Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage

United Technologies Research Center

DOE Hydrogen Program
Annual Merit Review
Washington, DC
May 11, 2011

Project ID: ST006

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Overview

Timeline
- Start: February 2009
- End Phase 1: March 2011
- End Phase 2: July 2013
- End Phase 3 / Project: June 2014
- Percent complete: 32% (spending)

Barriers*
- A – J
- A. System Weight & Volume
- E. Charging / Discharging Rates
- J. Thermal Management

Budget
- $6.86M Total Program
  - $5.32M DOE
  - $1.55M (22.5%) UTRC
- FY10: $1.00M DOE
- FY11: $950k DOE

Targets*
- All

Partners

* DOE EERE HFCIT Program Multi-year Plan for Storage

IEA HIA Task 22
Objectives

- Design of materials based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles

<table>
<thead>
<tr>
<th>Performance Measure</th>
<th>Units</th>
<th>2010</th>
<th>2015</th>
<th>Ultimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Gravimetric Capacity</td>
<td>g H₂ /kg system</td>
<td>45</td>
<td>55</td>
<td>75</td>
</tr>
<tr>
<td>System Volumetric Capacity</td>
<td>g H₂ /L system</td>
<td>28</td>
<td>40</td>
<td>70</td>
</tr>
<tr>
<td>System fill time (for 5 kg H₂)</td>
<td>minutes</td>
<td>4.2</td>
<td>3.3</td>
<td>2.5</td>
</tr>
<tr>
<td>Fuel Purity</td>
<td>% H₂</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Relevance**

- Performance Measure Units 2010 2015 Ultimate
- System Gravimetric Capacity  g H₂ /kg system  45 55 75
- System Volumetric Capacity  g H₂ /L system  28 40 70
- System fill time (for 5 kg H₂)  minutes  4.2 3.3 2.5
- Fuel Purity  % H₂  SAE J2719 guideline (99.97% dry basis)

- Major project impact:
  - H₂ storage systems comparison on common basis for Go/No-Go decision:
    - Integrated Power Plant Storage System Modeling
    - Volumetric capacity (compaction)
    - System fill time (thermal conductivity, HX design)
    - Fuel purity (purification cartridge to remove NH₃)
    - Qualitative risk analysis (QLRA)
Approach

- Leverage in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials based H₂ storage for automotive applications.

<table>
<thead>
<tr>
<th>Month/Year</th>
<th>Go/No-Go Decision</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feb-11</td>
<td>Provide a system model for each material sub-class (metal hydrides, adsorption, chemical storage) which shows:</td>
<td>Completed</td>
</tr>
<tr>
<td></td>
<td>● 4 of the DOE 2010 system storage targets are fully met</td>
<td></td>
</tr>
<tr>
<td></td>
<td>● Status of the remaining targets must be at least 40% of the target or higher</td>
<td></td>
</tr>
</tbody>
</table>
IPPSSM framework development

System Results for comparison with DOE targets

Vehicle-Level Model (NREL)
- System performance
  - Drive cycle
  - Power requested to fuel cell
  - Power achieved by fuel cell

Fuel Cell System (Ford)
- H₂ stream in
- H₂ request
- Power requested
- Power achieved

H₂ Storage Systems
- UTRC NaAlH₄ Powder
- 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

Quantitative comparison of H₂ storage systems on a common basis achieved by team effort
Compaction of (complex) metal hydrides

Address low volumetric capacity issue due to low powder density through compaction and higher capacity materials.

Li-Mg-N-H system requires binder (e.g. Expanded Natural Graphite (ENG)).
Mesh reinforcement reduces volumetric expansion and yields stronger pellets after absorption/desorption cycles but DOE target is 1,500 cycles.
Thermal conductivity enhancement

- Fast refueling time with SAH requires an effective bed thermal conductivity of 4-8 W/m/K

- Compaction of SAH without additives is not sufficient (AMR 2010)

Aluminum powder is ineffective; Use aluminum fins. Expanded Natural Graphite can be effective when used as ‘worms’ causing thermal conductivity anisotropy.
Technical Accomplishments and Progress

