Overview

Timeline

• Start: February 1, 2009
• End: June 30, 2014
• 70% Complete (as of 3/31/13)

Budget

• Total Center Funding:
  • DOE Share: $36,232,765
  • Contractor Share: $3,591,709
  • FY ’12 Funding: $5,930,000
  • FY ’13 Funding: $5,150,000
• Prog. Mgmt. Funding
  • FY ’12: $400,000
  • FY ’13: $300,000

Barriers

A. System Weight and Volume
B. System Cost
C. Efficiency
D. Durability
E. Charging/Discharging Rates
G. Materials of Construction
H. Balance of Plant (BOP) Components
J. Thermal Management
K. System Life-Cycle Assessment
O. Hydrogen Boil-Off
P. Understanding Physi/Chemi-sorption
S. By-Product/Spent Material Removal

Partners

[Logos of various partners for the project]
HSECoE Technical Objectives

Using systems engineering concepts, design innovative material-based hydrogen storage system architectures with the potential to meet DOE performance and cost targets.

- Develop and validate system, engineering and design models that lend insight into overall fuel cycle efficiency.
- Compile all relevant materials data for candidate storage media and define required materials properties to meet the technical targets.
- Design, build and evaluate subscale prototype systems to assess the innovative storage devices and subsystem design concepts, validate models, and improve both component design and predictive capability.
Why Perform Materials Development and System Engineering in Parallel?

Materials → Thermal Management → H₂ Storage → Fuel Cell → Vehicle → Wheels

Continuous feedback with system design identifying materials requirements

Materials → Engineered Materials Properties → Heat Transfer Designs → BoP Component Requirements → What is Needed of the Hydrogen Storage Media & System
## Technical Matrix

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>System Architects</td>
<td>Thornton Weimar</td>
<td>Tamburello</td>
<td>Hardy Corgnali, Sulic, Ortman, Drost</td>
<td>Veenstra Chahine Simpson</td>
<td>Simmons Newhouse Reiter</td>
<td>Chahine</td>
</tr>
<tr>
<td>Adsorbent System <em>Siegel</em></td>
<td>Thornton Weimar</td>
<td>Brooks</td>
<td>Brooks Semelsberger</td>
<td>Rönnebro Semelsberger</td>
<td>van Hassel Holladay Simmons</td>
<td>Semelsberger</td>
</tr>
<tr>
<td>Chemical Hydride System <em>Semelsberger</em></td>
<td>NREL</td>
<td>SRNL</td>
<td>GM OSU Oregon State</td>
<td>JPL HEXAGON LINCOLN</td>
<td>Pacific Northwest National Laboratory</td>
<td>Pacific Northwest National Laboratory</td>
</tr>
</tbody>
</table>

*Approach*
Phased Approach

**Phase I:**
System Requirements & Novel Concepts

- Where are we and where can we get to?
  - Model development
  - Benchmarking
  - Gap Identification
  - Projecting advances

**Phase II:**
Novel Concept Modeling Design & Evaluation

- How do we get there (closing the gaps) and how much further can we go?
  - Component development
  - Concept validation
  - Integration testing
  - System design
  - Materials requirements

**Phase III:**
Sub-Scale Prototype Construction, Test and Evaluation

- Put it all together and confirm claims.
  - System integration
  - System assessments
  - Model validation
  - Gap analysis
  - Performance projections
Important Dates Phase 2

- **Duration:** 5.5 years
  - Phase 1 Start: Feb. 1, 2009
  - Phase 1-2 Transition: March 31, 2011
  - Phase 1 End: June 30, 2011
  - Phase 2 Start: **July 1, 2011**
  - Phase 3 Go/No-Go Determination: **March 31, 2013**
  - **Phase 2 End:** June 30, 2013
  - Phase 3 Start: July 1, 2013
  - Completion Date: June 30, 2014 ⇒ 3/31/15?
Phase 1-2 State-of-the-Art

State-of-the-Art Identified for Chemical and Adsorbent Hydrogen Storage Systems

- Current status vs targets
- Identification of critical technical barriers
- Identification of potential solutions to barriers
- Summary of projected system performance vs targets

Approach
## HSECoE Phase 2 Go/NoGo Milestones

### Chemical Hydrides

<table>
<thead>
<tr>
<th>Target</th>
<th>Units</th>
<th>2015 DOE Goal (System)</th>
<th>Phase 1 HSECoE Baseline (System)</th>
<th>Phase 2 HSECoE Go/No-Go Targets (full scale)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gravimetric Capacity</td>
<td>kg H2/kg system</td>
<td>0.055</td>
<td>0.076 (Material)</td>
<td>0.042 (Material)</td>
</tr>
<tr>
<td>Volumetric Capacity</td>
<td>kg H2/L system</td>
<td>0.04</td>
<td>0.074 (Material)</td>
<td>0.039 (Material)</td>
</tr>
<tr>
<td>System Cost *</td>
<td>$/kWh net</td>
<td>3</td>
<td>25.6</td>
<td>25.6</td>
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<tr>
<td>Fuel Cost</td>
<td>$/gge at pump</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Min Operating Temp °C</td>
<td>°C</td>
<td>-40</td>
<td>2</td>
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<tr>
<td>Max Operating Temp °C</td>
<td>°C</td>
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<tr>
<td>Min Delivery Temp °C</td>
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<td>-40</td>
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<tr>
<td>Max Delivery Temp °C</td>
<td>°C</td>
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<td>85</td>
<td>85</td>
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<tr>
<td>Cycle Life</td>
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<td>1500</td>
<td>1000</td>
<td>1000</td>
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<tr>
<td>Min Delivery Pressure bar</td>
<td>bar</td>
<td>5</td>
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<tr>
<td>Max Delivery Pressure bar</td>
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<tr>
<td>Onboard Efficiency %</td>
<td>%</td>
<td>90</td>
<td>97</td>
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<tr>
<td>Well to Power Plant Efficiency %</td>
<td>%</td>
<td>60</td>
<td>37</td>
<td>37</td>
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<tr>
<td>System Fill Time min</td>
<td>min</td>
<td>3.3</td>
<td>2.7</td>
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<tr>
<td>Min Full Flow Rate g/s/kW</td>
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<tr>
<td>Fuel Purity %H2</td>
<td>%</td>
<td>99.97</td>
<td>99.97</td>
<td>99.99</td>
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<tr>
<td>Permeation, Toxicity, Safety scc/h</td>
<td>Meets or Exceeds Standards</td>
<td>s</td>
<td>s</td>
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</tr>
<tr>
<td>Loss of Useable Hydrogen (g/h)/kg H2 stored</td>
<td>0.05</td>
<td>0.1</td>
<td>0.1</td>
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</table>

