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

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DOE Fuel Cell Technology Program
Annual Merit Review

June 8, 2010
Technology Development Manager: Monterey Gardiner

Project ID: ST005
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

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Innovation for Our Energy Future

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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
# Accomplishment: Milestones FY10

<table>
<thead>
<tr>
<th>Quarter</th>
<th>Task</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>Task 7</td>
<td>Provide Rev.0 cost model, structure details and spreadsheet to Center partners for their evaluation.</td>
</tr>
<tr>
<td>Q2</td>
<td>Task 1</td>
<td>Complete preliminary design for fuel element transfer system (solids handling coupled to reactor).</td>
</tr>
<tr>
<td>Q2</td>
<td>Task 2</td>
<td>Complete COMSOL modeling of configurations</td>
</tr>
<tr>
<td>Q2</td>
<td>Task 2</td>
<td>Down select systems to be modeled for transient response</td>
</tr>
<tr>
<td>Q3</td>
<td>Task 3</td>
<td>Complete test station for monolithic fuel element and hydrogen release measurement</td>
</tr>
<tr>
<td>Q3</td>
<td>Task 1</td>
<td>Determine functional criteria and design rules based on modeling performance predictions and hydride system needs.</td>
</tr>
<tr>
<td>Q3</td>
<td>Task 2</td>
<td>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>Task 3</td>
<td>Determine bulk kinetics measurements and impact on performance.</td>
</tr>
<tr>
<td>Q3</td>
<td>Task 6</td>
<td>Complete modeling and establish pressure vessel design rules for use with prototypes.</td>
</tr>
<tr>
<td>Q4</td>
<td>Task 4</td>
<td>Complete assessment on the probability of integrating a heat exchanger within storage vessel.</td>
</tr>
<tr>
<td>Q4</td>
<td>Task 5</td>
<td>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.

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

![Graph showing the comparison between 2010 and 2015 systems, with different bed void fractions and volumetric capacities for close-packed spheres and loose powder.](image)

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 → Metal → 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 → Metal → Oil, No axial conduction

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

Oil Energy Equation

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

Metal Energy Equation

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

AB Energy Equation

\[
\pi r_{in}^2 \rho_{bulk,AB} c_{p,AB} \left( \frac{\partial T_{AB}}{\partial t} + u_{AB} \frac{\partial T_{AB}}{\partial x} \right) + 2\pi r_{in} \phi h_{metal-AB} \left( T_{AB} - T_{metal} \right) = 0
\]
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.
Baseline AB Bead Reactor 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)

Main components in the reactor system:

1. Hot Auger
2. Ballast Tank & Reactor
3. Cold Auger
4. Radiator
5. H₂ Burner
6. Control System
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
- \( \text{H}_2 \) 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

<table>
<thead>
<tr>
<th>Adsorbents</th>
<th>Developed Materials</th>
<th>Tier 1</th>
<th>Developing Materials</th>
<th>Tier 2</th>
<th>Down-selected Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOF 5</td>
<td>AX-21</td>
<td>MOF 5</td>
<td>Pt/AC-IRMOF 8</td>
<td>MOF 177</td>
<td></td>
</tr>
<tr>
<td>NH$_3$BH$_3$(s)</td>
<td>NH$_3$BH$_3$(l)</td>
<td></td>
<td>LiAlH$_4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AlH$_3$</td>
<td>NiAlH$_4$</td>
<td></td>
<td>Mg(NH$_2$)$_2$+MgH$_2$+2LiH</td>
<td>MgH$_2$</td>
<td></td>
</tr>
<tr>
<td>Metal Hydrides</td>
<td>NaAlH$_4$</td>
<td></td>
<td>TiCr(Mn)H$_2$</td>
<td>Mg$_2$NiH$_4$</td>
<td></td>
</tr>
<tr>
<td>2LiNH$_2$+MgH$_2$</td>
<td>TiCr(Mn)H$_2$</td>
<td></td>
<td>TiCr(Mn)H$_2$</td>
<td>Mg$_2$NiH$_4$</td>
<td></td>
</tr>
</tbody>
</table>

- **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.

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**Pacific Northwest National Laboratory**

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# Storage Material Screening Criteria

## Metal Hydrides

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula and reversible reaction formula</td>
<td></td>
</tr>
<tr>
<td>Capacity (% H₂ and kg H₂/L) as measured at what pressure (bar) and temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>Desorption: give temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>Enthalpy, ΔH (J/mol): formation</td>
<td></td>
</tr>
<tr>
<td>Enthalpy of formation (J/mol)</td>
<td></td>
</tr>
<tr>
<td>Crystal density (g/cm³)</td>
<td></td>
</tr>
<tr>
<td>Cost raw material + additive</td>
<td></td>
</tr>
<tr>
<td>Availability (g)</td>
<td></td>
</tr>
<tr>
<td>Availability (g)</td>
<td></td>
</tr>
</tbody>
</table>

## Chemical Hydrides

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula and decomposition reaction formula</td>
<td></td>
</tr>
<tr>
<td>Capacity (% H₂ and kg H₂/L) as measured at what temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>Desorption: give temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>Cost raw material (precursor)</td>
<td></td>
</tr>
<tr>
<td>Cost for raw material (precursor) and estimate for processing ($/g)</td>
<td></td>
</tr>
<tr>
<td>Availability (g)</td>
<td></td>
</tr>
</tbody>
</table>