Thermal conductivity anisotropy with ENG ‘worms’

- **Thermal conductivity experiment**

  ![Graph showing temperature rise vs. time for axial and radial directions.](Image)

  - **Objective** = \((\text{Experiment}_\text{axial} - \text{Comsol}_\text{axial})^2 + (\text{Experiment}_\text{radial} - \text{Comsol}_\text{radial})^2\)

  - Matlab® optimizer

- **COMSOL™ model development**

  - Applied load during compaction

- **Fit to experimental data**

- **Results for 8 LiH : 3 Mg(NH₂)₂**

<table>
<thead>
<tr>
<th>ENG wt.%</th>
<th>k radial [W/m/K]</th>
<th>k axial [W/m/K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAH</td>
<td>5</td>
<td>10.8</td>
</tr>
<tr>
<td>LiMgNH</td>
<td>5</td>
<td>1.56</td>
</tr>
<tr>
<td>LiMgNH</td>
<td>10</td>
<td>2.64</td>
</tr>
<tr>
<td>LiMgNH</td>
<td>15</td>
<td>11.6</td>
</tr>
</tbody>
</table>

Induce high thermal conductivity towards the heat exchanger tube
Heat exchanger optimization for fast refueling

- Refueling time target 10.5 minutes (40% of DOE 2010 target)
- 90% of materials capacity (SAH) equals 3.06 wt.%
- $T_{\text{max}} = 170^\circ\text{C}$
- $P_{H_2} = 100$ bar:
  - Low pressure system
  - Less carbon fiber, lower cost

Determined minimum HX mass inside SAH bed that would allow 90% of $H_2$ storage capacity in 10.5 minutes.
Performance modeling (COMSOL™)

- **Gravimetric capacity**
- **Volumetric capacity**

Pelletized SAH kinetics (updated) in combination with HX design enables 90% of storage capacity in 10.5 minutes.
Concept evaluation (Lab-scale)

- Integration with HX
- SAH pellets around HX tube

Technical Accomplishments and Progress
Concept evaluation (Lab-scale)

- Repaired/Modified PCT control system
- Adjusted COMSOL™ model with updated kinetics and axi-symmetry of test article

Validate key components and concepts at an appropriate scale for Phase 2
**Technical Accomplishments and Progress**

**Framework results**

**NaAlH$_4$ powder and compacted pellets systems**
- Maximum operating temperature: 170°C
- System starts at 20°C and delivers 5.6 kg H$_2$ to fuel cell
- Back-to-back EPA Fuel Economy test drive cycles
- Pressure drops during heat-up as gas in voids is sent to combustor to bring the system to operating temperature.

**NaAlH$_4$ powder system running Fuel Economy Test drive cycles**

**Initial pressure drop:** H$_2$ gas in voids is sent to combustor to heat up the system.

Buffer size can be reduced by 30% if buffer at 20°C instead of 140°C.

**H$_2$ buffer requirement for startup limits benefits of compaction**
**Framework results**

<table>
<thead>
<tr>
<th>Form</th>
<th>Amount [kg]</th>
<th>Buffer Volume [Liter]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NaAlH₄</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.1 wt.% in 10.5 min.</td>
<td>243</td>
<td>-</td>
</tr>
<tr>
<td>Pellet</td>
<td>255</td>
<td>53</td>
</tr>
<tr>
<td><strong>1:1 LiMgNH</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7 wt.%</td>
<td>92</td>
<td>90</td>
</tr>
<tr>
<td>Pellet</td>
<td>93</td>
<td>90</td>
</tr>
</tbody>
</table>

**Considered (complex) metal hydride systems are heavy and occupy a large volume**
Framework results

Weight and volume*: main contributors

- Effect of increased capacity:
  - BOP weight and volume become increasingly important when using a higher capacity material.

