Systems Engineering of Chemical Hydride, Pressure Vessel, and Balance of Plant for On-Board Hydrogen Storage

*D. Herling, K. Brooks, E. Ronnebro, S. Rassat, K. Simmons, M. Weimar*

DOE Fuel Cell Technology Program
Annual Merit Review

June 8, 2010
Technology Development Manager: Monterey Gardiner
Overview

Timeline
- Start: Feb. 2009
- Project End: Jan. 2014
  - End Phase 1: 2011
  - End Phase 2: 2013
  - End Phase 3: 2014

Budget
- $6.2M Total (PNNL) anticipated
  - DOE direct funded
  - No cost-share required for National Lab
- FY09: $600k
- FY10: $1.5M

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
- O. Hydrogen Boil-Off
- S. By-Product/Spent Material Removal

Partners

Proudly Operated by Battelle Since 1965
Introduction: PNNL Scope in HSECoE

Roles Supporting Engineering Center Structure
- Technology Area Lead (TAL) for Materials Operating Requirements
- Coordinate activities as the Technology Team Lead (TTL)
  - Bulk Materials Handling (Transport Phenomena)
  - Pressure Vessels (Enabling Technologies)
  - Manufacturing and Cost Analysis (Performance Analysis)
- Liaison to VT Program projects and resources

Technology Development and System Engineering Tasks
- Solid Chemical Hydride System Design
- Process Modeling & Engineering
- Kinetics & Materials Characterization
- Microarchitectures Device Development
- Materials Reactivity & Compatibility
- Containment and Pressure Vessel Design
- Manufacturing & Cost Analysis
Relevance: Hydrogen Storage

► Impact to FCT Program
  ■ Demonstrate high level of performance that meets DOE 2015 targets using solid chemical hydrogen storage
  ■ Apply materials discoveries and knowledge developed as part of the Materials Centers of Excellence

► Hydrogen Storage Community at Large
  ■ Develop and/or advanced modeling and simulation tools for the optimum design and engineering of on-board storage systems
  ■ Functional prototype systems available to OEMs
  ■ Engineering methodologies, analysis tools, and designs applicable to stationary storage and portable power applications
  ■ U.S. demonstration of on-board storage to advance state of the art globally
Approach: Objectives and Deliverables

► Technical Objectives of PNNL Scope
  ■ Design of chemical hydride hydrogen storage system & balance of plant (BoP) components
  ■ Reduce system volume and weight and optimize storage capability, fueling, and hydrogen supply performance
  ■ Mitigate materials incompatibility issues associated with hydrogen embrittlement, corrosion, and permeability
  ■ Demonstrate the performance of economical, compact, lightweight vessels for hybridized storage
  ■ Guide design and technology down selection through cost modeling and manufacturing analysis

► Program and annual Deliverables established
► Phased/gated progressions aligning with HSECoE go/no-go decisions

Focus is on Process Engineering, System Design and Functional Integration
<table>
<thead>
<tr>
<th>Quarter</th>
<th>Task</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>7</td>
<td>Task 7: Provide Rev.0 cost model, structure details and spreadsheet to Center partners for their evaluation.</td>
</tr>
<tr>
<td>Q2</td>
<td>1</td>
<td>Task 1: Complete preliminary design for fuel element transfer system (solids handling coupled to reactor).</td>
</tr>
<tr>
<td>Q2</td>
<td>2</td>
<td>Task 2: Complete COMSOL modeling of configurations.</td>
</tr>
<tr>
<td>Q2</td>
<td>2</td>
<td>Task 2: Down select systems to be modeled for transient response.</td>
</tr>
<tr>
<td>Q3</td>
<td>3</td>
<td>Task 3: Complete test station for monolithic fuel element and hydrogen release measurement.</td>
</tr>
<tr>
<td>Q3</td>
<td>1</td>
<td>Task 1: Determine functional criteria and design rules based on modeling performance predictions and hydride system needs.</td>
</tr>
<tr>
<td>Q3</td>
<td>2</td>
<td>Task 2: Complete a conceptual design for a solid chemical hydride reactor that will provide input to the HSECoE’s Phase 1 Go/No-go decision making process, and insight into the ability of such a system to meet the 2015 volumetric capacity target of 1.5 kWh/L.</td>
</tr>
<tr>
<td>Q3</td>
<td>3</td>
<td>Task 3: Determine bulk kinetics measurements and impact on performance.</td>
</tr>
<tr>
<td>Q3</td>
<td>6</td>
<td>Task 6: Complete modeling and establish pressure vessel design rules for use with prototypes.</td>
</tr>
<tr>
<td>Q4</td>
<td>4</td>
<td>Task 4: Complete assessment on the probability of integrating a heat exchanger within storage vessel.</td>
</tr>
<tr>
<td>Q4</td>
<td>5</td>
<td>Task 5: Complete identification of known materials compatibility issues and establish corrective action plan for component designs.</td>
</tr>
</tbody>
</table>
Chemical Hydride System Status
Solid Ammonia-Borane: 2010 Targets