## Adsorbents

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material and Synthetic Process</td>
<td></td>
</tr>
<tr>
<td>Desorption: give temperature (°C) and rate (g H₂/s) to reach max desorption capacity</td>
<td></td>
</tr>
<tr>
<td>Hydrogen uptake: give temperature (°C), pressure (bar) and rate (g H₂/s) to reach max adsorption capacity</td>
<td></td>
</tr>
<tr>
<td>BET Specific surface area (m²/g) and pore size distribution and/or bulk density (g/cm³)</td>
<td></td>
</tr>
<tr>
<td>Cost for raw material (precursor) and estimate for processing ($/g)</td>
<td></td>
</tr>
<tr>
<td>Availability (g)</td>
<td></td>
</tr>
</tbody>
</table>
**TABLE 1:** Isothermal Decomposition Rate Constants (s\(^{-1}\)) for α-, β-, and γ-AlH\(_3\)^a

<table>
<thead>
<tr>
<th>Polymorph</th>
<th>(h(60 , ^\circ C))</th>
<th>(h(80 , ^\circ C))</th>
<th>(h(90 , ^\circ C))</th>
<th>(h(120 , ^\circ C))</th>
<th>(h(138 , ^\circ C))</th>
</tr>
</thead>
<tbody>
<tr>
<td>α-AlH(_3)</td>
<td>(1.35 \times 10^{-6})</td>
<td>(9.14 \times 10^{-6})</td>
<td>(4.21 \times 10^{-5})</td>
<td>(2.80 \times 10^{-4})</td>
<td>(1.39 \times 10^{-3})</td>
</tr>
<tr>
<td>β-AlH(_3)</td>
<td>(4.41 \times 10^{-6})</td>
<td>(1.36 \times 10^{-5})</td>
<td>(5.99 \times 10^{-5})</td>
<td>(4.88 \times 10^{-4})</td>
<td>(2.46 \times 10^{-3})</td>
</tr>
<tr>
<td>γ-AlH(_3)</td>
<td>(3.97 \times 10^{-8})</td>
<td>(1.18 \times 10^{-7})</td>
<td>(3.94 \times 10^{-6})</td>
<td>(2.71 \times 10^{-5})</td>
<td>(7.98 \times 10^{-4})</td>
</tr>
</tbody>
</table>


**Figure 6.** Arrhenius plot for large crystallites of α-AlH\(_3\) (Dow)^4 and small crystallites of α-AlH\(_3\), β-AlH\(_3\), and γ-AlH\(_3\). Reaction rates for the large crystallites of α-AlH\(_3\) were measured at 135 °C ≤ \(T\) ≤ 160 °C and are extrapolated down to \(T \sim 60 \, ^\circ C\).
Summary & Proposed Future Work
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 - microarchitectecture device concept development and thermodynamic analysis
- UTRC - develop solutions for H₂ impurities filtering
- LANL - AB system design and measure H₂ 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 H₂

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 ($\rho$, $C_p$, $k$, $zh2$)
- 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
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Don Anton – HSECoE, Director
Monterey Gardiner – DOE EERE, Technology Development Manager
Extra Details & Back-up Slides
Responses to Previous Year Reviewers’ Comments

- FY2010 first full year for HSECoE activities
- 2010 is first AMR review – no previous reviewer comments
Publications and Presentations (FY2010)

► Publications


► Presentations


Background Information on Solid AB Thermal Stability
Ammonia Borane Shows Promise

Hydrogen Densities of Materials

Hydrogen mass density (mass %) vs. Hydrogen volume density (kgH₂ m⁻³)

Materials plotted:
- Mg₂NH₄
- TiH₂
- MgH₂
- Mg(OMe)₂ H₂O
- AlH₃
- LiNH₂(1)
- LiNH₂(2)
- NH₃BH₃(1)
- NH₃BH₃(2)
- NH₃BH₄(1)
- NH₃BH₄(4)
- NH₄BH₄(4)
- FeTiH₁.₇
- 11M aq NaBH₄
- KBH₄
- LiAIH₄
- LiBH₄
- C₂H₅OH
- C₃H₈
- C₄H₁₀
- C₅H₁₂
- C₆H₁₄
- C₇H₁₈
- C₈H₁₈
- CH₄ (liq)
- liquid hydrogen

2010 system targets:
- 700 bar
- 350 bar

2015 system targets:

Courtesy of G. Thomas

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AB Thermal Stability Calculations – Assumptions and Insight

- 1st equivalent only – Avrami kinetics
- 70-90 °C isothermal DSC data* used for initial fit of parameters
- Adiabatic assumed as a worst case

Model AB bed properties:
- 1000 mol AB = 4 kg H₂ (2 H₂ equiv.)
- 6.0 wt% H₂ in a storage unit including >50 wt% structure
- No temperature gradients

Extrapolation of DSC Data to Lower Isothermal Temperatures

* Wolf et al., Thermochimica Acta 343, (2000) 19
Source: PNNL CHCoE
Heat Management to Stabilize Stored AB

Under adiabatic conditions, the AB bed temperature and reaction rate increases due to the heat evolved as H₂ is released (e.g., -22 kJ/mol)

Small amounts of cooling and lower temperatures greatly increase the thermal stability of the packed AB bed (e.g., storage tank)

Computationally, cooling was not allowed to decrease T below the initial value

Source: PNNL CHCoE
Solid CH Kinetics Model Development
Initial Kinetics Model

► AB → AB* ↔ P + 3H₂

► Rate Equations

- \( r_{AB} = -k_1 y_{AB} \)
- \( r_{AB}^* = (k_1 y_{AB} - k_2 (y_{AB}^* - K_{eq} (y_{AB, initial} - y_{AB} - y_{AB}^*))) \)
- \( r_{H₂} = 3(k_2 (y_{AB}^* - K_{eq} (y_{AB, initial} - y_{AB} - y_{AB}^*))) \)

where \( k_1 = A_1 e^{E_1/RT} \) and \( k_2 = A_2 e^{E_2/RT} \)