- Guidance:
  - BOP weight and volume reduction important when using higher capacity material
  - Make buffer tank separate from hydride storage system

* Using BOP components library developed by PNL
Enabling technology: $H_2$ quality

- **Objective:** Develop system methods to improve discharged hydrogen purity / quality for acceptable PEM fuel cell durability (SAE J2719 APR2008 guideline)

**Technical Accomplishments and Progress**

- **Particulates:** $<10\mu m$, $<1\mu g/l$, ASTM D7650

**Ammonia adsorbent (UTRC)**

**Chemical hydrides**
- LiMgNH

**Complex metal hydrides**

**Adsorbents**
- AX21

**Consensus Concentration [ppm]**

<table>
<thead>
<tr>
<th></th>
<th>Borazine</th>
<th>Diborane</th>
<th>Ammonia</th>
</tr>
</thead>
<tbody>
<tr>
<td>AB</td>
<td>1000</td>
<td>-</td>
<td>619</td>
</tr>
</tbody>
</table>

**Quantification:** Ammonia, Diborane, Borazine, Solvents (LANL, PNL)
**Objective:** Identify the critical risks, failure modes and technical challenges of three \( \text{H}_2 \) storage systems.

<table>
<thead>
<tr>
<th></th>
<th>On-board sodium alanate system (UTRC)</th>
<th>Off-board solid AB system (PNNL)</th>
<th>On-board cryo-adsorption system (ANL)</th>
<th>On-board cryo-adsorption system (GM)</th>
</tr>
</thead>
</table>

### Examples of Critical Risks, Failure Modes and Technical Challenges

**Risk:** Potential for dust explosion in air (wet/dry). Also, fire and/or explosion of released \( \text{H}_2 \) gas.

**Failure mechanism:** accidental rupture of storage vessel upon collision.

**Risk:** material reactivity with water and subsequent fire and vessel failure by overpressurization.

**Failure mechanism:** water intrusion in-vessel.

**Risk:** Runaway chemical reaction during AB thermolysis.

**Failure mechanism:** Loss of thermolysis exothermic heat removal capability.

**Risk:** Release of toxic gases (diborane and borazine) during solid AB thermolysis.

**Failure mechanism:** Rupture of the on-board spent fuel tank or pipe leaks from the system.

**Risk:** Loss of vacuum insulation enhances heat influx through the tank wall causing boil off of stored \( \text{H}_2 \), pressurizing the storage tank, loss of \( \text{H}_2 \) inventory via PRD venting and potential for tank failure by overpressurization if PRD venting rate is not sufficient.

**Note:** Loss of \( \text{H}_2 \) via PRD venting and permeation through the tank wall reduce the mass of stored \( \text{H}_2 \) available to feed the on-board fuel cells.

**Failure mechanism:** Stored \( \text{H}_2 \) gradually permeates / diffuses to the vacuum insulation gap leading to pressurizing the gap with \( \text{H}_2 \).
Safety categorization of $H_2$ storage media

**Objective:** develop a framework for safety categorization of $H_2$ storage media for on-board vehicular applications.

- The storage media can be solid, liquid, or slurry and include: Metal hydrides, chemical hydrides and adsorbents
- Categorization is based on risk assessment of: Material reactivity, pyrophoricity, sensitivity to mechanical impact, toxicity, chemical stability, ability to cause runaway chemical reaction, on-board vehicular use & handling and off-board regeneration/recycling.
- Material risk includes adverse impact on human safety, health and environment impact.
- Four categories of material risk: Green, Yellow, Orange and Red.