### Responsible Organization

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Media</td>
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<td>Tank</td>
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<tr>
<td>BoP</td>
<td></td>
<td></td>
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<tr>
<td>Pumps</td>
<td></td>
<td></td>
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<tr>
<td>Heat Exchanger</td>
<td></td>
<td></td>
</tr>
<tr>
<td>GLS</td>
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<td></td>
</tr>
<tr>
<td>Purification</td>
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</tr>
<tr>
<td>Fluid AB at 50wt%</td>
<td>Fl</td>
<td>Bladder Tank</td>
</tr>
<tr>
<td>Bladder Tank</td>
<td>Flow Through Reactor</td>
<td>Feed/Recycle/Transfer Pumps</td>
</tr>
<tr>
<td>Flow Through Reactor</td>
<td>Gas/Liquid Separator</td>
<td>Hydrogen Purification mass and volume cut</td>
</tr>
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</table>
# HSECoE Phase 2 Go/NoGo Milestones

<table>
<thead>
<tr>
<th></th>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td><strong>Target</strong></td>
<td><strong>Units</strong></td>
<td><strong>Phase 1 HSECoE Baseline (System)</strong></td>
</tr>
<tr>
<td>Gravimetric Capacity</td>
<td>kg H2/kg system</td>
<td>0.055</td>
</tr>
<tr>
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<td>kg H2/L system</td>
<td>0.04</td>
</tr>
<tr>
<td>System Cost *</td>
<td>$/kWh net</td>
<td>25.6</td>
</tr>
<tr>
<td>Fuel Cost</td>
<td>$/gge at pump</td>
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<td>Min Operating Temp</td>
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<td>min</td>
<td>3.3</td>
</tr>
<tr>
<td>Min Full Flow Rate</td>
<td>g/s/kW</td>
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<td>Transient Response</td>
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<td>Fuel Purity</td>
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</table>

*System Cost is the sum of Fuel Cost and System Cost.*

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<thead>
<tr>
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<tbody>
<tr>
<td>LANL, PNNL</td>
<td>Media</td>
<td>Fluid AB at 50wt%</td>
</tr>
<tr>
<td>PNNL Tank</td>
<td>Bladder Tank</td>
<td>Flow Through Reactor</td>
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<tr>
<td>LANL Reactor</td>
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<td>BoP</td>
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<td>Gas/Liquid Separator</td>
<td>Heat Exchanger mass and volume cut</td>
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<td>UTRC GLS</td>
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<tr>
<td>UTRC Purification</td>
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<th>Phase 1 HSECoE Baseline (BOP only)</th>
<th>Phase 1 HSECoE Baseline (System)</th>
<th>Phase 2 HSECoE Actuals (Material)</th>
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<td>0.076</td>
<td>0.109</td>
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<td></td>
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<td>133</td>
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<td>0.074</td>
<td>0.074</td>
<td>0.102</td>
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<thead>
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<td>Gas/Liquid Separator</td>
<td></td>
</tr>
<tr>
<td>UTRC purification</td>
<td>Purification</td>
<td></td>
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</tbody>
</table>
## Approach

### Phase 2 Adsorbent System Milestones

<table>
<thead>
<tr>
<th>Adsorbent System Component</th>
<th>Partner</th>
<th>S<em>M</em>A<em>R</em>T Milestone</th>
<th>Status</th>
<th>Desired Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Materials Development</strong></td>
<td>Ford</td>
<td>Report ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/L.</td>
<td>Yes</td>
<td>Meets the metric.</td>
</tr>
<tr>
<td></td>
<td>BASF</td>
<td>Report ability to develop an adsorbent system having a total hydrogen material density of greater than or equal to 0.3 g/L.</td>
<td>Yes</td>
<td>Meets the metric.</td>
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<td><strong>Materials Development</strong></td>
<td>OSU</td>
<td>Report ability to develop an adsorbent system having a total hydrogen material density of greater than or equal to 0.3 g/L.</td>
<td>Yes</td>
<td>Meets the metric.</td>
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<tr>
<td></td>
<td>GM</td>
<td>Report ability to develop a high performance thermal insulation design having a mass less than 11 kg.</td>
<td>Yes</td>
<td>Meets the metric.</td>
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<tr>
<td></td>
<td>JPL</td>
<td>Report ability to develop a thermal insulation design having a mass less than 11 kg.</td>
<td>Yes</td>
<td>Meets the metric.</td>
</tr>
<tr>
<td></td>
<td>Lincoln</td>
<td>Report ability to develop a thermal insulation design having a mass less than 11 kg.</td>
<td>Yes</td>
<td>Meets the metric.</td>
</tr>
<tr>
<td><strong>Integrated Components</strong></td>
<td>OSU</td>
<td>Report ability to develop an adsorbent system having a total hydrogen material density of greater than or equal to 0.3 g/L.</td>
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<td>Meets the metric.</td>
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<td>Lincoln</td>
<td>Report ability to develop a high performance thermal insulation design having a mass less than 11 kg.</td>
<td>Yes</td>
<td>Meets the metric.</td>
</tr>
</tbody>
</table>

**Report on ability to identify a system design having a mass less than 6 liters.**

**Report on ability to develop and demonstrate a 1 kW catalytic adsorber capable of raising the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a compacted HX.**

**The kinetic response of the MOF-5 material will achieve the desired performance while the volumetric performance will continue to be a challenge with densities greater than 0.3 g/L.**

**Exceeded metric**

These results will be validated with lab experiments. The kinetic characterization of MOF-5 and Type 1 tanks will be performed at 77K and adding the capability of cryogenic cyclic testing capturing exceeding the metrics at this temperature.

**Met metric**

These results will be validated with lab experiments. The kinetic characterization of MOF-5 and Type 1 tanks will be performed at 77K and adding the capability of cryogenic cyclic testing capturing exceeding the metrics at this temperature.
Table 1 Adsortent System Component