► Species Equations

\[
\frac{\partial y_{AB}}{\partial t} = r_{AB} - \frac{\dot{m}_{AB, out}}{\rho_b A} \frac{\partial y_{AB}}{\partial x}
\]

\[
\frac{\partial y_{H₂}}{\partial t} = r_{H₂} + D_{H₂} \frac{\partial^2 y_{H₂}}{\partial^2 x}
\]

► Heat Equation

\[
\rho_b C_p \frac{\partial T}{\partial t} = \Delta H_{rxn} r_{H₂} - \frac{C_p \dot{m}_{AB, out}}{A} \frac{\partial T}{\partial x}
\]
Heat Transfer/Reaction in Packed Bed (Auger)

Auger Properties
- 1” Diameter, 5 ft long
- Residence Time 36 sec @ 80 kWe

Outer Surface Heating
- 100°C → Reaction initiates at 130 sec, duration ~ 10 sec, $T_{\text{max}} = 317°C$
- 200°C → Reaction initiates at 34 sec, duration ~ 10 sec, $T_{\text{max}} = 570°C$

Lessons Learned
- Auger length reasonable if 200°C oil temperature
- Reaction very rapid and results in high temperature
- Must not exceed ~ 700°C or boron nitride is formed ($\Delta T_{\text{adiabatic}} = 482°C$)
Solid “Block” of AB System Design Concept
Heating Outside of AB Block

- 1-D model \( \frac{1}{2}'' \) thick AB (\( L,W \gg \frac{1}{2}'' \))
- Heat outer 0.04'', inner remains at 20°C
- Although bulk temperature is low, reaction initiates

<table>
<thead>
<tr>
<th>Heated Section Temp (°C)</th>
<th>Ave Bulk Temp (°C)</th>
<th>Reaction Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>33</td>
<td>160</td>
</tr>
<tr>
<td>200</td>
<td>50</td>
<td>120</td>
</tr>
<tr>
<td>300</td>
<td>67</td>
<td>90</td>
</tr>
</tbody>
</table>
Improved AB Kinetic Model

- Ammonia Borane reaction kinetics represented by Avrami kinetics:

\[ \chi = 1 - \exp\left\{ - [k(t - \tau)]^n \right\} \]

0 for \( t \leq \zeta \)

\[ \chi_{tot} = 1.1\left[1 - \exp\left[-(k_1 t)^3\right]\right] + 1.4\left[1 - \exp\left[-(k_2 t)\right]\right] \]

Note: Experimental data maximum only 160°C

Predicted H₂ Release at 130°C

Predicted H₂ Release at 180°C

- Global Model, Film Data
- Global Model, Powder Data
- Global Model, All Data

130°C Film Data
- Individual Fit, 130C
- Global Model, Film Data
- Global Model, All Data

Molar Equivalents H₂

Time (min)
Approach

- For a given conversion ($\chi$) and temperature ($T$), obtain $t^*$ (pseudo-reaction time) from look-up table.

$$\chi_{tot} = 1.1\{1 - \exp[-(k_1 t)^3]\} + 1.4\{1 - \exp[-(k_2 t)]\}$$

- Calculate the derivative of $\chi$ with respect to $t^*$ to obtain reaction rate for isothermal case.

$$\frac{d\chi}{dt^*} = R_{rxn} = 3.3k_1^3 t^2 \exp[-(k_1 t^*)^3] + 1.4k_2 \exp[-(k_2 t^*)]$$

- Use $R_{rxn}$ to calculate $\chi$ for new time and position step

$$\frac{\partial \chi}{\partial t} = -u_{AB} \frac{\partial \chi}{\partial x} + R_{rxn}$$

- Calculate new temperature ($T$) from energy equation

$$\rho_{bulk,AB} C_{p,AB} \frac{\partial T_{AB}}{\partial t} = \frac{\Delta H_{rxn} R_{rxn} \rho_{bulk,AB}}{MW_{AB}} - \frac{C_{pAB} \dot{m}_{AB,in}}{A} \frac{\partial T_{AB}}{\partial x}$$
## Hydrogen Loss and Purity Issues with AB

- Moving material between pressurized and unpressurized parts of the system
  - H₂ loss increases with system pressure
  - Air infiltration constant with gap size

<table>
<thead>
<tr>
<th>System Pressure (atm)</th>
<th>Beads Random Packing H₂ Loss (gH₂/hr*kgH₂)</th>
<th>Purity impact from Air (%)</th>
<th>PEZ Block 1/8&quot; Gap H₂ Loss (gH₂/hr*kgH₂)</th>
<th>Purity (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.9</td>
<td>99.93%</td>
<td>1.0</td>
<td>99.91%</td>
</tr>
<tr>
<td>10</td>
<td>1.7</td>
<td>99.93%</td>
<td>2.1</td>
<td>99.91%</td>
</tr>
<tr>
<td>50</td>
<td>8.7</td>
<td>99.93%</td>
<td>10.3</td>
<td>99.91%</td>
</tr>
<tr>
<td>100</td>
<td>17.4</td>
<td>99.93%</td>
<td>20.6</td>
<td>99.91%</td>
</tr>
<tr>
<td>500</td>
<td>86.9</td>
<td>99.93%</td>
<td>103.0</td>
<td>99.91%</td>
</tr>
</tbody>
</table>