1. Fuel Purity
2. Fill Time
3. Full Flow Rate
4. Loss of useable H₂
5. Delivery Temp.

- 17 Targets Above 40%
- 4 Targets Undetermined or Below 40% Minimum

Source: Anton 2010 HSECoE program AMR
Primary Engineering Barriers for Chemical Hydride Systems

- Chemical Hydrides are not ‘reacted’ in the fuel tank
  - Solids handling engineering key part of any system concept
  - Exothermic reaction of most systems requires different thermal management solutions compared to MH or absorbents
  - AB thermolysis at <100°C; long term storage in hot climates?

- DOE Technical Targets:
  - BoP components and will add to
  - Performance impact of impurities needs a solution
  - Loss of Useable Hydrogen (g/hr)/kg H2 stored: 0.1 (2010) & 0.05 (2015); loss includes venting, if required

- Re-fueling vehicle logistics can be a challenge
- Ammonia Borane foams on reaction – potential limitation to practical engineering application
Engineered Form-Factor for Solid AB

- System targets are difficult for granulated materials
- AB foams when it releases hydrogen – not conducive to engineering
- Antifoaming approaches key
  - More than 50 additive formulations tested with 2-3 successful (CHCoE study)
  - Scaffold materials also demonstrate foam suppression at lower AB:scaffold loadings
  - Paves way for system with monolithic fuel & high volumetric density

Additive suppresses foaming and enables monolithic fuels

Source: PNNL CHCoE
Integrated System Design and Process Modeling for Solid Ammonia Borane
System Modeling Approach

- **Ballast Tank**
  - Provides H2 for start-up and transients

- **No Heat Addition**
  - Exothermic reaction heat warms incoming AB

- **Issues/Assumptions**
  - High heat transfer required between oil and AB in augers (heat/cool)
  - Extrapolation of kinetic data at 160°C to > 500°C
  - Modeling counterflow in Simulink
  - High Pressures in Ballast Tank—need for carbon fiber tank
  - No reaction in heated auger
  - Sticky AB during phase change
  - Impurity Borazine
BoP Equipment Equations/Assumptions

- **Heated Auger**
  - Psuedo Counterflow (co-flow section configured in counterflow)
  - Transient (includes metal thermal mass)
  - Assumes HT Oil $\rightarrow$ Metal $\rightarrow$ AB, No axial conduction

- **Cooled Auger**
  - Counterflow Heat Exchanger
  - Steady State (NTU-Effectiveness Method)

- **Burner**
  - Co-Flow
  - Transient (includes metal thermal mass)
  - Assumes HT Gas $\rightarrow$ Metal $\rightarrow$ Oil, No axial conduction

- **Radiator**
  - Cross Flow Heat Exchanger
Example Simulink Component Modeling

Oil Energy Equation

\[
\pi \left( R_{in}^2 - r_{out}^2 \right) \rho_{oil} C_{p,oil} \left( \frac{\partial T_{oil}}{\partial t} + u_{oil} \frac{\partial T_{oil}}{\partial x} \right) + 2\pi \rho_{oil} h_{oil-metal} (T_{oil} - T_{metal}) = 0
\]

Metal Energy Equation

\[
\pi \left( r_{out}^2 - r_{in}^2 + r_{auger}^2 \right) \rho_{metal} C_{p,metal} \left( \frac{\partial T_{metal}}{\partial t} \right) + 2\pi \rho_{metal} h_{metal-oil} (T_{metal} - T_{oil}) + 2\pi \left( r_{in} + r_{auger} \right) \phi_{metal-AB} (T_{metal} - T_{AB}) = 0
\]

AB Energy Equation

\[
\pi r_{in}^2 \rho_{bulk,AB} C_{p,AB} \left( \frac{\partial T_{AB}}{\partial t} + u_{AB} \frac{\partial T_{AB}}{\partial x} \right) + 2\pi \rho_{bulk,AB} \phi_{metal-AB} (T_{AB} - T_{metal}) = 0
\]
Integrated System Simulation