<table>
<thead>
<tr>
<th>Component</th>
<th>Partner</th>
<th>5% MAFIV Milestones</th>
<th>Status</th>
<th>Potential Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Materials Development</td>
<td>Ford</td>
<td>Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/cc, HD density of 11.5% and 33 g/liter and thermal conductivity of 0.5 W/mK at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency.</td>
<td>Not Met</td>
<td>- The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to identify volumetric mass density which will meet all of the metric.</td>
</tr>
<tr>
<td>Materials Development</td>
<td>Ford/NIK</td>
<td>Report on ability to demonstrate a composite MOF-5 adsorbent materials having a total hydrogen material density of greater than or equal to 0.3 g/cc, HD density of 11.5% and 33 g/liter and thermal conductivity of 0.5 W/mK at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency.</td>
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</tr>
<tr>
<td>Materials Development</td>
<td>SNPE/LQTR</td>
<td>Report on ability to develop a composite MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/cc, HD density of 11.5% and 33 g/liter and thermal conductivity of 0.5 W/mK at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency.</td>
<td>Not Met</td>
<td>- The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to identify volumetric mass density which will meet all of the metric.</td>
</tr>
<tr>
<td>Structured Bed</td>
<td>GM</td>
<td>Report on ability to develop MOF-5 powder bed having a total hydrogen density of 15.6 % (g MOF/20 g H2/0.25 liter HX) at P = 60 - 65 bar and T = 80 - 160C. The bed is 40 - 50 mm thick with a void fraction of 0.45.</td>
<td>Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>Composite Tank</td>
<td>JPL</td>
<td>Report on ability to test building capacity to burst test Type 1 composite and Type 1 (metal) tanks at 400 and demonstrate design and fabrication of a cryogenic pressure test/external system capable of bursting at 77K has been completed. Soft tooling and documentation is currently 75% complete. Operating this system at 40K is not feasible. The modified testing will be conducted using a new design in a cryogenic test system capable of bursting at 77K.</td>
<td>In progress</td>
<td>- Compressed hydrogen (CH2) pressure test/external system is to be used for testing Type 1 CO2 tanks. Pressure testing of Type 1 tanks will be performed at 77K and adding the capability of the cryogenic system.</td>
</tr>
<tr>
<td>Internal MA/5 HX</td>
<td>OSU</td>
<td>Report on ability to build and demonstrate a 1000 bar hydrogen system capable of achieving less than 0.3 g/cc, HD density of 11.5% and 33 g/liter and thermal conductivity of 0.5 W/mK at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency. HD vol. density of the MOF-5 material = 33 g/l be possible with 5 gic (&lt;5%) ENG at P = 60-65 bar and T = 80-160K with 68% packing efficiency.</td>
<td>Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>Internal non-MAS/HHX</td>
<td>LSI/SFPE</td>
<td>Report on ability to develop and demonstrate a heat exchange loop capable of allowing less than 3 min. time and HD vol. density of 0.02 g/l (g MOF/20 g H2/0.25 liter HX) with a mass less than 6.5 g/liter and a volume less than 6 liters.</td>
<td>In progress</td>
<td>- Compressed hydrogen (CH2) pressure test/external system is to be used for testing Type 1 CO2 tanks. Pressure testing of Type 1 tanks will be performed at 77K and adding the capability of the cryogenic system.</td>
</tr>
<tr>
<td>Internal flow through HX</td>
<td>SNPE/LQTR</td>
<td>Report on ability to develop and demonstrate an internal flow through HX system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 2.5 mbar and heated using a 185kW laser (uncompressed) GCD=15 V, VCD=26.5 V, GCD=40 bar, VCD=33.5 bar, GCD=0.17 bar, VCD=10 bar, with the HX being heated to maintain the temperature at 77K. The total mass of the HX is less than 0.5 kg and a volume less than 0.25 liters.</td>
<td>Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>Internal flow through HX</td>
<td>GM</td>
<td>Report on ability to develop and demonstrate an internal flow through HX system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 2.5 mbar and heated using a 185kW laser (uncompressed) GCD=15 V, VCD=26.5 V, GCD=40 bar, VCD=33.5 bar, GCD=0.17 bar, VCD=10 bar, with the HX being heated to maintain the temperature at 77K. The total mass of the HX is less than 0.5 kg and a volume less than 0.25 liters.</td>
<td>Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>External HX</td>
<td>JPL</td>
<td>Report on ability to develop and demonstrate a high temperature reactor capable of heating 80K hydrogen stream to 233K flowing at 1.0 g/sec with no icing at 50% RH with a mass increase of less than 2.5 kg and a volume increase of less than 5 liters.</td>
<td>Not Met</td>
<td>The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to identify volumetric mass density which will meet all of the metric.</td>
</tr>
<tr>
<td>Catalytic Reactor</td>
<td>OSU</td>
<td>Report on ability to develop and demonstrate a 1 kW catalytic reactor capable of augmenting partial H2 preconditioning by an existing FC reactor with 100% efficiency and a mass less than 0.6 kg and volume less than 0.4 liters.</td>
<td>In progress</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>BoP</td>
<td>PNNL</td>
<td>Report on ability to identify BoP materials (excluding internal HX, external HX, and combustor) suitable for 40 bar cryogenic. Adsorbent system having mass less than 0.7 kg and a volume less than 0.15.8 liters.</td>
<td>Not Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
<tr>
<td>System Design</td>
<td>SNPE/LQTR</td>
<td>Report on ability to identify a system design having a mass less than 137 kg and a volume less than 279 liters meeting the all of the criteria of the HSEC CoE design cycles</td>
<td>Exceeded</td>
<td>- Compressed hydrogen (CH2) pressure test/external system is to be used for testing Type 1 CO2 tanks. Pressure testing of Type 1 tanks will be performed at 77K and adding the capability of the cryogenic system.</td>
</tr>
<tr>
<td>Efficiency Analysis</td>
<td>NREL</td>
<td>Calculate and model the well-to-powerplant (WTP) efficiency for two adsorbtion system designs and compare results relative to the 65% technical target.</td>
<td>Not Met</td>
<td>The kinetic response of the MOF-5 material will achieve the desired response while the permanence will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
</tbody>
</table>
**Phase 2 Adsorbent System Milestones**

<table>
<thead>
<tr>
<th>Adsorbent System Component</th>
<th>Partner</th>
<th>S<em>M</em>A<em>R</em>T Milestone</th>
<th>Status 10/12</th>
<th>Projected Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Materials Development</strong></td>
<td>Ford</td>
<td>Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/L, HD density of 1.1 g/L and 33 g/L and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.</td>
<td>GC density of the MOF-5 material &gt;11% is possible with 3 g/L (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. HD vol. density of the MOF-5 material &gt;33 g/L is possible with 5 g/L (+5% ENG) at P = 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of 0.5 W/m-K is possible with 3 g/L and 5 g/L ENG with temperatures = 100-120 K.</td>
<td>The capability of achieving specific metrics with a given configuration is possible, investigations will be continued to devise a media morphology which will meet all of the metrics.</td>
</tr>
<tr>
<td></td>
<td>SunII</td>
<td>Evaluation of materials provided by Ford for initial B and final system: 180kg/m³ (uncompacted) GCD=0.05 ∆V=25.5 kg/m³ (uncompacted) GCD=0.10 ∆V=33.0 kg/m³ (uncompacted) GCD=0.15 ∆V=40.5 kg/m³ (uncompacted) GCD=0.20 ∆V=48.0 kg/m³ (uncompacted) GCD=0.25.</td>
<td></td>
<td>Met Metric</td>
</tr>
<tr>
<td></td>
<td>SRC</td>
<td>Adsorption experimental work show that the adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the HD temperature high enough, however the final MLI-HX has higher mass and volume than a comparable MATI.</td>
<td></td>
<td>Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.</td>
</tr>
<tr>
<td></td>
<td>GM</td>
<td>Optimization for the adsorber: HD 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) is possible with 60% packing efficiency. Thermal conductivity of .5 W/m-K is possible with .3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160K.</td>
<td></td>
<td>Exceeded metric</td>
</tr>
<tr>
<td></td>
<td>JPL</td>
<td>Detailed modeling and coupon-scale validation experiments have been completed showing that the thermal isolation system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 1e+4 Torr, reduces parasitic heat load to 2W far exceeding the metric.</td>
<td></td>
<td>Exceeded metric</td>
</tr>
<tr>
<td></td>
<td>JPL</td>
<td>System design exceeding metrics:</td>
<td></td>
<td>Exceeded metric</td>
</tr>
<tr>
<td></td>
<td>NREL</td>
<td>Detailed modeling and coupon-scale validation experiments have been completed showing that the thermal isolation system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 1e+4 Torr, reduces parasitic heat load to 2 W far exceeding the metric.</td>
<td></td>
<td>Exceeded metric</td>
</tr>
</tbody>
</table>

### Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).