(Assuming ideal gas law, 2.5 equivalents produced)
(Block is assumed to be 3" x 3" x 1/2" thick)
Approach to Solid CH System Modeling
Slurry Reactor

14kW @ 80 kW e
3 kW @ 15 kW e
0 kW @ startup

120 scfm Air

Fuel Cell

Feed Tank
27 gallons/hr @ 80 kW e
5 gallons/hr @ 15 kW e

Coolant Pump

Combustor
e = 0.7

Recirculation Pump

Heat Exchanger
T = 160°C
P= 200 atm
800 atm (standby)

Slurry Feed Pump

60°C

Fresh

Spend

70 wt% Slurry AB in Mineral Oil

Recuperator

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Ballast Tank Equations

► **AB → AB* ↔ P + 3H₂**

► **Rate Equations**
  - \( r_{AB} = -k_1 y_{AB} \)
  - \( r_{AB}^* = (k_1 y_{AB} - k_2(y_{AB}^* - K_{eq}(y_{AB,initial} - y_{AB} - y_{AB}^*))) \)
  - \( r_{H₂} = 3(k_2(y_{AB}^* - K_{eq}(y_{AB,initial} - y_{AB} - y_{AB}^*))) \)
  - where \( k_1 = A_1 e^{-E_1/RT} \) and \( k_2 = A_2 e^{-E_2/RT} \)

► **Species Equations**

\[
\frac{\partial y_{AB}}{\partial t} = r_{AB} - \frac{\dot{m}_{AB,\text{out}}}{\rho_b A} \frac{\partial y_{AB}}{\partial x}
\]

\[
\frac{\partial y_{AB}^*}{\partial t} = r_{AB}^* - \frac{\dot{m}_{AB,\text{out}}}{\rho_b A} \frac{\partial y_{AB}^*}{\partial x}
\]

\[
\frac{\partial y_{H₂}}{\partial t} = r_{H₂} + D_{H₂} \frac{\partial^2 y_{H₂}}{\partial x^2}
\]

► **Heat Equation**

\[
\rho_b C_p \frac{\partial T}{\partial t} = \Delta H_{\text{rxn}} r_{H₂} - \frac{C_p \dot{m}_{AB,\text{out}}}{A} \frac{\partial T}{\partial x}
\]
Heated/Cooled Auger

**Heat Transfer Equations**

\[
NTU = \frac{UA}{C_{p,AB} \dot{m}_{AB,\text{in/out}}}
\]

\[
C_r = \frac{C_{pAB} \dot{m}_{AB,\text{in/out}}}{C_{p,oil} \dot{m}_{oil}}
\]

\[
\varepsilon = \frac{1}{1 - C_r e^{(-NTU(1-C_r))}}
\]

\[
q_{HA} = \varepsilon C_{p,AB} \dot{m}_{AB,\text{in}} \left( T_{oil,\text{hot}} - T_{\text{ambient}} \right)
\]

\[
q_{CA} = \varepsilon C_{p,AB} \dot{m}_{AB,\text{in}} \left( T_{BT} - T_{oil,\text{cool}} \right)
\]

\[
T_{oil,HA} = T_{oil,\text{hot}} - \frac{q_{HA}}{C_{p,oil} \dot{m}_{oil}}
\]

\[
T_{oil,CA} = T_{oil,\text{cool}} + \frac{q_{CA}}{C_{p,oil} \dot{m}_{oil}}
\]

\[
T_{AB,HA} = T_{\text{ambient}} + \frac{q_{HA}}{C_{p,AB} \dot{m}_{AB,\text{in}}}
\]

\[
T_{AB,CA} = T_{AB,BT} - \frac{q_{CA}}{C_{p,AB} \dot{m}_{AB,\text{out}}}
\]
Ancillary Equipment

**Burner**

\[ C_{P,oil} \dot{m}_{oil} \left( T_{oil,hot} - T_{oil,CA} \right) = \dot{m}_{H_2, burn} \Delta H_{rxn,H_2} \varepsilon_{burner} \]

**Radiator**

\[ C_{P,oil} \dot{m}_{oil} \left( T_{oil,HA} - T_{oil,cool} \right) = U A \Delta T_{lm} \]

\[ \Delta T_{lm} = \frac{\left( T_{oil,HA} - T_{oil,cool} \right)}{\ln \left( \frac{T_{oil,HA} - T_{ambient}}{T_{oil,cool} - T_{ambient}} \right)} \]
Materials Compatibility
Storage Media Relationship to Reactivity and Compatibility

Materials Operating Requirements

<table>
<thead>
<tr>
<th>D. Herling, PNNL</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Materials Centers of Excellence Collaboration – SRNL, LANL, NREL</td>
</tr>
<tr>
<td>• Reactivity &amp; Compatibility – UTRC</td>
</tr>
<tr>
<td>• Adsorption Properties – NREL</td>
</tr>
<tr>
<td>• Metal Hydride Properties – SRNL</td>
</tr>
<tr>
<td>• Chemical Hydride Properties – LANL</td>
</tr>
<tr>
<td>• Media Structure - GM</td>
</tr>
</tbody>
</table>