<table>
<thead>
<tr>
<th>Safety Categories of Storage Media</th>
<th>Classification Criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>GREEN</td>
<td>Material's chemistry is green, i.e., causes no risks to human health and/or the environment. Qualifying features: 1) No release of toxic chemicals during its manufacturing, on-board vehicular use or regeneration/recycling. 2) Material is chemically stable, i.e., non-ignition, non-explosive, non-reactive. 3) Non-corrosive and no material compatibility concerns. 4) Not sensitive to mechanical impact.</td>
</tr>
<tr>
<td>YELLOW</td>
<td>Low-to-moderate-risk material. Qualifying features: 1) Material may release very low concentrations of toxic chemicals during its manufacturing, use or regeneration/recycling. Releases are of no harm to human and/or the environment. 2) Risk can be eliminated through risk mitigation. Examples: a) Material's pyrophoricity and water reactivity can be eliminated by powder compaction. b) Material's temperature sensitivity can be eliminated by stabilizing the material using additives with green chemistry features.</td>
</tr>
<tr>
<td>ORANGE</td>
<td>High risk material. Qualifying features: 1) Material releases high concentrations of toxic chemical during its manufacturing, use or regeneration/recycling. Releases are harmful to human health and/or the environment. 2) Risk may be eliminated/reduced through risk mitigation but cost would be high, process is complex, additives are of non-green chemistry, additives adversely impact the volumetric and/or gravimetric storage capacity.</td>
</tr>
<tr>
<td>RED</td>
<td>Material’s risk is unacceptable to human health and/or the environment. Qualifying features: 1) Material may release unacceptably high concentrations of toxic chemicals during its manufacturing, use or regeneration/recycling. Releases are harmful to human health and/or the environment. 2) Risk cannot be eliminated through risk mitigation. Examples: a) Material's pyrophoricity and water reactivity cannot be eliminated by powder compaction. b) Material's temperature sensitivity cannot be eliminated by stabilizing the material using additives with green chemistry features. c) Material may cause a runaway chemical reaction.</td>
</tr>
</tbody>
</table>

**Phase-II risk analysis activities**
- Perform failure modes and effects analysis (FMEA) to rank material and system risks based on the probability of occurrence and severity of consequences.
- Populate the safety categorization framework.

**Collaborations**
- Continue to incorporate risk insights from UTRC materials reactivity contract.
- Continue to incorporate quantitative insights from SNL and SRNL reactivity contracts.
## FY11 and FY12 Plan

<table>
<thead>
<tr>
<th>FY11</th>
<th>FY12</th>
</tr>
</thead>
<tbody>
<tr>
<td>2Q</td>
<td>3Q</td>
</tr>
<tr>
<td><strong>Go/No-Go meeting for Phase 1 to Phase 2 transition</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Design FMEA of H₂ storage systems: improve levels of quantitative risk assessment</strong></td>
<td></td>
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<tr>
<td><strong>Improve understanding of DOT requirements</strong></td>
<td></td>
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<tr>
<td><strong>Framework maintenance and support and updating models</strong></td>
<td></td>
</tr>
<tr>
<td><strong>LiMgNH system implementation in Framework</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Enable sensitivity studies with Framework</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Address data gaps in material properties</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Further develop internal mesh reinforcement path of compacted hydrides</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Evaluation hydride pellet / HX tube concept</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Screen NH₃ sorbent with higher capacity that is regenerable</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Fabricate and evaluate test article for impurity mitigation</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Evaluate particulate mitigation strategies</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Prioritize tasks after DOE’s review of Go/No-Go presentation materials</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Solid transport quantification with surrogate material</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Gas/liquid separation design for liquid chemical hydride system</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Engineer specialty components and their evaluation</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Support material and system selection of best technology for Phase 3</strong></td>
<td></td>
</tr>
</tbody>
</table>
## Summary

### Relevance:
Design of materials based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles.

### Approach:
Leverage in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials based H$_2$ storage for automotive applications.

### Technical Accomplishments and Progress:
- Simulink framework generated a quantitative comparison of all three hydrogen storage systems on a common basis for the Go/No-Go decision.
- Compaction know-how transferred from SAH to LiMgNH system; Identified need for binder; SAH pellet stabilization with internal mesh demonstrated.
- Additives evaluated for thermal conductivity enhancement; introduced preferred thermal conductivity enhancement towards HX tube (anisotropy).
- Designed heat exchanger with minimal weight for fast refueling of SAH tank.
- Revitalized PCT for evaluating concept of SAH pellet integration with HX tube.
- Screened ammonia sorbents and particulate filter to enable sufficient H$_2$ purity.
- Qualitative risk assessment of all three H$_2$ storage systems.

### Collaboration:
Simulink framework recognized as successful effort of HSECoE as it enabled a team effort and yielded results at a critical time (Go/No-Go).