**Exceeded metric**

### Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.

**Exceeded metric**

**Metric not achievable**

**Not Met**

### After evaluating 8 different materials it was concluded that the liner separates from the shell when the pressure is decreased below 35bar with a liner thickness of 2.55mm. With current materials this metric is not feasible and either a Type 1 or 3 tank design is necessary.

**Exceeded metric**

25% scale experimental verification has been started, and preliminary results are being analyzed which should provide exceeding of the metric.
**Chemical Hydride System Projection**

**End of Phase 1**

**2017 Targets**
- Media: Fluid Phase Ammonia Borane: 50wt.% AB in BMIMCl (1-n-butyl-3-methylimidazolium chloride)
- 12 Components:
  - Bladder Tank
  - Flow Through Reactor
  - Gas Liquid Separator/Ballast Tank
  - Radiator
  - Hydrogen Purification

1. Gravimetric Density
2. On-Board Efficiency
3. System Cost
4. H₂ Purity
Accomplishment

Chemical Hydride: Slurry Development

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric</th>
<th>Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>develop a 40 wt% slurry AB</strong> material having viscosity less than 1500cP pre- and post-dehydrogenation and kinetics comparable to the neat.</td>
<td></td>
<td>Exceeded metrics</td>
</tr>
</tbody>
</table>

Ammonia Borane Slurry Development

Milestone Metric Outcome

- **Report on ability to develop a 40 wt% slurry AB** material having viscosity less than 1500cP pre- and post-dehydrogenation and kinetics comparable to the neat.

Exceeded metrics

**Weylchem AB Slurry After Sonication**

- Particle Size Distribution

**Weylchem AB Slurry Spent Slurry**

- Particle Size Distribution

**45w/o AB in silicon oil ~7 w/o H₂**

- **45wt% AB slurry before H-release**
- **45wt% AB slurry after H-release**
Accomplishment

Chemical Hydride: Reactor

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
</table>
| Report on ability to **develop a flow through reactor** capable of discharging 0.8 g/s H₂ from a 40 wt.% AB fluid-phase composition having a mass of no more than 2 kg and a volume of no more than 1 liter. | Reactor performance tests with kinetics will be performed on
  • 35-40 wt% AB slurries
  • 40-60 wt.% Alane slurries with the anticipation of meeting the target |

Flow-Through Reactor

**Media**
- Ammonia Borane Slurries
- Alane Slurries
- Methoxy-propyl amine borane (MPAB)

Liquid Helical Reactors

Alane Auger Reactor Results

---

**Graphs**

1. **Temperature vs. Time**
   - Reactor inlet
   - Reactor slurry
   - Reactor outlet
   - Avg Reactor Temp

2. **Conversion vs. Temp**
   - Alane = 1.09 mL/min
   - Alane = 0.55 mL/min
Chemical Hydride: BoP-Gas/Liquid Separator

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric</th>
<th>Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to develop a GLS capable of handling 720 mL/min liquid phase and 600 L/min of H2 @ STP (40 wt% AB @ 2.35 Eq H2 and max H2 flow of 0.8 g/s H2) fluid having a viscosity less than 1500cp with resulting in a gas with less than 100ppm aerosol having a mass less than 5.4 kg and volume less than 19 liters.</td>
<td>Could not meet mass but far exceeded volume metric</td>
<td>Demonstrated operation meeting metrics utilizing spent fuel simulant.</td>
</tr>
</tbody>
</table>

Accomplishment

Gas-Liquid Separator Efficiency Modeling

Milestone Metric Outcome
Could not meet mass but far exceeded volume metric
Demonstrated operation meeting metrics utilizing spent fuel simulant.
## Chemical Hydride: BoP-Gas Purification

### Accomplishment

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>develop a borazine scrubber</strong> with a minimum replacement interval of 1800 miles of driving resulting in a minimum outlet borazine concentration of 0.1 ppm (inlet concentration = 4,000 ppm) having a maximum mass of 3.95 kg and maximum volume less of 3.6 liters.</td>
<td><strong>Mass metric achieved but volume metric missed.</strong> Compaction of adsorbent media could be conducted to meet the volume metric but emphasis will be placed on reactor testing.</td>
</tr>
<tr>
<td>Report on ability to <strong>develop an ammonia scrubber</strong> with a minimum replacement interval of 1800 miles of driving resulting in a minimum ammonia outlet concentration of 0.1 ppm (inlet concentration = 500 ppm) having a maximum mass of 1.2 kg and a maximum volume of 1.6 liters.</td>
<td><strong>Met Metric</strong></td>
</tr>
</tbody>
</table>

### Ammonia & Borazine Filters

![Graphs of ammonia and borazine concentration over time](image)

- **NH₃-dynamic sorption capacity [wt. %]**
- **Dynamic adsorption cycle number [-]**
- **Wavenumber (cm⁻¹)**

![Graphs of ammonia and borazine mass and volume](image)
Accomplishment

Chemical Hydride: System Design

### Milestone

Report on ability to **identify BoP materials** suitable for the Chemical Hydrogen system having a system mass no more than 41 kg and a system volume no more than 57 liters.

**Metric Outcome**

Volumetric metric met.
Gravimetric metric not met. The requirements for the Hydrogen purification system increased from 4.3 kg to 19.1 kg.

Report on ability to **identify a system design** having a mass less than 97 kg and a volume less than 118 liters meeting the all of the HSECoE drive cycles.

**Metric Outcome**

Metric not met. A path to minimize the mass and volume of the system to meet the targets has been identified, but higher slurry concentration (64\% AB) or a slurry with a higher hydrogen loading (9.8 \%wt) will be required to meet the metric.