Chemical Hydride Properties – LANL

Metal Hydride Properties – SRNL

Adsorption Properties – NREL

Media Structure - GM

Reactivity & Compatibility – UTRC, PNNL

ET-Pressure Vessels & Containment – PNNL

Bulk Materials Handling
# H₂ Storage Materials

<table>
<thead>
<tr>
<th>Adsorbents</th>
<th>Prototypical Material</th>
<th>Developed Materials</th>
<th>Potential Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>AX-21</td>
<td>(UQTR/ANL/GM/UTRC)</td>
<td>MOF 5 (Ford)</td>
<td>Duke PEEK (NREL)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MOF 177 (Ford)</td>
<td>UMO AC (NREL)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IRMOF 8 (Ford)</td>
<td>LLNL AeroGel (NREL)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Pt/AC-IRMOF 8 (NREL)</td>
</tr>
<tr>
<td>NH₃BH₃(s)</td>
<td>(PNNL/UTRC)</td>
<td>NH₃BH₃(l) (LANL)</td>
<td>N-Ethyl Carbazole</td>
</tr>
<tr>
<td></td>
<td></td>
<td>AIH₃ (SRNL)</td>
<td>(LANL)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>LiAIH₄ (PNNL)</td>
<td></td>
</tr>
<tr>
<td>Metal Hydrides</td>
<td>NaAIH₄ (UTRC/Sandia)</td>
<td>LiNH₄+MgH₂ (SNL)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2Mg(NH₂)₂+MgH₂+LiH</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(SRNL)</td>
<td></td>
</tr>
</tbody>
</table>

*Initial systems foci*

*Performance analysis*

*Further assessment needed*
## Material Operating Requirements

<table>
<thead>
<tr>
<th>Category</th>
<th>Material</th>
<th>Operating Temperature</th>
<th>Material Form</th>
<th>Pellet/Powder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adsorbents</td>
<td>AX-21 (UQTR)</td>
<td>77K</td>
<td>Material Form</td>
<td>Pellet/Powder</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical Hydrides</td>
<td>NH₃BH₃(s) (PNNL)</td>
<td>160°C</td>
<td>Material Form</td>
<td>Pellet/Solid</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Metal Hydrides</td>
<td>NaAlH₄ (UTRC)</td>
<td>&lt;200°C</td>
<td>Material Form</td>
<td>Pellet/Powder</td>
</tr>
</tbody>
</table>
Material Hydrogen Effects

- Hydrogen Embrittlement
  - Internal
  - External
- Hydrogen Attack
- Hydrogen Permeability
- Temperature considerations are very important
Hydrogen Embrittlement

Microvoids (internal corrosion pits)

Intergranular Crack

Stainless Pipe

Temperature Effects


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Difference in Materials Relative to Hydrogen Embrittlement

The materials which can be used without any specific precautions are:
- Brass and most of the copper alloys
- Aluminum and aluminum alloys (some high strength aluminum alloys are known to be sensitive to hydrogen embrittlement)
- Cu-Be (this material is particularly interesting because of its very high mechanical properties and good fatigue resistance e.g. spring or membrane)

The materials which are known to be very sensitive to HE are:
- Ni and high Ni alloys (contrary to steels, unacceptable HE behavior may remain even at rather high temperature)
- Ti and Ti alloys
Hydrogen Attack

- Hydrogen attack increases when temperature and pressure increase. In addition, the higher the Cr and Mo content, the better the binding of carbon, which reduces risks of HA by decarburization or formation of methane.

- Hydrogen attack increases when the level of mechanical stresses increase.
Polymers

- Limited data on most polymers
- HDPE is common, but current storage materials exceed the working temperature range
- Higher temperature material candidates under consideration
- Diffusion is highly dependent on the degree of crystallinity
- Higher density materials with lower free-volumes also have lower diffusion rates
- Hydrogen impurities and mixed gases can have an effect on different polymers compatibility
Recommendations on Communication Compatibility and Reactivity Group

- The “scope”, i.e. the hydrogen pressure, the temperature and the hydrogen purity,
- The “material”, i.e. the mechanical properties, chemical composition and heat treatment,
- The stress level of the equipment, vessels, or containment
- The surface defects and quality of finish, and
- The welding procedures
- Component database for all pressure vessels, containments, and BOP.
  - Tubing
  - Valves
  - Heat exchangers
  - Pumps
  - others
Containment & Pressure Vessel
## Tier 1 Material Operating Requirements

<table>
<thead>
<tr>
<th>Operating Temperature</th>
<th>Adsorbents AX-21 (UQTR/GM/UTRC)</th>
<th>Chemical Hydrides NH$_3$BH$<em>3$$</em>{s}$(PNNL/UTRC)</th>
<th>Metal Hydrides NaAlH$_4$ (UTRC/Sandia)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>70K LH$_2$ 77K LN 100K LH$_2$</td>
<td>160°C</td>
<td>&lt;200°C</td>
</tr>
<tr>
<td>Material Form</td>
<td>Pellet/Powder</td>
<td>Pellet/Solid</td>
<td>Pellet/Powder</td>
</tr>
<tr>
<td>Vessel Requirements</td>
<td>Subambient</td>
<td>Thermal control/Ballast Tank</td>
<td>Thermal control</td>
</tr>
<tr>
<td></td>
<td>Cryogenic material requirements</td>
<td>Materials handling</td>
<td>Material handling</td>
</tr>
<tr>
<td></td>
<td>Thermal control</td>
<td>Storage material impurities</td>
<td>Gas diffusion (O$_2$)</td>
</tr>
<tr>
<td></td>
<td>H$_2$ Permeability</td>
<td>Balance of plant</td>
<td></td>
</tr>
</tbody>
</table>

Each design must meet the DOE goals
NaAlH4 Initial Tank Design

Assumptions: 5.6 wt%, 200 Bar, 95% Solid hydride inside tank, Maximum theoretical performance of hydride.

Not Included: Liner, Insulation, Temperature Control Systems, etc.

