Overview

Timeline
HSECoE start date: FY09
HSECoE end date: FY15
Percent complete: 70%

Budget
Total funding $1.8M
DOE Share 100%
Funding Received in FY12: $110K
Funding for FY13: $100K

Barriers
• System cost
• Charge/discharge rate
• System mass
• Systems volume
• Transient response
• Well-to-power plant efficiency
• Vehicle performance

Partners
Savanna River National Lab (SRNL), 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) the DOE Vehicle Technologies Program.

- 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 tradeoffs 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 an onboard systems.
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, acceleration, 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
Objectives: Energy Analysis

Perform hydrogen storage system energy analysis to evaluate well-to-power-plant (WTPP) efficiency, Energy requirements, hydrogen cost and green house gas (GHG) emissions

- Develop vehicle a level models and obtain fuel economy (FE) figures for energy analysis.
- Obtain data from center partners on storage system designs (mass, volume, operating temperature (T) and pressure (P))/fuel interface/dispensing/station energy requirements.
- Work with other teams (e.g. Hydrogen Delivery and Systems Analysis) and use existing data for H\textsubscript{2} production and distribution and tank production and carbon dioxide equivalent (CO\textsubscript{2}e) emission factors (from GREET, H\textsubscript{2} A, etc.) to calculate WTPP efficiencies etc.
- Adjust model inputs based on changes in storage system design and data to obtain final results.
- FY13 focus is on accounting for and understanding the impact of the thermal management (i.e. flow through cooling design for adsorbents) and off-board regeneration cycles for chemical hydride systems.
## Milestones

<table>
<thead>
<tr>
<th>Date</th>
<th>Milestone or Go/No-Go Decision</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>2/13</td>
<td>NREL will work center partners to set up and run vehicle simulations to evaluate the key volumetric, gravimetric, and on-board efficiency trade-offs over three test cases (drive cycles) and progress towards 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.</td>
<td>100%</td>
</tr>
<tr>
<td>8/13</td>
<td>Provide summary of scaled H2 storage system engineering material property input.</td>
<td>30%</td>
</tr>
<tr>
<td>9/13</td>
<td>Provide HSECoE appropriate engineering properties</td>
<td>30%</td>
</tr>
<tr>
<td>9/13</td>
<td>Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.</td>
<td>50%</td>
</tr>
<tr>
<td>9/13</td>
<td>Calculate and model the well-to-powerplant (WTPP) efficiency for two chemical hydrogen (CH) storage system designs and compare results relative to the 60% technical target.</td>
<td>100%</td>
</tr>
</tbody>
</table>
Approach: Develop HSSIM (Vehicle Model)

Output
- Fuel economy (mpgge) based on EPA adjusted five cycle estimate
- Range (miles) from adjusted mpgge
- Onboard efficiency (%)
- Hydrogen flow (moles/s)
- Vehicle performance (e.g. 0-60 mph time)

Validation

- EPA Urban Dynamometer Driving Schedule

Structure

Drive Cycles

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### Approach: Vehicle Assumptions

**Midsize Car Class (Family Sedan):**

<table>
<thead>
<tr>
<th>Vehicle Attribute</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glider mass(^1)</td>
<td>kg</td>
<td>1,104</td>
</tr>
<tr>
<td>Frontal area</td>
<td>m(^2)</td>
<td>2.2</td>
</tr>
<tr>
<td>Drag coefficient</td>
<td>–</td>
<td>0.29</td>
</tr>
<tr>
<td>Rolling Resistance</td>
<td>–</td>
<td>0.008</td>
</tr>
<tr>
<td>Tires</td>
<td>–</td>
<td>P195/65R15</td>
</tr>
<tr>
<td>Electric Motor</td>
<td>kW</td>
<td>100 (~85% eff.)</td>
</tr>
<tr>
<td>Energy Storage</td>
<td>kW/kWh</td>
<td>20/1 (40-80% SOC)</td>
</tr>
</tbody>
</table>

\(^1\) Excludes fuel cell, hydrogen storage system, electric motor, power electronics, and energy storage system

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**Image:**
- Image of a red sedan
- Image of a white sedan

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**Source:** NATIONAL RENEWABLE ENERGY LABORATORY
A tool used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent assumptions.
Approach: Energy and WTPP Analysis