---

**Legend**

- Slurry
- Tankage
- Pumps
- Tank Mixers
- Leak-Up Beds & Filters
- Radiators
- Reactor
- Valves and Piping
- Instruments

= 137 kg
Accomplishment

Chemical Hydride: BoP-Displacement Tank

One liter volume displacement tank designed/built/tested

Exposure testing of membrane materials to AB and silicon oil before and after dehydrogenation

Pleated membrane design validated to minimize strain and allow flexibility in membrane materials
Accomplishment

Chemical Hydride System Waterfall Charts

Achieving Mass target through increased fluid loading and reduced clean-up system will result in achievement of volume target.
Accomplishment

Chemical Hydride System Projection
End of Phase 2

2017 Targets
- Media Type: 50wt% Slurry Ammonia Borane in silicon oil
- Primary Components:
  - Bladder Tank
  - Flow Through Reactor
  - Gas Liquid Separator/Ballast Tank
  - Radiator
  - Purification

1. Gravimetric Density
2. On-Board Efficiency
3. System Cost
4. H₂ Purity
Accomplishment

Chemical Hydride System Projection
End of Phase 2

2017 Targets

- Media Type: 50wt% Slurry Ammonia Borane in silicon oil
- Primary Components:
  - Bladder Tank
  - Flow Through Reactor
  - Gas Liquid Separator/Ballast Tank
  - Radiator
  - Purification

1. Gravimetric Density
2. On-Board Efficiency
3. System Cost
4. $\text{H}_2$ Purity
Accomplishment

Adsorbent System Projection
End of Phase 1

2017 Targets

- AX-21, no thermal enhancement, 80 K initial fill
- Type 3 CF/Al lined pressure vessel, 6 mm liner, 200 bar
- Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K
- Porous-bed "flow-through" cooling/fueling design for adsorption
- Desorption heat via tank-integral electrical resistance elements/HX

1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H₂
**Accomplishment**

**Adsorbent System: Media Engineering**

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>develop compacted MOF-5 adsorbent media</strong> having a total hydrogen material density of greater than or equal to 0.3 g/L, H₂ density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.</td>
<td>The capability of achieving individual metrics with a given configuration has been demonstrated. <strong>No one structure has been identified achieving all of the metrics.</strong></td>
</tr>
<tr>
<td>Report on ability to <strong>demonstrate a composite MOF-5 adsorbent monoliths</strong> having H₂ effective kinetics equivalent to 5.6 kg usable H₂ over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.</td>
<td><strong>Met Metric</strong> The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.</td>
</tr>
</tbody>
</table>

**Volumetric Density**

- $\rho = 0.3 \text{ g/cc}$

- $\rho = 0.5 \text{ g/cc}$

**Permeability Measurements**
## Adsorbent System: BoP-Composite Tank

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>develop testing capability</strong> to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure.</td>
<td>The cryogenic test facility was completed, but funding was exhausted prior to tank testing. Cimeron composites has been identified as having the capability to perform these tests within budget. <strong>Metric Met.</strong></td>
</tr>
<tr>
<td>Report on ability to <strong>develop Type 4 (composite) and Type 1 (metal) tanks</strong> capable of use between 40 and 160K meeting ASME pressure vessel code for use at 60 bar having a mass less than 10 kg and a volume less than 120 liters.</td>
<td>Based on these results single piece 120 liter Type 1 and Type 4 tanks will be designed and masses calculated. It is anticipated that the Type 1 tank will not meet the mass target while the <strong>Type 4 tank will meet the mass metric.</strong></td>
</tr>
<tr>
<td>Report on ability to <strong>identify Type IV tank liner materials</strong> suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).</td>
<td><strong>Metric not achievable</strong></td>
</tr>
</tbody>
</table>

- **Cryogenic Tank Testing**
- **Composite tank design**
- **Segmented Al tank design**
- **Cryo-burst test facility competed**
Accomplishment

**Adsorbent System: BoP-Insulation Development**

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.</td>
<td>25% scale experimental verification has been started, and preliminary results are being analyzed which should prove exceeding of metric.</td>
</tr>
</tbody>
</table>

![Bell Jar Diagram]

![Graphs showing q_total vs. P for different layer counts]

- 20 Layers
- 40 Layers
- 60 Layers
- 80 Layers

![Graphs showing Heat vs. P for experiment and prediction]

- Experiment: 30 Layers
- Prediction: 30 Layers, 43/cm
Adsorbent System: BoP-Internal Heat Exchange

Accomplishment

Report on ability to **develop and demonstrate a Modular Adsorption Tank Insert** capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.

**Milestone**

**Metric Outcome**

- Exceeded metric
  Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.

Modular Adsorption Tank Insert (MATI)

**System Concept**

- Cross-flow HX
- Heat of adsorption removed by LN2
- Radial H2 access to adsorption bed

**MATI v1 – Combined LN2 cooling and H2 distribution**

![MATI Diagram](image)

**Graphs**

- TC1, TC2, TC3: Evolution of Red Temperature (°C)
- TC4, TC5, TC6: Evolution of Red Temperature (°C)
- Time [s]: 0 to 300
Accomplishment

Adsorbent System: BoP-Internal Heat Exchange

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>develop and demonstrate an internal flow</strong> through <strong>HX</strong> system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.</td>
<td>Met metric</td>
</tr>
</tbody>
</table>

Powder & Pellet HexCell HX
### Adsorbent System: System Design

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Metric Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report on ability to <strong>identify BoP materials</strong> (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbent system having mass less than 17 kg and a volume less than 18.5 liters.</td>
<td>Metric exceeded</td>
</tr>
<tr>
<td>Report on ability to <strong>identify a system design</strong> having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles</td>
<td>Metric exceeded</td>
</tr>
</tbody>
</table>

### Metric Outcome

<table>
<thead>
<tr>
<th>Internal HX and Media</th>
<th>Helical Coil + powder MOF-5</th>
<th>HexCell + powder MOF-5</th>
<th>HexCell + 0.32 g/cc MOF-5 pellets</th>
<th>MATI + 0.32 g/cc MOF-5 pucks</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Mass [kg]</td>
<td>178.4</td>
<td>159.2</td>
<td>175.0</td>
<td>164.3</td>
</tr>
<tr>
<td>System Volume [L]</td>
<td>328.7</td>
<td>320.2</td>
<td>288.8</td>
<td>270.4</td>
</tr>
<tr>
<td>Estimate System Cost [$]</td>
<td>$2,486</td>
<td>$2,376</td>
<td>$2,671</td>
<td>$2,883</td>
</tr>
<tr>
<td>System Rank (Ford)</td>
<td>5.742</td>
<td>6.020</td>
<td>5.699</td>
<td>5.964</td>
</tr>
<tr>
<td>Gravimetric Capacity [g/g]</td>
<td>0.0314</td>
<td>0.0352</td>
<td>0.0320</td>
<td>0.0341</td>
</tr>
<tr>
<td>Volumetric Capacity [g/L]</td>
<td>17.04</td>
<td>17.49</td>
<td>19.40</td>
<td>20.72</td>
</tr>
</tbody>
</table>

**Source:** Pacific Northwest National Laboratory

**Approach:** From over ½ Billion combinations... down to 4 Systems

<table>
<thead>
<tr>
<th>From over ½ Billion combinations... down to 4 Systems</th>
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</thead>
<tbody>
<tr>
<td>- Innovative screening of all combinations</td>
</tr>
<tr>
<td>- System screening</td>
</tr>
</tbody>
</table>

**Final System:**

1. Three phase through testing with diverse HX options
2. HX 300x400 with MOF-5
3. HX 300x400 with MOF-5 and HX 500x500
4. HX 300x400 with MOF-5 and HX 500x500
5. Different HX configuration
6. Different testing criteria
7. Different HX design
8. Different HX material

**Metric exceeded**
Accomplishment

HexCell Adsorbent System Projection
End of Phase 2

2017 Targets

- MOF-5, no thermal enhancement, 80 K initial fill
- Type 1 Al pressure vessel, 100 bar
- Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K
- Adsorption: Porous-bed “flow-through” cooling/fueling
- Desorption: Electrical resistance heater/honeycomb HX 140K