Gravimetric Capacity (kg H2/kg system) vs. Volumetric Capacity (kg H2/L system) chart showing different tank materials:
- Titanium Tank
- Carbon Fiber Tank
- High Strength Steel Tank
- Low Cost Aluminum Tank

DOE 2010 Goals
- DOE 2015 Goals
- DOE Ultimate Goals

Notes:
- Carbon Fiber Tank is at the highest capacity for both gravimetric and volumetric values.
- Titanium Tank is at the lowest capacity for both gravimetric and volumetric values.

Assumptions:
- 5.6 wt% hydride
- 200 Bar pressure
- 95% Solid hydride inside tank
- Maximum theoretical performance of hydride

Not Included:
- Liner
- Insulation
- Temperature Control Systems
- etc.
NaAlH4 Design Performance Estimates

Four sets of hydride performance assumptions. The worst set is less desirable than comparable pressurized tanks.

Gravimetric Capacity (kg H₂/kg system) vs. Volumetric Capacity (kg H₂/L system)

- DOE 2010
- DOE 2015
- DOE Ultimate
- Hydride Tanks
- 200 Bar PV
- 300 Bar PV

DOE 2010 Goals
- 0.028
- DOE 2015 Goals
- 0.045
- DOE Ultimate Goals
- 0.070

Theoretical Maximum
- 5.6% Solid
- 5.6 wt% Dense Powder

3.5 wt% Solid
- 0.028

3.5 wt% Loose Powder
- 0.01

Lightweight Carbon Fiber Tanks
Possible Hybrid Tank to Meet 2015 Goal?

If a hydride tank can achieve a high volumetric capacity, there could be a way to meet the 2015 goal with a two-tank system, or one hybrid tank that combines pressurized gas storage with a partial hydride system.
Pressure Tanks Compared to Hydride Goals

Note: Temperature is assumed to be 100°C

<table>
<thead>
<tr>
<th>Hydride</th>
<th>100 Bar</th>
<th>200 Bar</th>
<th>300 Bar</th>
<th>400 Bar</th>
<th>500 Bar</th>
<th>600 Bar</th>
<th>700 Bar</th>
</tr>
</thead>
</table>

Gravimetric Capacity (kg H₂/kg system)

Volumetric Capacity (kg H₂/L system)

DOE 2010 Goals

DOE 2015 Goals

DOE Ultimate Goals

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Combined Tank Performance, 100-700 Bar

Note: Temperature is assumed to be 100°C

**Gravimetric Capacity (kg H₂/kg Sys.)**

**Volumetric Capacity (kg H₂/L Sys.)**

- **DOE Ultimate Gravimetric Goal (0.075)**
- **DOE Ultimate Volumetric Goal (0.070)**

**Titanium and Steel Tanks**

**Carbon Fiber Tanks**

**Aluminum Tanks**

- **DOE 2015 Cost Goal ($2)**
- **DOE 2010 Cost Goal ($4)**

Cost ($/kWh)
Temperature Example: 700 Bar Carbon Fiber Tank

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Cost ($/kWh)</th>
<th>Gravimetric Capacity (kg H2/kg sys.)</th>
<th>Volumetric Capacity (kg H2/L sys.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>6.220</td>
<td>0.091</td>
<td>0.033</td>
</tr>
<tr>
<td>50</td>
<td>7.000</td>
<td>0.081</td>
<td>0.029</td>
</tr>
<tr>
<td>100</td>
<td>7.775</td>
<td>0.074</td>
<td>0.026</td>
</tr>
</tbody>
</table>
Critical Commonalities of the Pressure and Containment Task Vessels

- Thermal management
- Safety-material compatibility, etc.
- Low cost
- Lightweight
- Volumetric capacity
- On-board vs. off-board recharging
Trends

Lower temperature is better.
- High temperature reduces material strength.
- High temperature lowers hydrogen gas density.

Higher pressure is better.
- Gains in gas density are greater than need for thicker tank.
- Higher hydrogen density is needed or DOE’s ultimate volumetric goal is unobtainable.

Carbon fiber has greatest potential to meet all goals.
- But high temperature requirements lead to unacceptable costs because of resin expense.
Conclusions

- Note: Storage Enhancement due to metal hydride will drastically affect the results.
- Carbon fiber is the lowest-weight option in all scenarios, but looks cost-prohibitive at 300C.
- High-strength titanium and steel are heavier but lower-cost options.
- Aluminum is the lowest-cost option of them all, but the weight is a detraction.
- Low-strength steel and magnesium do not compare well to the others in cost or weight.
Preliminary Calculations for Hybrid Metal Hydride Tank On-Board Storage
Introduction

These calculations investigate a range of values for the design of a pressurized hydrogen storage vessel.

Since the details of the internal structure are not yet known, this study focuses on a constant internal volume to contain 5.6 kg of hydrogen at a specified temperature and pressure.

Metal hydrides can increase the actual storage capacity by up to a factor of 6, so the effective storage capacity of the tanks in this study is expected to be between 5.6 kg and 33.6 kg.
Geometry of Simple Tanks

\[ L = \text{Inside Length} \]

\[ D = \text{Inside Diameter} \]

\[ T = \text{Constant Wall Thickness} \]

Internal volume is chosen based on hydrogen density at the specified temperature and pressure to hold 5.6 kg.

L/D = 3, so dimensions are determined by volume requirement.

