H₂ 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

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Relevance – Original Framework Does Not Provide Entire Solution

Materials Research
H₂ Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Storage System Design & Operating Parameters

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

- H₂ 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

- Improved GUI!

Stand-Alone System Design Tools

- Component and System Mass & Volume
- Stand-Alone Values

Estimated Gravimetric & Volumetric Capacity

Improved Website

- Isotherm Fitting Tool
- DA Parameters
### Approach – Modeling Tools Available / In Progress

#### Finite Element Models:
- **Metal Hydride (MH)**: SRNL
- **Adsorbent (AD) – HexCell**: SRNL
- **Adsorbent (AD) – MATI**: SRNL

#### Framework Model with:
- **Physical Storage**: UTRC/NREL
- **Metal Hydride (MH)**: UTRC/SRNL/NREL
- **Chemical Hydrogen (CH)**: PNNL/NREL
- **Adsorbent (AD)**: SRNL/NREL
- **Compressed/Cryo-Compressed H₂**: SRNL/NREL

#### Stand-alone System Design Tool:
- **Adsorbent (AD)**: SRNL
- **Chemical Hydrogen (CH)**: PNNL
- **Metal Hydride (MH)**: PNNL
- **Compressed/Cryo-Compressed H₂**: SRNL

#### Additional Tool / Models:
- **MH Acceptability Envelope**: SRNL
- **Tank Volume/Cost Model**: PNNL
- **AD Isotherm Fitting Tool**: SRNL

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**Estimate performance of light-duty vehicles with four drive cycles for each storage system**

- **Tank Heat and Mass Transfer Models**
- **Evaluate Material Properties**
- **Estimate tank material, design and cost**
- **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

Hydrogen Storage Engineering CENTER OF EXCELLENCE

Home Mission Partners Approach Technology Areas Progress Technical Gap Models Contact

Models

- Hydrogen Vehicle Simulation Framework
- 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-SAM)
- Hydrogen Storage Tank Analysis and Cost Estimation Model
- CH Storage System Design - Standalone
- Adsorbent Storage System Design - Standalone
- Downloads
- Model Support and Feedback
- Publications, Presentations and Model Verification
- News

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Accomplishments and Progress – **Stand-Alone Design Tools**

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 H₂-based estimate
- Use calculated useable H₂ in Framework to estimate vehicle range

![Graph showing vehicle range vs. storage system volume](image-url)
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
  o With original cryogenic temperature system operation
• UNILAN-based system design formulation (In Progress)
  o With original Dubinin-Astakhov (D-A) system design formulation
• Total $\text{H}_2$ storage system volume-based system design
  o 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

<table>
<thead>
<tr>
<th>Adsorbent Material</th>
<th>Gravimetric Capacity [g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}]</th>
<th>Volumetric Capacity [g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}]</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOF-5 Powder [130 kg/m\textsuperscript{3}]</td>
<td>0.0338 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>18.6 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>SRNL / HSECoE</td>
</tr>
<tr>
<td>MOF-5 Compact [406 kg/m\textsuperscript{3}]</td>
<td>0.0314 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>21.3 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>SRNL / HSECoE</td>
</tr>
<tr>
<td>MOF-5 Powder [200 kg/m\textsuperscript{3}]</td>
<td>0.0332 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>19.6 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>SRNL / HSECoE</td>
</tr>
<tr>
<td>UMCM-9 Powder* [200 kg/m\textsuperscript{3}]</td>
<td>0.0345 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>20.5 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>Ford / U. of Michigan</td>
</tr>
<tr>
<td>MOF-177 Powder* [200 kg/m\textsuperscript{3}]</td>
<td>0.0340 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>20.2 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>Ford / U. of Michigan</td>
</tr>
<tr>
<td>SNU-70 Powder* [200 kg/m\textsuperscript{3}]</td>
<td>0.0341 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>20.2 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>Ford / U. of Michigan</td>
</tr>
<tr>
<td>DUT-23 (Co) Powder* [200 kg/m\textsuperscript{3}]</td>
<td>0.0340 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>20.2 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>Ford / U. of Michigan</td>
</tr>
<tr>
<td>IRMOF-20 Powder* [200 kg/m\textsuperscript{3}]</td>
<td>0.0336 g\textsubscript{H\textsubscript{2}}/g\textsubscript{sys}</td>
<td>19.9 g\textsubscript{H\textsubscript{2}}/L\textsubscript{sys}</td>
<td>Ford / U. of Michigan</td>
</tr>
</tbody>
</table>