1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H₂
HexCell Adsorbent System Projection
End of Phase 2
2017 Targets

- MOF-5, no thermal enhancement, 80 K initial fill
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Accomplishment
Accomplishment

MATI Adsorbent System Projection
End of Phase 2
2017 Targets

- Compacted MOF-5, no thermal enhancement, 80 K initial fill
- Type 1 Al pressure vessel, 100 bar
- Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K
- Adsorption: LN2 chilled plates
- Desorption: BoP heated H2/140K

1. Gravimetric Density
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1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H2
Waterfall Charts for 80 K, 100 bar HexCell System

Step Description

A Phase 1 Baseline – Activated Carbon; Type 3 tank; Full at 80K, 200 bar; FT Cooling + Generic Resistance Heater

B Set Operating Conditions to 80 K, 100 bar and Type 1 Al Tank

C Identify Internal Heat Exchanger Design: HexCell w/ Resistance Heater

D Change Material from Activated Carbon to Powder MOF-5

E Improve BOP Components (reduce mass & volume by 25%)

F Maintain Capacity with increased Operating Temperature (reduce MLVI by 50%; remove LN2)

G Increase Material Capacity to 140% of Powdered MOF-5

H Increase Material Capacity to 200% of Powdered MOF-5

Accomplishment
Adsorbent System FMEA Updated
Failure Modes and Effects Analysis

Accomplishment

- Highest risk items identified from initial FMEA
- Corrective actions taken
- Example actions during phase 2 for reducing the Risk Priority Number (RPN)
  - Completed initial homogenous material analysis and heat exchanger testing
  - Revised tank construction from composite to aluminum and completed cryogenic testing
  - Developed designs with deep-dive technical reviews, controls, and test plans for Phase 3

Initial Phase 2 RPN values
- High: 720
- Mean: 188

Final Phase 2 RPN values
- High: 512
- Mean: 113
Wells-to-Power Plant Analyses

Milestone | Metric Outcome
---|---
Calculate and **model the well-to-power plant (WTPP) efficiency** for two adsorbent and one chemical storage system designs and compare results relative to the 60% technical target. | Met metric for one adsorbent system in process of completion.

Energy Efficiency

GHG Emissions

Drive Cycles

Integrated System Modeling
Technical Target Prioritization

- **All targets must still be met simultaneously**
- Prioritization identifies *performance must-have* vs. *design choice* targets
- Guides design trade-offs to optimize overall system/vehicle performance to meet customer expectations
- QFD approach originally taken

**Method for the refined analysis**
- Quantify the storage system linkage to vehicle attributes
- Subjective scale of cause-effect relationships are revised based on correlation analysis
- Limited to the key system targets: *gravimetric density, volumetric density, and cost*

**Refined Analysis**
- **System Score** = Grav. Score + Cost Score + Vol. Score
- **Target Score** = (% of Target Obtained)*\(\sum (\text{Importance} \times \text{Correlation Constant})\)
- Gravimetric Score = \(S_{GD}\% (I_{FE} \times C_{GFE} + I_{DR} \times C_{GDR} + I_{VA} \times C_{GVA} + I_{VC} \times C_{GVC})\)
- Cost Score = \(S_{C}\% \times I_{VC} \times C_{CVC}\)
- Volumetric Score = \(S_{VD}\% \times I_{VDR} \times C_{VDR}\)
WEB Czar (Ted) responsible for updating
Load models on site for public dissemination
New models being implemented continually
R. Bowman and T. Johnson (SNL) agreed to β-test models
WEB Czar (Ted) responsible for updating
Load models on site for public dissemination
New models being implemented continually
R. Bowman and T. Johnson (SNL) agreed to β-test models
WEB Site Models Added

WEB Czar (Ted) responsible for updating load models on site for public dissemination. New models being implemented continually.

R. Bowman and T. Johnson (SNL) agreed to β-test models.
Accomplishment

Metal Hydride FEM Model

Input data – Constants and functions
Input data – Geometry and regions definition
Input data – Mass, energy balance models
Accomplishment

Metal Hydride FEM Model
Accomplishment

Metal Hydride FEM Model

Spatial & Temporal Temperature Distribution
Accomplishment

Metal Hydride FEM Model

Spatial & Temporal Concentration Distribution
### HSECoE Website Status/Plan

<table>
<thead>
<tr>
<th>Model Name</th>
<th>Lead</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 MH Acceptability Envelope</td>
<td>SRNL</td>
<td>Complete</td>
</tr>
<tr>
<td>2 MH Finite Element Model</td>
<td>SRNL</td>
<td>Complete</td>
</tr>
<tr>
<td>3 MH Framework Model</td>
<td>UTRC</td>
<td>Model complete (TBR)</td>
</tr>
<tr>
<td>4 Tank Volume/Cost Model Electric/Hybrid Vehicle</td>
<td>PNNL</td>
<td>Model Complete (TBR)</td>
</tr>
<tr>
<td>5 Performance*</td>
<td>NREL</td>
<td>6/13</td>
</tr>
<tr>
<td>6 AD Finite Element Model</td>
<td>SRNL</td>
<td>9/13</td>
</tr>
<tr>
<td>7 AD Framework Model</td>
<td>SRNL</td>
<td>3/14</td>
</tr>
<tr>
<td>8 Chemical Hydride Model(s)</td>
<td>PNNL</td>
<td>6/14</td>
</tr>
</tbody>
</table>

* NREL model to be linked to HSECoE website
Phase 3 Go/NoGo Review Held

• **Where we are now?**
  • Phase 2 Spider Charts
  • Phase 2 SMART Milestone Status
  • Phase 2 Waterfall Charts

• **Why this demonstration will be valuable?**
  • Validate models
  • Materials Properties Requirements
  • Demonstrate Engineering Concepts

• **What will be demonstrated in Phase 3?**
  • Scale of test and justification
  • Specific designs/components (mass/volume/cost)
  • Design status/plan

• **How will it be demonstrated in Phase 3?**
  • Specific test plan for each target
  • What will be learned from each test
  • Test facility status/plan
  • Decommissioning plan

• **Who will participate and how?**
  • Partner’s roles
  • Phase 3 Draft SMART Milestones

• **When will this come about?**
  
  
  Planned Phase 3 Gantt chart

Green text indicates deliverable to DOE
### System Test Matrices

<table>
<thead>
<tr>
<th>Phase 3 ideas for testing specific targets: MOF-S cryoadsorbent system</th>
</tr>
</thead>
</table>
## System Test Matrixes

<table>
<thead>
<tr>
<th>Target</th>
<th>Gravimetric capacity</th>
<th>Volumetric capacity</th>
<th>System cost</th>
<th>Fuel cost</th>
<th>Ambient temperature °C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>wt%</td>
<td>g-H₂/L</td>
<td>$/kWh net</td>
<td>$/gge at pump</td>
<td></td>
</tr>
<tr>
<td>Ultimate</td>
<td>2017</td>
<td>5.5</td>
<td>7.5</td>
<td>40</td>
<td>-40 - 60 (sun)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>70</td>
<td>2-6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2-3</td>
<td></td>
</tr>
</tbody>
</table>

### Table Notes:
- **Target** column indicates the phase target for each system.
- **Gravimetric capacity** and **Volumetric capacity** are key performance indicators for each system.