### Future Work:
Work towards milestones and next phase Go/No-Go decision.
Acknowledgements

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Technical Back-Up Slides
**Center structure – roles & collaborations**

### Hydrogen Storage Engineering Center of Excellence

- **D. Anton, SRNL**
- **T. Motyka, SRNL**

#### Materials Operating Requirements
- **D. Herling, PNNL**
  - Materials Centers of Excellence Collaboration – SRNL, LANL, NREL
  - Reactivity & Compatibility – UTRC
  - Adsorption Properties – UQTR
  - Metal Hydride Properties – SRNL
  - Chemical Hydride Properties – LANL
  - Media Structure - GM

#### Transport Phenomena
- **B. Hardy, SRNL**
  - Bulk Materials Handling – PNNL
  - Mass Transport – SRNL
  - Thermal Transport – SRNL

#### Enabling Technologies
- **J. Reiter, JPL**
  - Thermal Insulation – JPL
  - Hydrogen Purity – UTRC
  - Sensors – LANL
  - Thermal Devices - OSU
  - Pressure Vessels - PNNL

#### Performance Analysis
- **M. Thornton, NREL**
  - Vehicle Requirements – NREL
  - Tank-to-Wheels Analysis – NREL
  - Forecourt Requirements - UTRC
  - Manufacturing & Cost Analysis - PNNL

#### Integrated Power Plant / Storage System Modeling
- **B.A. van Hassel, UTRC**
  - Off-Board Rechargeable - PNNL
  - On-Board Rechargeable – GM
  - Power Plant – Ford

#### Subscale Prototype Construction, Testing & Evaluation
- **T. Semelsberger, LANL**
  - Risk Assessment & Mitigation – UTRC
  - System Design Concepts and Integration - LANL
  - Design Optimization & Subscale Systems – LANL, SRNL, UQTR
  - Fabricate Subscale Systems Components – SRNL, LANL
  - Assemble & Evaluate subscale Systems – LANL, JPL, UQTR

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**Leading / Project Tasks**

**Additional Project Tasks**

**Supporting**

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[Image of the diagram]
Vibration packing

Objective: Evaluate whether vibration packing of adsorbent material like AX21/Maxsorb can improve density from 0.3 g/cm³ to 0.6 g/cm³ without binder additions

Expectations for packing density:

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
<th>Packing density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dense regular packing</td>
<td>Monodisperse spheres</td>
<td>0.7405</td>
</tr>
<tr>
<td>Random close packing</td>
<td>Bimodal particle size distribution</td>
<td>0.75-0.68</td>
</tr>
<tr>
<td>Random close packing</td>
<td>E.g. the bed vibrated</td>
<td>0.641-0.625</td>
</tr>
<tr>
<td>Random loose packing</td>
<td></td>
<td>0.58</td>
</tr>
</tbody>
</table>
Vibration packing principle

Shakers in two directions

Maxsorb

Accelrometer
Vibration packing did not improve density of AX21/Maxsorb above 0.3 g/cm³. AX21/Maxsorb needs to be kept under compression to yield 0.6 g/cm³.
Kinetics of NaAlH₄ + 4 mol% TiCl₃ remeasured

- H₂ Absorption Rate
- Capacity loss upon aging at 180°C, 110-100 bar H₂ partial pressure

**SAH + 4 mol% TiCl₃ has considerably higher kinetics than Prototype 2 material. Consider 170°C upper limit for SAH to avoid capacity loss.**
Kinetics and heat transfer for LiMgNH system

- Requirement
  - A fast system fill time
  - Enablers:
    - Kinetics yields 90% of materials capacity at targeted fill time
    - Not reduced by compaction
    - (Complex) metal hydride bed effective thermal conductivity 4-8 W/m/K

<table>
<thead>
<tr>
<th>System Fill Time [min]</th>
<th>2010</th>
<th>3.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ultimate</td>
<td>2.5</td>
<td></td>
</tr>
</tbody>
</table>

![Graph showing Wt. % H2 and Time in minutes for different systems and conditions.](chart)

*HSECoE United Technologies Research Center*
Objectives:
- Functionally demonstrate solid hydride transport
- Identify key challenges to on board bulk material handling
- Support March 2011 go/no-go decision (BMH)