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

System Design Assumptions:

- 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\textsubscript{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 H₂ 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)
## Material Properties

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydcap</td>
<td>0.08</td>
<td>decimal</td>
<td>Hydride Carrying capacity</td>
</tr>
<tr>
<td>kbed</td>
<td>6</td>
<td>W/m-K</td>
<td>Thermal Conductivity of Hydride Bed</td>
</tr>
<tr>
<td>rhobed</td>
<td>600</td>
<td>kg/m^3</td>
<td>Density of Hydride Bed</td>
</tr>
<tr>
<td>dH</td>
<td>-30000</td>
<td>J/mol</td>
<td>Enthalpy per mole H2</td>
</tr>
<tr>
<td>dS</td>
<td>-110</td>
<td>J/mol-K</td>
<td>Entropy</td>
</tr>
<tr>
<td>dHcombust</td>
<td>241950</td>
<td>J/mol</td>
<td>Enthalpy of Combustion H2</td>
</tr>
<tr>
<td>WH2</td>
<td>0.002</td>
<td>kg/mol</td>
<td>Molar Mass H2</td>
</tr>
<tr>
<td>Rgas</td>
<td>8.314</td>
<td>J/mol-K</td>
<td>Universal Gas Constant</td>
</tr>
</tbody>
</table>

## System Parameters

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

Model Operator Interface

Results Excel Table

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

System Diagram

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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

Storage Volume and Mass Outputs

- In Progress
- In Progress
- Public version
- Public version
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
Accomplishments and Progress – Adsorbent System Design Tool in the Framework

Storage Volume and Mass Outputs
Accomplishments and Progress – **Metal Hydride Tool Integration with the Vehicle Framework**

![MH Storage System Design](image)

### Input file

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Units</th>
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</tr>
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<tbody>
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<tr>
<td>HemObl</td>
<td>1</td>
<td>option</td>
<td>Hemispherical end cap option</td>
</tr>
</tbody>
</table>

### Material Options

- Material Option 1 = 6061-T6
- Material Option 2 = 316 SS
- Material Option 3 = Composite Type III (AL liner)
- Material Option 4 = Composite Type IV (plastic liner)

<table>
<thead>
<tr>
<th>Name</th>
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<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>L/d</td>
<td>4</td>
<td>decimal fraction</td>
<td>Desired Ltank over dtank Enter Zero to Calculate</td>
</tr>
<tr>
<td>Ltube</td>
<td>0</td>
<td>m</td>
<td>Desired tank length Enter 0 to calculate</td>
</tr>
<tr>
<td>dtank</td>
<td>0</td>
<td>m</td>
<td>Desired tank inner diameter Enter 0 to calculate</td>
</tr>
<tr>
<td>dt</td>
<td>300</td>
<td>sec</td>
<td>Target Refueling time (300 s = DOE 2020 target)</td>
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<td>Vessel</td>
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<td>0</td>
<td>m</td>
<td>Insulation thickness</td>
</tr>
<tr>
<td>eff</td>
<td>0.7</td>
<td>decimal fraction</td>
<td>Combustion Efficiency if required</td>
</tr>
</tbody>
</table>

Options that should be specified:
- Type
- L/d
- Ltube
- dtank
- dt
- Vessel
- th_Lns
- eff

Options that can be left at the default values:
- TH_Lns

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

Sessions

- July 2017: 80
- October 2017: 80
- January 2018: 40
- April: 40

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%

New Visitor Returning Visitor
- 10.9%
- 0.0%
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