Utilize H₂A Hydrogen Delivery Scenario Model (HDSAM)

• Standardized Excel spreadsheet tool with the same H₂A approach to cost, energy efficiency and GHG emissions analysis but more complex
• Pre-loaded with current capital costs and utility costs of hydrogen delivery components – pipelines, tube trailers, liquid hydrogen (LH₂) trucks, terminals, refueling stations, etc.
• User specifies a delivery scenario:
  • Urban or city and which city
  • Market penetration (%)
  • Transport mode (to terminal) and distance
  • Distribution mode (terminal to refueling stations)
• Model calculates: delivery cost ($/kg-H₂), energy efficiency (WTPP), and GHGs (gms/mile)
Approach: Energy Analysis Assumptions for HDSAM

Production: Steam Methane Reforming (SMR)
Market: Sacramento, 15% market penetration
Plant (and Regen.): 62 miles (100 km) from city gate
Electricity: U.S. grid
Large scale storage: Geologic, LH$_2$, liquid
Transport: Plant to city gate terminal
  • GH2 – pipeline
  • LH2, liquid carrier – truck
Distribution: City gate terminal to refueling stations – truck
Refueling Station Size: 1000 kg/day maximum (may be limited by one delivery per day or 9% coverage)
Work with engineering center partners to identify potential materials and configurations that can be optimized with the appropriate thermal conductivity, sorption, and mechanical properties needed for integration in a hydrogen storage system.

- Provide measurements of relevant metal organic framework (MOF)-5 samples to validate models.

NREL's Sitaram PCTPro System with Temperature Stability Improvements to Measure Hydrogen Isotherms
Accomplishments: Vehicle Performance Summary-End of Phase I

Simulated vehicle performance results for Phase I hydrogen storage systems with fixed on-board H2 (from framework)

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

Phase I Results from 2012 AMR Presentation

Fixed on-board usable H2 = 5.6kg
### Accomplishments: Vehicle Performance Summary-End of Phase II

Simulated vehicle performance results for Phase II hydrogen storage systems with fixed on-board H2 (from framework)

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

*Preliminary Model Results  **Off Model Calculations

Fixed on-board usable H2 = 5.6kg
Accomplishment: US06-Aggressive Dive Cycle
H2 Delivery Requirements Exothermic AB Slurry

System meets drive cycle demands under aggressive driving conditions
Accomplishment: US06-Aggressive Dive Cycle H2 Delivery Requirements
Endothermic Alana Slurry

System meets drive cycle demands under aggressive driving conditions
### Accomplishment: WTW Storage Systems Results

#### Draft—Preliminary Results

<table>
<thead>
<tr>
<th></th>
<th>WTW H2 Cost ($/kg-H2)</th>
<th>WtW Energy Efficiency (%)</th>
<th>WTW GHG Emissions (gms/mile)</th>
<th>Volumetric Efficiency (gms-H2/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2010 700 bar Gas-250 bar Tube Trailer</td>
<td>$5.28</td>
<td>54.7%</td>
<td>240</td>
<td>25.6</td>
</tr>
<tr>
<td>2010 CcH2 - Liq. H2 Truck</td>
<td>$4.92</td>
<td>43.2%</td>
<td>322</td>
<td>41.8</td>
</tr>
<tr>
<td>2020 700 bar Gas - T520</td>
<td>$3.91</td>
<td>56.4%</td>
<td>230</td>
<td>25.6</td>
</tr>
<tr>
<td>2020 CcH2 - Liq. H2 Truck</td>
<td>$4.49</td>
<td>46.5%</td>
<td>289</td>
<td>41.8</td>
</tr>
<tr>
<td>2020 Liquid AB - Liq. Truck</td>
<td>$13.96</td>
<td>16.5%</td>
<td>915</td>
<td>41.4</td>
</tr>
<tr>
<td>2020 Liquid Alane: Liq. Truck</td>
<td>$7.89</td>
<td>24.7%</td>
<td>642</td>
<td>32.2</td>
</tr>
<tr>
<td>2020 Absorbent 60 bar 80 K gas-T340</td>
<td>$6.00</td>
<td>39.9%</td>
<td>407</td>
<td>24.1</td>
</tr>
</tbody>
</table>
Accomplishment: Isotherm Measurement Method Calibration

Provided isotherm measurements on MOF-5 powder at 40 K and 60 K

- Systematic evaluation requiring the use of a He cyrostat cooler that can be adjusted to hold the sample at a temperature between 20 K and 330 K.
  - Calibration indicates appropriate temperature control & self-consistent zero measurements.
  - With a stainless steel tube sample holder, the thermal conductivity is an issue and a pressure dependence of the different volumes is observed, especially at lower temperatures.
  - This pressure dependence should not occur; not known why it is affecting the measurement.