Scope:
- Material: surrogate representative of solid candidate fuels
- Engineering forms: powder and encapsulated pellets
- Through reactor and fuel tanks

Evaluation metric:
- Distance over which the material is transported
- Elevation that one needs to be able to achieve
- Section with curvature and hot zone
- Rate at which the material is transported
- Absolute pressure and/or pressure difference
- Scalability
Flexible rectangular coil screw as primary propulsion element

Teflon outer tube and inner core forming an annular passage to minimize flow back

Curved material passage to mimic for reactor

Low speed feeding and metering by variable speed drive (up to 600 rpm of screw speed)

*Microthene G polyolefin powders* (50 mesh) used as surrogated material for Ammonia Borane
Weight & volume correlation for 100 bar pressure vessels

- To quickly obtain weight and volume of a Type IV pressure vessel, Lincoln Composites provided some cases for different internal volumes at 100 bar.
  - Type IV tank.
  - Rated for 100 bar (2.25 FS)

- A simple linear correlation is used to determine the additional weight and volume due to the pressure vessel at intermediate points.

\[
y = 0.137x + 3.7408 \\
R^2 = 0.9938
\]

\[
y = 0.142x - 1.3099 \\
R^2 = 0.9963
\]
## Drive cycles & test conditions for use in the framework

<table>
<thead>
<tr>
<th>Case</th>
<th>Test Schedule</th>
<th>Cycles</th>
<th>Description</th>
<th>Test Temp (°F)</th>
<th>Distance per cycle (miles)</th>
<th>Duration per cycle (minutes)</th>
<th>Top Speed (mph)</th>
<th>Average Speed (mph)</th>
<th>Max. Acc. (mph/sec)</th>
<th>Stops</th>
<th>Idle</th>
<th>Avg. H2 Flow (g/s)*</th>
<th>Peak H2 Flow (g/s)*</th>
<th>Expected Usage</th>
</tr>
</thead>
</table>
| 1    | Ambient Drive Cycle | UDDS   | Low speeds in stop-and-go urban traffic          | 75 (24 C)      | 7.5                         | 22.8                         | 56.7            | 19.6                | 3.3                 | 17    | 19%  | 0.09                | 0.69                | 1. Establish baseline fuel economy (adjust for the 5 cycle based on the average from the cycles)
|      |                     |        |                                                  |                |                             |                              |                 |                     |                     |       |      |                     |                     | 2. Establish vehicle attributes                                              |
|      |                     |        |                                                  |                |                             |                              |                 |                     |                     |       |      |                     |                     | 3. Utilize for storage sizing                                                |
| 2    | Aggressive Drive    | US06   | Higher speeds; harder acceleration & braking      | 75 (24 C)      | 10.26                       | 12.75                        | 60              | 48.3                | 3.2                 | 0     | 0%   | 0.15                | 0.56                | Confirm fast transient response capability – adjust if system does not perform function |
| 3    | Cold Drive Cycle    | FTP-75 (cold) | FTP-75 at colder ambient temperature  | -4 (-20 C)    | 11.04                       | 31.2                         | 56              | 21.1                | 3.3                 | 23    | 18%  | 0.07                | 0.66                | 1. Cold start criteria
|      |                     |        |                                                  |                |                             |                              |                 |                     |                     |       |      |                     |                     | 2. Confirm cold ambient capability – adjust if system does not perform function |
| 4    | Hot Drive Cycle     | SC03   | AC use under hot ambient conditions              | 95 (35 C)      | 3.6                         | 9.9                          | 54.8            | 21.2                | 5.1                 | 5     | 19%  | 0.09                | 0.97                | Confirm hot ambient capability - adjust if system does not perform function |
| 5    | Dormancy Test       | n/a    | Static test to evaluate the stability of the storage system | 95 (35 C)      | 0                           | 31 days                      | 0               | 0                   | 0                   | 100%  | 100% |                     |                     | Confirm loss of useable H2 target                                            |

*Based on NREL simulation with compact vehicle, 5.6 kg usable H2, 80 kW fuel cell with a 20 kW battery
**NaAlH$_4$ (uncompacted powder) system diagram**

- **243** kg hydride needed to deliver 5.6 kg to the fuel cell.
- System: **410 kg, 438 liters = 1.37 wt%, 13 g-H$_2$/L**
- No separate buffer tank. All gas comes from the pores.