### Additional Notes:
- **System cost** and **Fuel cost** are critical for assessing the economic viability of each system.
- The **Ambient temperature** column highlights the operational range for each target system.

### Technical Specifications:
- The table includes a comprehensive list of technical specifications for each system, including gravimetric and volumetric capacities, system cost, fuel cost, and ambient temperature.
- Each system is evaluated against a set of criteria to ensure it meets the specified requirements.

---

**Accomplishment**

**HSECoE**

---

**38**
### System Test Matrices

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### Accomplishment

**Will this target be tested?**

**What is the test or model approach?**

**What exactly should be measured in this test to verify the target or model?**

---

*Note: The table above summarizes the system test matrices for different targets, including their gravimetric and volumetric capacities, system and fuel costs, and ambient temperature conditions. The test and model approaches, as well as the specific measurements to be made for each target, are also detailed.*
## Accomplishment

### System Test Matrixes

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</tr>
</tbody>
</table>

### Will this target be tested?

- Yes-Partial
- Yes-Partial
- Maybe
- No

### What is the test or model approach?

- Actual weights instrumented BOP list; Instrumentation and hardware adds to system; What we could build today; Alternate list of what it could be; actual capacity of system
- Separate lists of volumes (as for weights)
- Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI
- Cost to refuel will be estimated by Paster and Thornton

### What exactly should be measured in this test to verify the target or model?

- Usable capacity
- Usable capacity
- Estimated costs of lab scale system to actual cost of lab scale system
- Amount of LN₂ and H₂ consumed during refill

- External temperature
- Test will be at room temperature
## System Component Specification

<table>
<thead>
<tr>
<th>Component</th>
<th>Assumed Validation in Phase II</th>
<th>Responsible Design Organization</th>
<th>What can be validated with modeling rather than experimental work?</th>
<th>Rationale for including/excluding from Phase III</th>
<th>Areas of Concern Requiring Testing</th>
<th>Limitations on Scaling</th>
<th>Include in Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal Heat Exchanger: HexCell Resistance Heater with Flow-Through Cooling</td>
<td>Modeling and partial experimental validation of individual components/capabilities</td>
<td>SRNL / UQTR</td>
<td>1st-order thermal behavior (already completed).</td>
<td>Simple, low-cost design; Verify capability for rapid cooling; dynamic behavior (such as channeling) can only be evaluated experimentally</td>
<td>Cool-down time; non-uniform temperature distribution; robustness of HX with respect to temperature/pressure cycling; efficiency (energy consumed during fill)</td>
<td>N/A</td>
<td>Yes</td>
</tr>
<tr>
<td>Cryo-Adsorbent Material: Powder MOF-5</td>
<td>Modeling and experimental validation</td>
<td>SRNL / UQTR / Ford (BASF)</td>
<td>Theoretical H2 uptake; heat transfer (partial)</td>
<td>Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non-uniform packing)</td>
<td>Packing density, heat transfer, and adsorption capacity</td>
<td>N/A</td>
<td>Yes</td>
</tr>
<tr>
<td>Inter-Wall LN2 Pre-chiller: “Thermos Bottle”</td>
<td>Modeling only; Constant wall temperature models to show the need/benefit</td>
<td>PNNL / Lincoln Composites</td>
<td>1st-order thermal behavior can be modeled</td>
<td>Validate system thermal models; Phase-change within the channel must be evaluated experimentally</td>
<td>Choked flow due to LN2 phase change</td>
<td>Channel cross-section must remain intact</td>
<td>Yes – partially</td>
</tr>
<tr>
<td>Internal Heat Exchanger: MATI with Isolated-H2 Heating and Isolated-LN2 Cooling</td>
<td>Modeling and partial experimental validation of individual components/capabilities</td>
<td>OSU</td>
<td>1st-order thermal behavior has already been verified.</td>
<td>Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance</td>
<td>Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness</td>
<td>N/A</td>
<td>Yes – partially</td>
</tr>
<tr>
<td>Cryo-Adsorbent Material: Compacted MOF-5 “pucks” (0.32 g/cc)</td>
<td>Modeling and partial experimental validation</td>
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<td>Integral part of system; validate capacity and kinetic projections; Assess robustness and heat transfer limitations</td>
<td>Cracking/crumbling, heat transfer, and adsorbent behavior</td>
<td>N/A</td>
<td>Yes – partially</td>
</tr>
<tr>
<td>Type 1 Aluminum pressure vessel</td>
<td>Design and partial experimental validation</td>
<td>LC</td>
<td>Mass, volume, and cost</td>
<td>Integral part of system; validate capacity projections</td>
<td>Cryo-burst testing</td>
<td>N/A</td>
<td>Yes</td>
</tr>
<tr>
<td>Multi-layer vacuum insulation</td>
<td>Modeling of heating rate/dormancy performance</td>
<td>JPL</td>
<td>Partial dormancy performance</td>
<td>Validate dormancy model; vacuum level stability; robustness of design</td>
<td>No supplier (JPL work scope reduction)</td>
<td>N/A</td>
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Adsorbent System Phase 3 Proposal

Heat Exchange Systems
- HexCell/MOF-5 Powder
- Flow-Through Cooling
- Resistance Heating

Containment
- 2 Liter Type 1
- Segmented Al Tank

Test Facilities
- 0.3g/cc MOF-5 Puck
- MATI Heating/Cooling
- Type 1 SS
- Pressure Vessel
Future Work

Chemical System Phase 3 Proposal

Materials

20-40\(^{\circ}/_{\circ}\) AB/Si-oil

20-40\(^{\circ}/_{\circ}\) AlH\(_3\)/Si-oil

MPAB

System

Ammonia & Borazine Scrubbers

Gas/Liquid Separator

Reactor

Feed

Auger

TC1

TC cont

TC2

TC3

Effluent
Phase 3 Approach

- Design subscale prototype systems
- Synthesize materials
- Complete test facilities
- Acquire BoP components
- Fabricate/assemble prototype system
- Evaluate prototype under static conditions assessing performance against targets
- Compare to and refine models
- Modify test apparatus/prototype
- Post updated models on WEB
- Decommission prototypes as necessary
- Write Final Report
# Phase 3 Gantt Chart