Hydrogen adsorption of empty sample holder at 75 K. The data show that the instrument is providing a reasonable measure of zero adsorption as a function of pressure. Red: Adsorption per Step (left axis). Blue: Total Adsorption (right axis).

Adsorption system calibration measurements with He show a pressure dependence for the volume that increases as the temperature decreases below 200K.
Accomplishment: Isotherm Measurement

Improved isotherm measurements at less than 75 K.

- Developed a “difference” technique that removes He calibration.
  - Measures H2 adsorption difference between 303 K (RT) and 40 K to 75 K. 303 K (RT) adsorption usually negligible.
  - Preliminary results: measured adsorption at 40 K with difference method is similar to the models.

- Redesigned cryostat sample holder to minimize pressure dependent effects.

- At this time, no additional work to improve the measurements is planned.

<table>
<thead>
<tr>
<th>Pressure (Bar)</th>
<th>Difference Method 100*(gH2/gsample)</th>
<th>A-D Model 100*(gH2/gsample)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.3</td>
<td>8.2</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>8.3</td>
<td>8.5</td>
</tr>
<tr>
<td>1.8</td>
<td>8.5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>10.5</td>
</tr>
</tbody>
</table>

Preliminary difference method results compared with model at 40 K. The maximum adsorption from the model is approximately 10.5 g/gX100 at 4 bar. Additional measurements are needed to measure intermediate pressures.
Collaboration and Coordination

Key Collaborators:
- UTRC-Model integration and model Framework
- Ford-FC model, model integration and MOF-5 data
- SRNL-Adsorbent models
- PNL-Chemical Hydride models
- GM-Metal Hydride models
- LANL-Chemical Hydride data
- UM-Adsorbent data
- ANL-System/energy analysis

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

– Continue to run vehicle simulations to:
  ▪ Evaluate the impact of changes to phase III storage system designs and refinements
  ▪ Determine system demand/flow rate for phase III systems (based on US06 cycle)
  ▪ Assist with public release and access of all center models

– Energy Analysis
  ▪ Work complete

– Media engineering properties
  ▪ Possibly provide hydrogen storage engineering properties for selected sorbent materials/pellets at the appropriate conditions to validate models.
Summary

– Manage HSECoE vehicle performance, cost and energy analysis technology area

– Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance tradeoffs at the vehicle system level.

– Energy Analysis: Coordinate hydrogen storage system 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 sorbent materials that have the potential for meeting DOE technical targets for an onboard systems.
Technical Back-Up Slides
FE Validation,

CDP#6: Fuel Economy

Fuel Economy (miles/kg H₂)

Dyno (1)  Window-Sticker (2)  On-Road (3)(4)

Gen 1  Gen 2

(1) One data point for each make/model. Combined City/Highway fuel economy per DRAFT SAE J2372.
(2) Adjusted combined City/Highway fuel economy (0.78 x High, 0.3 x City).
(3) Excludes trips < 1 mile. One data point for on-road fleet average of each make/model.
(4) Calculated from on-road fuel cell stack current or mass flow readings.
Adjusted Five Cycle Fuel Economy Calculation (Window Sticker)

\[
Adjusted\_City\_MPGGE = \frac{1}{0.003259 + \frac{1.1805}{Model\_City\_MPGGE}}
\]

\[
Adjusted\_Highway\_MPGGE = \frac{1}{0.001376 + \frac{1.3466}{Model\_Highway\_MPGGE}}
\]

\[
Adjusted\_Combined\_MPGGE = (Adjusted\_City\_MPGGE \cdot 0.55) + (Adjusted\_Highway\_MPGGE \cdot 0.45)
\]