Adapted from the GM alanate system diagram.
NaAlH₄ powder system: Case 1 for sizing

- **Main parameters**
  - Usable H₂: 5.6 kg
  - Total weight: 410.2 kg
  - Total volume: 438 L
  - Gravimetric capacity: 1.37%
  - Volumetric capacity: 12.8 g/L

- **Material (pelletized)**
  - Gravimetric capacity: 3.1%
  - Porosity: 56%

- **Weights**
  - Material: 243 kg
  - Heat exchanger: 41.6 kg
  - Pressure vessel (additional): 45.8 kg
  - Heat transfer fluid loop: 70.53 kg
  - Hydrogen loop: 7.61 kg
  - Isolation valve: 1.65 kg

- **Volumes**
  - Tank internal volume: 307 L
  - Pressure vessel (additional): 42.3 L
  - Heat transfer fluid loop: 47.7 L
  - Hydrogen loop: 40.2 L
  - Isolation valve: 0.26 L

- **Other targets**
  - On-board efficiency: 70%
  - Cold/hot cases: OK
  - Dormancy: N/A
  - Delivery temperature: < 85°C
  - Min delivery pressure: 5 bar
  - Min full flow rate: 1.6 g/s
NaAlH₄ (compacted pellets) system diagram

- 255 kg hydride needed to deliver 5.6 kg to the fuel cell.
- System: 395 kg, 377 liters = 1.42 wt%, 15 g-H₂/L
- No separate buffer tank: additional 53 L in-tank provided.

Adapted from the GM alanate system diagram
NaAlH$_4$ compacted system: Case 1 for sizing

- **Main parameters**
  - Usable H$_2$: 5.6 kg
  - Total weight: 394.8 kg
  - Total volume: 376.6 L
  - Gravimetric capacity: 1.42%
  - Volumetric capacity: 15 g/L

- **Material (pelletized)**
  - Gravimetric capacity: 3.1%
  - Porosity: 29%

- **Weights**
  - Material: 255 kg
  - Heat exchanger: 21.5 kg
  - Pressure vessel (additional): 38.5 kg
  - Heat transfer fluid loop: 70.53 kg
  - Hydrogen loop: 7.61 kg
  - Isolation valve: 1.65 kg

- **Volumes**
  - Tank internal volume: 253.7 L
  - Pressure vessel (additional): 34.7 L
  - Heat transfer fluid loop: 47.7 L
  - Hydrogen loop: 40.2 L
  - Isolation valve: 0.26 L

- **Other targets**
  - On-board efficiency: 69%
  - Cold/hot cases: OK
  - Dormancy: N/A
  - Delivery temperature: < 85°C
  - Min delivery pressure: 5 bar
  - Min full flow rate: 1.6 g/s
Comparison of NaAlH$_4$ powder and compacted pellets systems

- There is a trade-off in compacting the material.
  - A reduction in pore volume can be effective up to a point.
  - Further compaction results in insufficient gas initially to heat the system to operating conditions → additional buffer space must be provided.
1:1 Li-Mg-N-H (uncompacted powder) system

- 92 kg hydride needed to deliver 5.6 kg to the fuel cell.
- System: 240 kg, 348 liters = 2.33 wt%, 16.1 g-H₂/L
- No separate buffer tank: additional 90 L in-tank provided for cold start.