- Components in the model are coded as ‘C’ s-functions and simulated in Matlab/Simulink
- Control scheme is based on fuel cell demand and ballast tank states
- Start-Up assumed with 60 kWe power requirement
- Drive Cycle assumed after start-up
Integrated System Simulation

Components in the model are coded as ‘C’ s-functions and simulated in Matlab/Simulink. The control scheme is based on fuel cell demand and ballast tank states. Start-Up is assumed with a 60 kWe power requirement, and the drive cycle is assumed after start-up.
Baseline AB Bead Reactor System

Main components in the reactor system:

1. Hot Auger
2. Ballast Tank & Reactor
3. Cold Auger
4. Radiator
5. H₂ Burner
6. Control System

- Developing, refining system concepts
- Intrinsic kinetic models developed
- Developing reactor sub-models for use in system model
- Investigate auger / reactor heat transfer coefficients
- Determine “rheology”, “stickiness” of reacting AB with and without additives (e.g., using DMA and/or rheometers)
Simulation Results: Start-Up from 20°C

- Constant power 60 kWe
- AB begins to react at ~3 min
- Heat of reaction drives ballast tank reaction to maximum
- Reaction in ballast tank very small—will go away
- H₂ burner turns off at ~3 min
- Radiator not needed after hot auger, required for H₂ product
- Ballast Tank pressure drops to below 100 atm but rises again to 450 atm set point
Simulation Results: Start-Up from -20°C (cold)

- Constant power 40 kWe
- AB begins to react at ~3.5 min
- Cold AB forces burner on after initial start-up
- Instability needs to be investigated
- Ballast Tank pressure drops to 100 atm but rises again to near 450 atm set point
Simulation Results: Drive Cycle after Warm-Up

- US06 Drive Cycle with 0% Hybridization
- Pressure in Ballast Tank maintained ~500 atm
- Heated auger slowly cools at low flows
- H₂ burner turned on intermittently between 380 and 450 sec
## System Weight and Volume Estimate

- **Target:** Total Mass 111 kg and Total Volume 178 liters

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>AB Storage</td>
<td>30.8kg</td>
<td>0L</td>
</tr>
<tr>
<td>Feed/Product Tanks</td>
<td>14kg</td>
<td>140L</td>
</tr>
<tr>
<td>Ballast Tank (carbon fiber)</td>
<td>29.7kg</td>
<td>9L</td>
</tr>
<tr>
<td>Hot Auger (steel)</td>
<td>10.8kg</td>
<td>3.2L</td>
</tr>
<tr>
<td>Cold Auger (steel)</td>
<td>20.2kg</td>
<td>6.3L</td>
</tr>
<tr>
<td>Burner/Blower</td>
<td>6.3kg</td>
<td>5.7L</td>
</tr>
<tr>
<td>Radiator</td>
<td>1kg</td>
<td>1.8L</td>
</tr>
<tr>
<td>NH₃ Filter</td>
<td>2.2kg</td>
<td>2.7L</td>
</tr>
<tr>
<td>Oil Piping/Pump/Tank</td>
<td>4.7kg</td>
<td>3.5L</td>
</tr>
<tr>
<td>Valves/Actuators</td>
<td>5kg</td>
<td>3.5L</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>125kg</td>
<td>176L</td>
</tr>
</tbody>
</table>
Better Engineered Solution

To address weight/volume constraints, a new design of the bead reactor is proposed:

- Kinetics in the augers rather than ballast tank
- Combined Feed and Product Tank
- Better thermal control through multiple heat exchanger loops and through control logic.

Hot hydrogen heats incoming AB feed.
Materials Characterization
Accomplishments

- Materials Centers of Excellence recommended top storage materials
  - Based on multiple criteria
  - Available data and access to materials

- Materials properties of 12 materials posted on HSECoE Share point: MOR/Shared documents/Materials data base
  - Identified materials properties needed for modeling
  - Populated with literature and partner known and validated property data and kinetics
  - Gap analysis completed and plan established to augment data

- Screening criteria/Questionnaire created
  - Material must pass this rough assessment to be further considered
  - Provided to organizations who have a material of interest
## HSECoE Materials Categories

### Developed Materials
- System analysis is being performed on up-selected candidates and necessary engineering properties measured.

### Developing Materials
- Up-selected materials under performance evaluation and materials properties collected and measured if necessary.