<table>
<thead>
<tr>
<th>MODEL</th>
<th>DOWNLOADS (Since AMR17)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$ Storage Tank Mass and Cost Model</td>
<td>194 (44)</td>
</tr>
<tr>
<td>MHAE Model</td>
<td>60 (14)</td>
</tr>
<tr>
<td>MHFE Model</td>
<td>92 (18)</td>
</tr>
<tr>
<td>Vehicle Simulator Framework Model</td>
<td>138 (31)</td>
</tr>
<tr>
<td>CH System Design Standalone</td>
<td>18 (18)</td>
</tr>
<tr>
<td>Adsorbent System Design Standalone</td>
<td>18 (18)</td>
</tr>
<tr>
<td>MH System Design Standalone</td>
<td>New</td>
</tr>
</tbody>
</table>

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

Answered: 4  Skipped: 20
# AMR Comments

<table>
<thead>
<tr>
<th>2017 AMR Comment</th>
<th>2018 Response/Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>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.</td>
<td>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.</td>
</tr>
<tr>
<td>The team should consider including raw test data that have been collected by the HSECoE partners.</td>
<td>Without permission from HSECoE partners, we cannot post their raw test data. Assuming permission can be obtained, a section will be added to <a href="http://www.hsecoe.org">www.hsecoe.org</a> where raw test data is made available.</td>
</tr>
<tr>
<td>It was not clear where and how different heat removal strategies could be explored within their models.</td>
<td>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.</td>
</tr>
</tbody>
</table>
| 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.                                                                                                                  |
<table>
<thead>
<tr>
<th>Organization</th>
<th>Relationship</th>
<th>Type</th>
<th>Responsibility</th>
</tr>
</thead>
<tbody>
<tr>
<td>NREL</td>
<td>Team Member</td>
<td>Federal Lab</td>
<td>Update Website and Framework</td>
</tr>
<tr>
<td>SRNL</td>
<td>Team Member</td>
<td>Federal Lab</td>
<td>Adsorbent and Compressed Gas Modeling</td>
</tr>
<tr>
<td>PNNL</td>
<td>Team Member</td>
<td>Federal Lab</td>
<td>Chemical Hydrogen and Metal Hydride Modeling</td>
</tr>
<tr>
<td>Ford</td>
<td>Consultant</td>
<td>Industry</td>
<td>Beta Testing, Fuel Cell Model, Adsorption Data</td>
</tr>
<tr>
<td>RCB Hydrides LLC</td>
<td>Consultant</td>
<td>Industry</td>
<td>Beta Testing, H₂ Storage Expertise</td>
</tr>
<tr>
<td>University of Michigan</td>
<td>Material</td>
<td>Academia</td>
<td>Adsorption Data</td>
</tr>
<tr>
<td>University of California Berkeley</td>
<td>Material Developer</td>
<td>Academia</td>
<td>Adsorption Data</td>
</tr>
<tr>
<td>Purdue University</td>
<td>Material</td>
<td>Academia</td>
<td>Chemical Hydrogen Storage Reaction Rate</td>
</tr>
<tr>
<td>HyMARC</td>
<td>Material</td>
<td>Federal Lab / Collaboration</td>
<td>Material development</td>
</tr>
</tbody>
</table>
Remaining Challenges and Barriers

• Increase the use of the models by material developers
  o *Expand the capability of the models to include other kinetic and thermodynamic expressions*
  o *Simplify the model use for non-modelers*

• Increase the use of the models by systems engineers
  o *Potential expansion of the model capabilities to other vehicle classes*

• Demonstrate the model’s utility to other researchers
  o *Applying the models to their applications*

• Find available data to validate the model
### Proposed Future Work – Recent Past and Proposed Future Milestones/Deliverables

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

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 H₂ 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

<table>
<thead>
<tr>
<th>Relevance</th>
<th>• Provide materials based hydrogen storage researchers with models and materials requirements to assess their material’s performance in an automotive application.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approach</td>
<td>• Improve framework utility by bridging the gap between the information generated by the materials researcher and the parameters required for the framework model.</td>
</tr>
</tbody>
</table>
| 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.