Gravimetric improvement is driven by the material. Volumetric improvement is marginal due to need for extra volume for cold start.
1:1 Li-Mg-N-H powder Case 1 for sizing

- **Main parameters**
  - Usable H2: 5.6 kg
  - Total weight: 240 kg
  - Total volume: 348 L
  - Gravimetric capacity: 2.33%
  - Volumetric capacity: 16.1 g/L

- **Material (pelletized)**
  - Gravimetric capacity: 7.5%
  - Porosity: 50%

- **Weights**
  - Material: 92 kg
  - Heat exchanger: 32 kg
  - Pressure vessel (additional): 35 kg
  - Heat transfer fluid loop: 70.5 kg
  - Hydrogen loop: 7.6 kg
  - Isolation valve: 1.65 kg

- **Volumes**
  - Tank internal volume: 229 L
  - Pressure vessel (additional): 31.1 L
  - Heat transfer fluid loop: 47.7 L
  - Hydrogen loop: 40.2 L
  - Isolation valve: 0.26 L

- **Other targets**
  - On-board efficiency: 75%
  - Cold/hot cases: OK
  - Dormancy: N/A
  - Delivery temperature: < 85C
  - Min delivery pressure: 5 bar
  - Min full flow rate: 1.6 g/s
1:1 Li-Mg-N-H (compacted pellets) system

- 92.5 kg hydride needed to deliver 5.6 kg to the fuel cell.
- System: 218 kg, 311 liters = 2.75 wt%, 18 g-H₂/L
- No separate buffer tank: additional 90 L in-tank provided for cold start.

Gravimetric improvement is driven by the material. Volumetric improvement is marginal due to need for extra volume.

- In-tank buffer is inefficient for this case: a separate buffer with colder H₂ may be more effective.
1:1 Li-Mg-N-H compacted Case 1 for sizing

- **Main parameters**
  - Usable H₂: 5.6 kg
  - Total weight: 218 kg
  - Total volume: 311 L
  - Gravimetric capacity: 2.75%
  - Volumetric capacity: 18 g/L

- **Material (pelletized)**
  - Gravimetric capacity: 7.5%
  - Porosity: 25%

- **Weights**
  - Material: 92.5 kg
  - Heat exchanger: 15 kg
  - Pressure vessel (additional): 30.7 kg
  - Heat transfer fluid loop: 70.53 kg
  - Hydrogen loop: 7.61 kg
  - Isolation valve: 1.65 kg

- **Volumes**
  - Tank internal volume: 196 L
  - Pressure vessel (additional): 26.7 L
  - Heat transfer fluid loop: 47.7 L
  - Hydrogen loop: 40.2 L
  - Isolation valve: 0.26 L

- **Other targets**
  - On-board efficiency: 75%
  - Cold/hot cases: OK
  - Dormancy: N/A
  - Delivery temperature: < 85°C
  - Min delivery pressure: 5 bar
  - Min full flow rate: 1.6 g/s
Capacity comparison summary

Gravimetric capacity (weight %)

- TiCrMn (GM)
- Alanate dual bed (GM)
- Alanate powder
- Alanate pellets
- 1:1 Li-Mg-N-H powder
- 1:1 Li-Mg-N-H pellets

2010 Target: 27.3
2015 Target: 28

Volumetric capacity (g-H₂/L)

- 2010 Target: 43
- 2015 Target: 40

- Independent alanate powder system analyses (GM & UTRC) give comparable results. The difference in gravimetric capacity is due to the pressure vessel assumption: Composite tank + Steel liner (GM) vs Type IV (UTRC).

- Most promising is the 1:1 Li-Mg-N-H compacted system:
  - Gravimetric capacity: 61% of 2010 target, 50% of 2015 target
  - Volumetric capacity: 64% of 2010 target, 45% of 2015 target
Weight and volume: main contributors

**NaAlH₄ powder**
- Total: 410 kg
- Hydride: 59%
- Pores: 11%
- Pressure vessel: 10%
- Oil heating loop: 17%
- Buffer: 6%
- Other: 4%

**NaAlH₄ pellets**
- Total: 395 kg
- Hydride: 65%
- Pores: 5%
- Pressure vessel: 10%
- Oil heating loop: 18%
- Buffer: 14%
- Other: 0%

**1:1 LiMgN powder**
- Total: 240 kg
- Hydride: 38%
- Pores: 50%
- Pressure vessel: 9%
- Oil heating loop: 11%
- Buffer: 14%
- Other: 0.4%

**1:1 LiMgN pellets**
- Total: 218 kg
- Hydride: 42%
- Pores: 32%
- Pressure vessel: 14%
- Oil heating loop: 32%
- Buffer: 29%
- Other: 1%