### Down-selected Materials
- Materials found to not improve system performance relative to up-selected materials, and thus not for further consideration.

<table>
<thead>
<tr>
<th>Adsorbents</th>
<th>Tier 1 Developed Materials</th>
<th>Tier 2 Developing Materials</th>
<th>Down-selected Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>AX-21</td>
<td>Pt/AC-IRMOF 8</td>
<td>MOF 177</td>
<td></td>
</tr>
<tr>
<td>MOF 5</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chemical Hydrides</th>
<th>Tier 1 Developed Materials</th>
<th>Tier 2 Developing Materials</th>
<th>Down-selected Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH₃BH₃ₜ(s)</td>
<td>NH₃BH₃(l)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AIH₃</td>
<td>LiAIH₄</td>
<td></td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Metal Hydrides</th>
<th>Tier 1 Developed Materials</th>
<th>Tier 2 Developing Materials</th>
<th>Down-selected Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaAlH₄</td>
<td>Mg(NH₂)₂+MgH₂+2LiH</td>
<td>MgH₂</td>
<td></td>
</tr>
<tr>
<td>2LiNH₂+MgH₂</td>
<td>TiCr(Mn)H₂</td>
<td>Mg₂NiH₄</td>
<td></td>
</tr>
</tbody>
</table>
### Storage Material Screening Criteria

**Metal Hydrides**

<table>
<thead>
<tr>
<th>Chemical formula and reversible reaction formula</th>
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<tbody>
<tr>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Capacity (wt% H₂ and kg H₂/L) as measured at what pressure (bar) and temperature (°C)</th>
</tr>
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<tbody>
<tr>
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</table>

<table>
<thead>
<tr>
<th>Absorption: give temperature (°C), pressure (bar) and rate (g H₂/s) to reach max absorption capacity</th>
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</table>

<table>
<thead>
<tr>
<th>Desorption: give temperature (°C) and rate (g H₂/s) to reach max desorption capacity</th>
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</table>

<table>
<thead>
<tr>
<th>Enthalpy, ΔH (J/mol): for formation and/or reaction</th>
</tr>
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<tbody>
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</table>

<table>
<thead>
<tr>
<th>Crystal density (g/cm³)</th>
</tr>
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<tbody>
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</table>

<table>
<thead>
<tr>
<th>Material and Synthetic Process</th>
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</table>

**Chemical Hydrides**

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<table>
<thead>
<tr>
<th>Desorption: give temperature (°C)</th>
</tr>
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<tbody>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Enthalpy of formation (J/mol)</th>
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<tbody>
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<td></td>
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<table>
<thead>
<tr>
<th>Desorption: give temperature (°C) and rate (g H₂/s) to reach measured capacity</th>
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<tbody>
<tr>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost raw material + additive ($/g)</th>
</tr>
</thead>
<tbody>
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</table>

<table>
<thead>
<tr>
<th>Availability (g)</th>
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<tbody>
<tr>
<td></td>
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</table>

**Adsorbents**

<table>
<thead>
<tr>
<th>Capacity as independently validated maximum Gibbs excess capacity (wt% H₂ and kgH₂/L) as measured at what pressure (bar) and temperature (°C). Provide isotherms at RT and 77K.</th>
</tr>
</thead>
<tbody>
<tr>
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</table>

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<thead>
<tr>
<th>Desorption: give temperature (°C) and rate (g H₂/s) to reach max desorption capacity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Hydrogen uptake: give temperature (°C), pressure (bar) and rate (g H₂/s) to reach max adsorption capacity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost for raw material (precursor) and estimate for processing ($/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>BET Specific surface area (m²/g) and pore size distribution and/or bulk density (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>

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<tr>
<th>Availability (g)</th>
</tr>
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<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>
### Chemical formula and reversible reaction formula

LiNH₂ + MgH₂ = LiMgN + 2H₂ etc

### Capacity (wt% H₂ and kg H₂/L) as measured at what pressure (bar) and temperature (°C) and cycle life (# of abs/des cycles and % capacity loss)

7.9wt% H₂ adsorbed at ?°C and ? bar; 5 cycles

### Absorption at RT-250 C at 1-700 bar: give temperature (°C), pressure (bar) and rate (g H₂/s) to reach max absorption capacity

?? Data not yet in data base, but in literature

### Desorption at 80-250 C at 1-3 bar: give temperature (°C), pressure (bar) and rate (g H₂/s) to reach max desorption capacity

?? Data not yet in data base, but in literature

### Enthalpy, ΔH (J/mol) <50kJ/mol: for formation and/or reaction

33.5kJ/mol

### Crystal density (g/cm³)

2.388mg/m³

### Availability (g)

2.388mg/m³

### Cost raw material + additive ($/g)

??