T is defined such that peak hoop stress equals material yield strength, including a safety factor of 2.0 for metals or 2.35 for composites.
Carbon Fiber Composite Assumptions

- **Toray 700S**
  - 370 ksi composite strength, 60% volume fraction

- **Translation Efficiency**
  - 90% translation efficiency for 2900 and 290 psi
    - Quantum reports 83% @ 5 ksi and 63% @ 10 ksi

- **Hoop Design Strength:**
  - 222 ksi \((\frac{370 \times 2}{3} \times 0.90)\)

- **Reducing Volume Fraction of Fiber is not Economical.**
  - Reduced volume fraction was considered, but is not effective.
Pressure Effect Assumptions

Calculated from: *Revised Standardized Equation for Hydrogen Gas Densities for Fuel Consumption Applications* (NIST, 2008)

<table>
<thead>
<tr>
<th></th>
<th>20 bar (290 psi)</th>
<th>200 bar (2900 psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen Gas Density @ 100 C</td>
<td>1.29 g/L</td>
<td>12.8 g/L</td>
</tr>
<tr>
<td>Hydrogen Gas Density @ 300 C</td>
<td>0.840 g/L</td>
<td>7.92 g/L</td>
</tr>
<tr>
<td>Internal Storage Volume for 5.6 kg of H2 @ 100 C</td>
<td>4353 L</td>
<td>475 L</td>
</tr>
<tr>
<td>Internal Storage Volume for 5.6 kg of H2 @ 300 C</td>
<td>6665 L</td>
<td>707 L</td>
</tr>
</tbody>
</table>
# Temperature Effect Assumptions

<table>
<thead>
<tr>
<th>Material</th>
<th>100 C Yield Strength (ksi)</th>
<th>300 C Yield Strength (ksi)</th>
<th>% Strength Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel</td>
<td>60</td>
<td>54</td>
<td>10%</td>
</tr>
<tr>
<td>Steel (High Strength)</td>
<td>250</td>
<td>225</td>
<td>10%</td>
</tr>
<tr>
<td>Titanium</td>
<td>120</td>
<td>80</td>
<td>33%</td>
</tr>
<tr>
<td>Titanium (High Strength)</td>
<td>165</td>
<td>110</td>
<td>33%</td>
</tr>
<tr>
<td>Carbon Fiber Composite</td>
<td>222</td>
<td>222*</td>
<td>100%</td>
</tr>
<tr>
<td>Aluminum</td>
<td>80</td>
<td>40</td>
<td>50%</td>
</tr>
<tr>
<td>Magnesium</td>
<td>18</td>
<td>10</td>
<td>45%</td>
</tr>
</tbody>
</table>

*Strength remains the same, but resin cost increases substantially.
## Cost Assumptions

<table>
<thead>
<tr>
<th>Material</th>
<th>Cost: $/lb</th>
<th>Cost Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel (60 ksi)</td>
<td>0.4</td>
<td>2006 Estimate</td>
</tr>
<tr>
<td>Steel (250 ksi)</td>
<td>2</td>
<td>2006 Estimate</td>
</tr>
<tr>
<td>Titanium (120 ksi)</td>
<td>2</td>
<td>2006 Estimate</td>
</tr>
<tr>
<td>Titanium (165 ksi)</td>
<td>2</td>
<td>2006 Estimate</td>
</tr>
<tr>
<td>Carbon Fiber (100C)</td>
<td>9.4</td>
<td>Current*</td>
</tr>
<tr>
<td>Carbon Fiber (300C)</td>
<td>74</td>
<td>Current*</td>
</tr>
<tr>
<td>Aluminum</td>
<td>1</td>
<td>2006 Estimate</td>
</tr>
<tr>
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</table>

*See next slide for carbon fiber composite material cost breakdown
Detailed Composite Cost Determination

- **Toray 700S Fiber**
  - 13 $/lb
  - 0.0650 lb/in³ (1.8 g/cc)

- **100 C Resin**
  - Non-specific Resin
  - 2 $/lb
  - 0.0477 lb/in³ (1.32 g/cc)
  - E=6.9E5 Pa

- **100 C composite**
  - 60% fiber volume fraction
  - 0.05808 lb/in³
  - 67.1% wt fiber, 32.9% wt resin
  - 9.4 $/lb

- **300 C Resin**
  - RP-46 (specific resin)
  - 199 $/lb
  - 0.0477 lb/in³ (1.32 g/cc)
  - E=6.9E5 Pa

- **300 C composite**
  - 60% fiber volume fraction
  - 0.05808 lb/in³
  - 67.1% wt fiber, 32.9% wt resin
  - 74 $/lb
General Loading Assumptions

- Safety Factor of 2.0 for metals, 2.35 for carbon fiber
- 25% overpressure: ignored
  - If necessary, it affects all designs equally
- 5mm HDPE liner: ignored
  - Assumed it affects all designs equally
- 1mm Glass fiber overwrap: ignored
  - Non functional
- Pressure Loads: 20 Bar (290 psi), 200 Bar (2,900 psi)
- Hydrides will increase storage capacity by 6x-1x
  - This is not reflected in results
  - 20 Bar results look unattractive when this is not accounted for
All Results: Bubble Chart

Bubble Size = Relative Cost ($418 Smallest to $13,000 Largest)
All Results: Volume/Weight Comparison

- 300C/20Bar
- 100C/20Bar
- 300C/200Bar
- 100C/200 Bar
Below 1000 lbs and $1500

<table>
<thead>
<tr>
<th>Material</th>
<th>Total wt (lbs)</th>
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<tbody>
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Proudly Operated by Battelle Since 1965
## 100°C Results

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<th>Total Volume (L)</th>
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<th>Temp</th>
<th>Press</th>
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# 300°C Results

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<td>200 Bar</td>
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</table>
DOE Goal Considerations