## Future Work

<table>
<thead>
<tr>
<th>Task Name</th>
<th>Resource Names</th>
<th>Duration</th>
<th>Start</th>
<th>Finish</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design subscale prototype systems</td>
<td>SRNL/OSU</td>
<td>66 days</td>
<td>Mon 7/1/13</td>
<td>Mon 9/30/13</td>
</tr>
<tr>
<td>Acquire BOP System Components</td>
<td>UCTR/OSU</td>
<td>60 days</td>
<td>Wed 10/9/13</td>
<td>Tue 12/31/13</td>
</tr>
<tr>
<td>Acquire BOP System Components</td>
<td>LANL/UTRC</td>
<td>50 days</td>
<td>Wed 10/9/13</td>
<td>Tue 12/31/13</td>
</tr>
<tr>
<td>Evaluate prototype &amp; assess performance</td>
<td>UCTR/OSU</td>
<td>197 days</td>
<td>Tue 4/14</td>
<td>Wed 12/31/14</td>
</tr>
<tr>
<td>Compare to and refine models</td>
<td>LANL/UTRC</td>
<td>197 days</td>
<td>Tue 4/14</td>
<td>Wed 12/31/14</td>
</tr>
<tr>
<td>Modify test apparatus/prototype</td>
<td>LANL/UTRC</td>
<td>197 days</td>
<td>Tue 4/14</td>
<td>Wed 12/31/14</td>
</tr>
<tr>
<td>Post updated models on WEB</td>
<td>LANL/UTRC/FAMILAREL</td>
<td>30 days</td>
<td>Thu 1/15</td>
<td>Wed 12/31/15</td>
</tr>
<tr>
<td>Decommission prototypes as necessary</td>
<td>UCTR/OSU</td>
<td>40 days</td>
<td>Thu 1/15</td>
<td>Wed 12/31/15</td>
</tr>
<tr>
<td>Performance/Cost Model Updates</td>
<td>LANL/UTRC</td>
<td>161 days</td>
<td>Fri 5/16/14</td>
<td>Wed 12/31/14</td>
</tr>
<tr>
<td>Materials’ Requirements Refinement</td>
<td>NREL/PRNL/FMC</td>
<td>195 days</td>
<td>Fri 5/16/14</td>
<td>Wed 12/31/14</td>
</tr>
<tr>
<td>Project Management</td>
<td>SPNL</td>
<td>457 days</td>
<td>Thu 1/15</td>
<td>Thu 4/28/15</td>
</tr>
<tr>
<td>Write Final Report</td>
<td>All</td>
<td>56 days</td>
<td>Thu 1/15</td>
<td>Thu 4/28/15</td>
</tr>
</tbody>
</table>
Phase 3 Gantt Chart

SMART Milestones Being Developed for Each Contribution in Resources
Future Work

**Preliminary vs. Demonstrated Spider Chart**

*Why Phase 3 demonstration is critical in model validation*

Chemical Hydrogen Storage System (2012)
Future Work

Preliminary vs. Demonstrated Spider Chart

*Why Phase 3 demonstration is critical in model validation*

Chemical Hydrogen Storage System (2012)
## Technology Readiness Levels

### Materials Based Hydrogen Storage Systems for Automotive Applications

<table>
<thead>
<tr>
<th>TRL 1</th>
<th>TRL 2</th>
<th>TRL 3</th>
<th>TRL 4</th>
<th>TRL 5</th>
<th>TRL 6</th>
<th>TRL 7</th>
<th>TRL 8</th>
<th>TRL 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basic Technology Research</td>
<td>Research to Prove Feasibility</td>
<td>Technology Development</td>
<td>Technology Demonstration</td>
<td>System Commissioning</td>
<td>System Operation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Basic Principals</td>
<td>Concept Formulation</td>
<td>Characteristic Proof of Concept</td>
<td>System Validation in Laboratory Environment</td>
<td>System Validation in Relevant Environment</td>
<td>Pilot Scale System Validation</td>
<td>Full Scale System Validation</td>
<td>Actual System Qualification</td>
<td>Actual System Operation</td>
</tr>
</tbody>
</table>

**Materials CoEs**

- Basic Technology Research
  - Basic Principles
  - Concept Formulation
- Research to Prove Feasibility
  - Characteristic Proof of Concept
- Technology Development
  - System Validation in Laboratory Environment
- Technology Demonstration
  - System Validation in Relevant Environment
- System Commissioning
  - Pilot Scale System Validation
- System Operation
  - Full Scale System Validation
  - Actual System Qualification
  - Actual System Operation

---

**Images:**
- Fuel cell and heat exchanger diagram
- Vacuum jacket insulation and high pressure vessel with resistance heating
- Waste heat recirculated
- Engine efficiency graph
- Temperature distribution diagram
- Laboratory setup for system validation
- Actual system validation setup
- Actual system operation of hydrogen storage system
Summary

• Adsorption Systems
  • Limited in volumetric density and dormancy at ~77K due to materials
  • Temperature assisted PSA using a Type I tank at 60 bar is proposed for subscale prototype demonstration.

• Chemical Systems
  • Limited in gravimetric density and efficiency due to materials.
  • Liquid/Slurry flow through reactors with GLS and purification is proposed for subscale prototype demonstration.

• Phase 3 Go/NoGo meetings held with DoE with results forthcoming.
Technical Back-Up Slides
Integrated Model Framework

\[ n_{\text{ex}} = n_{\text{acc}} \exp \left[ - \frac{RT}{(\alpha + \beta T)} \right] \ln \left( \frac{P_0}{P} \right) - \rho_a V_a \]

**Vehicle level model**
- Max power achievable by fuel cell [W]
- Power achieved by fuel cell [W]
- Storage aux power request [W]
- Aux power to storage [W]
- Storage system result output
- Power requested from fuel cell [W]
- Fuel cell system result output
- Storage tank state
- H2 use rate [mol/s]
- Vehicle level parameters

**Fuel cell system**
- H2 stream in
- H2 stream out
- Waste heat stream in
- Waste heat stream out
- Vehicle

**H2 storage system**
- UTRC NaAlH4 Powder
- H2 requested
- H2 stream out
- UTRC NaAlH4 Pellets
- UTRC/SRNL 1:1 Li-Mg-N-H
- GM NaAlH4
- GM/SRNL/JPL AX-21
- PNNL Solid AB
- PNNL/LANL Liquid AB
- 350 bar Compressed
- 700 bar Compressed

**SRNL 200 bar AX-21 Flow-Through**
Integrated Model Framework

Vehicle level model

Fuel cell system

Parameter input:

Vehicle level parameters
Fuel cell design parameters
Storage system design parameters

Vehicle speed [m/s]

H2 use rate [mol/s]

Power requested from fuel cell [W]

Power achieved by fuel cell [W]

Max power achievable by fuel cell [W]

Vehicle level model

SRNL 200 bar
AX-21
Flow-Through

UTRC NaAlH₄ Powder
H₂ requested
H₂ stream out

UTRC NaAlH₄ Pellets

UTRC/SRNL 1:1 Li-Mg-N-H

GM NaAlH₄

GM/SRNL/JPL AX-21

PNNL Solid AB

PNNL/LANL Liquid AB

350 bar Compressed

700 bar Compressed

Design parameters

Design results

Tank state

Aux power in [W]

Aux power request [W]

H₂ use rate [mol/s]

H₂ requested [mol/s]

H₂ stream out

Waste heat stream in

Waste heat stream out

Fuel cell system

Storage system

HSECoE