---

**Questionnaire applied to LiNH₂:MgH₂ 1:1**

**Adsorbents**

**Chemical Hydrides**

**Metal Hydrides**

**BET Specific surface area (m²/g) and pore size distribution and/or bulk density (g/cm³)**

??
## Example: Data Base for Sodium Alanate

<table>
<thead>
<tr>
<th>Category</th>
<th>Property</th>
<th>reported value</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Composition</strong></td>
<td></td>
<td>NaAlH₄ + 2m%TiCl₃ + 0.33m%AlCl₃ + 0.5m%FeCl₃</td>
<td>Mosher et al. UTRC Final Report (2007)</td>
</tr>
<tr>
<td><strong>Catalyst</strong></td>
<td></td>
<td>2m%TiCl₃ + 0.33m%AlCl₃ + 0.5m%FeCl₃</td>
<td></td>
</tr>
<tr>
<td><strong>Impurities/Ratios</strong></td>
<td></td>
<td>NaAlH₄: 86.3% NaAlH₄, 4.7%Na₃AlH₆, 7.5% free Al and 10.1% insoluble Al (in wt%).</td>
<td></td>
</tr>
<tr>
<td><strong>Synthesis</strong></td>
<td></td>
<td>SPEX ball milling under nitrogen for 6 hours</td>
<td>Mosher et al. UTRC Final Report (2007)</td>
</tr>
</tbody>
</table>
| **Decomposition Pathways** |   | \[
NaAlH₄ \iff \frac{1}{3} \text{Na}_3\text{AlH}_6 + \frac{2}{3} \text{Al} + H_2 \iff \text{NaH} + \text{Al} + \frac{3}{2} H_2
| **Intermediates** |                | 57.1 mol% NaH, 42.9 mol% Alrollment                                                                  | Srinivasan 377(2004)283                     |
|                   |                | 35.3 mol% NaH, 54.6 mol% Al, 8.7% Na₃AlH₆, 1.3% NaCl                                                | Srinivasan 377(2004)283                     |
| **Impurities**    |                | None                                                                                               |                                              |
| **Hydrogen**      |                |                                                                                                    |                                              |
| **Intrinsic properties** |   |                                                                                                    |                                              |
| **Kinetic Model** |                | \[
\left( \frac{dC_j}{dt} \right)_{r_i} = D_i \exp \left( - \frac{E_i}{RT} \right) \times \left( \frac{P_{e,i} - P}{P_{e,i}} \right) \times (C_k)^{x_i}
\] | Mosher et al. UTRC Final Report (2007)          |
Example: Data Base for Sodium Alanate

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<td>Synthesis Method</td>
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<td>Mosher et al. UTRC Final Report</td>
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<td></td>
<td>57.1 mol% NaH, 42.9 mol% Al, 35.3 mol% NaH, 54.6 mol% Al, 8.7% Na₃AlH₆, 1.3% NaCl</td>
<td>Srinivasan 377(2004)283</td>
</tr>
<tr>
<td>Hydrogen Impurities</td>
<td></td>
<td>None</td>
<td></td>
</tr>
<tr>
<td>Kinetic Model</td>
<td></td>
<td>Di Needs to be calculated, Eᵢ Needs to be calculated, χᵢ Needs to be calculated</td>
<td></td>
</tr>
</tbody>
</table>

MgH₂+0.1TiH₂ 6wt% reversible at 300°C for 80 cycles. Kinetics remain similar.

Absorption kinetics

Desorption kinetics

Jun Lu, Young Joon Choi, Zhigang Zak Fang, Hong Yong Sohn and Ewa Rönnebro, JACS 2010
<table>
<thead>
<tr>
<th>Category</th>
<th>Property reported value reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition</td>
<td>NaAlH$_4$+2m%TiCl$_3$+0.33m%AlCl$_3$+0.5m%FeCl$_3$</td>
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<tr>
<td>Catalyst</td>
<td>2m%TiCl$_3$+0.33m%AlCl$_3$+0.5m%FeCl$_3$</td>
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<tr>
<td>Impurities/Ratios</td>
<td>NaAlH$_4$: 86.3% NaAlH$_4$, 4.7%Na$_3$AlH$_6$, 7.5% free Al and 10.1% insoluble Al (in wt%).</td>
</tr>
</tbody>
</table>

**Synthesis**

Method

SPEX ball milling under nitrogen for 6 hours


**Decomposition Pathways**


**Intermediates**

57.1 mol% NaH, 42.9 mol% Al

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35.3 mol% NaH, 54.6 mol% Al, 8.7% Na$_3$AlH$_6$, 1.3% NaCl

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**Hydrogen Impurities**

None

**Intrinsic properties**

**Kinetic Model**


Di Needs to be calculated

E$_i$ Needs to be calculated

P$_e,i$ Needs to be calculated

$\chi$ Needs to be calculated

\[
HAlNaHHAlAlHNaNaAlH \leftrightarrow \leftrightarrow  \]

\[
(\ )_i \exp \frac{k_i}{RT} \exp \frac{E_i}{RT} dt \exp \frac{-\Delta H}{RT} dt \]
Summary & Proposed Future Work
Collaborative Activities

Hydrogen Storage Engineering Center of Excellence

- Lincoln Composites - study of CF cost and pressure vessel design modeling
- GM - design of structured media bed for MH
- Ford - characterization of absorbent materials
- UQTR - design and materials characterization of carbon absorbent
- OSU - microarchitectural device concept development and thermodynamic analysis
- UTRC - develop solutions for $H_2$ impurities filtering
- LANL - AB system design and measure $H_2$ impurities
- NREL - input for tank to wheels analysis and system cost models
- SRNL - study AB reactivity and kinetics model development

SAWGG

- Participate in group discussions and analysis

Materials ‘Reactivity’ Program

- Khalil (UTRC) and Anton (SRNL) - understand reactivity properties of AB
- Van Hassel (UTRC) - study impurities in $H_2$

Independent Analysis

- TIAX - provide design details for AB refueling cost and feasibility assessment, plus share cost parameters for system cost modeling
Summary of Accomplishments

- A representative systems model of a AB based bead reactor system was developed and successfully simulated in Matlab/Simulink environment.

- A COMSOL transport model was developed for a bead and a block system. The heat and mass transfer model used a simple reaction rate expression: (1) Bead reaction can occur within the auger that has been designed assuming a 200°C wall. (2) Heating the outside surface of a block can light off the reaction for the entire block.

- An improved kinetic model has been developed and implemented into the system model.

- Hydrogen loss and impurities assessed for solid AB as material is moved into and out of the pressurized reaction system.
Summary of Accomplishments (con’t)

- Materials properties database established for HSECoE partners
- Screening criteria/Questionnaire created
- Engineering cost model structure established
- Studies and analysis of pressure vessels performed:
  - Metal hydride hybrid
  - Vessel material of construction sensitivity analysis
  - Liner material assessment
- Materials compatibility and reactivity studies started
Future Work: Chemical Hydride System Design

Future work includes implementation of the new bead reactor design in Matlab/Simulink and corresponding simulation analysis

- Improve H2 Delivery Temperature
- Increase Volumetric/Gravimetric Density
- Include variable transport properties ($\rho$, $C_p$, $k$, $z_{H2}$)
- Address impurities and hydrogen losses in design

Investigation of alternate materials for chemical hydride hydrogen storage.

Implementation of the new kinetic model in Matlab/Simulink and corresponding simulation analysis

Include temperature dependent transport properties into models as they become available. Modify kinetic model with higher temperature experimental data.
Future Systems to be Evaluated

- Materials to be Studied
  - Ammonia Borane \((\text{NH}_3\text{BH}_3_{(s)})\) (Starting Material)
  - Alane \((\text{AlH}_3)\)
  - Lithium Aluminum Hydride \((\text{LiAlH}_4)\)
- Other System Configurations

Bulk Solids Configuration

Slurry Reactor Configuration
Future Work

- Complete system concept modeling efforts and provide initial component design for partner review
- Determine final reactor details and lock-in design
- Complete bulk kinetics modeling and validation studies
- Initiate heat exchanger modeling effort and provide initial component design for partner review
- Progression of cost model with system details and integrate component “catalog”
- Storage material bulk characterization
Darrell Herling – Pacific Northwest National Lab, Principal Investigator
darrell.herling@pnl.gov, (509) 375-6905

Don Anton – HSECoE, Director
Monterey Gardiner – DOE EERE, Technology Development Manager