- System Gravimetric and Volumetric Capacity targets are compared to set of potential designs.
- With ideal assumptions, a hydride enhancement factor greater than 1.0 is necessary to meet 2010 and higher targets.
- Assuming a 6.0 hydride enhancement factor, and ideal assumptions, a few designs meet the Ultimate Target.
### Maximum Potential Goals
6x Hydrogen Storage Efficiency
No Significant Insulation

<table>
<thead>
<tr>
<th>System</th>
<th>State</th>
<th>kWh/kg</th>
<th>kWh/L</th>
<th>$/kWh net</th>
<th>Weight GOAL</th>
<th>Volume GOAL</th>
<th>Cost GOAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel (250 ksi)</td>
<td>100 C, 200 Bar</td>
<td>2.19</td>
<td>2.24</td>
<td>0.78</td>
<td>2015</td>
<td>2015</td>
<td>&gt;2015</td>
</tr>
<tr>
<td>Aluminum (80 ksi)</td>
<td>100 C, 200 Bar</td>
<td>2.04</td>
<td>2.01</td>
<td>0.43</td>
<td>2015</td>
<td>2015</td>
<td>&gt;2015</td>
</tr>
<tr>
<td>Titanium (165 ksi)</td>
<td>100 C, 200 Bar</td>
<td>2.49</td>
<td>2.18</td>
<td>0.67</td>
<td>2015</td>
<td>2015</td>
<td>&gt;2015</td>
</tr>
<tr>
<td>Carbon Fiber</td>
<td>100 C, 200 Bar</td>
<td>5.81</td>
<td>2.20</td>
<td>1.00</td>
<td>Ultimate</td>
<td>2015</td>
<td>&gt;2015</td>
</tr>
<tr>
<td>Carbon Fiber</td>
<td>300 C, 200 Bar</td>
<td>4.47</td>
<td>1.48</td>
<td>16.68</td>
<td>Ultimate</td>
<td>2015</td>
<td>FAIL</td>
</tr>
</tbody>
</table>
## Maximum Potential Goals
### 6x Hydrogen Storage Efficiency
### Significant Insulation: Materials Unaffected by Temperature

<table>
<thead>
<tr>
<th>System</th>
<th>State</th>
<th>kWh/kg</th>
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<td>1.48</td>
<td>Ultimate</td>
<td>2015</td>
<td>&gt;2015</td>
</tr>
</tbody>
</table>
Weight Goal

- Weight goal depends largely on tank material, metal hydride material, and system components.
- These scoping calculations only consider tank shell material, not the hydride and not the system components.
- The calculations show that many materials have the potential to meet the 2015 goal, but only carbon fiber can meet the ultimate goal.
- Tank shell material strength and density are the key contributors to tank weight.
Volumetric Goal

There is no way to meet the ultimate volumetric goal with the current assumptions.

Possible fixes:
- Increase hydrogen storage efficiency above 6x
- Increase pressure above 200 Bar

There are potential options for meeting 2015 goal, but they have no hope of going higher.

This is fundamental and NOT related to tank material.
Tank Structure Scoping Analyses: Two Key Terms

**Tank Shell**: The outer casing of the proposed hydrogen tank is considered apart from the other system components. The function of containing the internal pressure dictates many requirements for the rest of the system. The assumed shape is cylindrical with hemispherical ends. The standard L/D ratio is 3, but others were considered (and made little difference).

![Diagram of tank shell](image)

**Hydride System**: In these calculations, the specific hydride system is treated as an unknown. Liners, insulation, valves, pipes, hydride material, and any other components other than the tank shell are all lumped together under this term. A pressure range of 20-200 Bar and a peak temperature range of 100°C to 300°C is considered, under the assumption that the hydride system will function in this range.
Methodology

- Tank Shell internal radius is determined by volume requirement for 5.6 kg of hydrogen gas at a given temperature, pressure, and hydride absorption factor.
  - Choosing an L/D ratio leaves R as the only variable.
- Tank Shell wall thickness is based on allowable hoop strength, which is based on material strength and a safety factor of 2 for metals and 2.35 for composites.
  - Thickness = Pressure*Radius/Hoop Stress Allowable
- Weight, volume, and cost are determined from Tank Shell volume.
  - Although the Hydride System particulars are not yet known, these results are useful in determining the system’s potential to meet DOE targets.
Carbon Fiber Composite Assumptions

▶ Toray 700S
- 370 ksi composite strength (60% volume fraction)
- 90% translation efficiency for 2900 and 290 psi
  - Quantum reports 83% @ 5 ksi and 63% @ 10 ksi
- Wrap 2/3 fibers hoop, 1/3 axial
- Hoop Design Strength = 222 ksi (370 ksi*2/3 *.90)

▶ Cost
- Carbon Fiber = 13 $/lb (1.8 g/cc)
- 100C Resin (generic) = 2 $/lb (1.32 g/cc)
- 300C Resin (RP-46) = 199 $/lb (1.32 g/cc)

▶ Composite
- 222 ksi hoop design strength
- .058 lb/in³ (1.61 g/cc)
- Cost at 100C = 9.4 $/lb
- Cost at 300C = 74 $/lb
## Results: Maximum Potential DOE Target Goals

Assumptions: 6x hydrogen storage efficiency (hydrogen density is 6x gaseous density at given temperature and pressure). Tank shell material strength or material cost is based on peak temperature. Insulation is not assumed.

<table>
<thead>
<tr>
<th>System</th>
<th>State</th>
<th>kWh/kg</th>
<th>kWh/L</th>
<th>$/kWh net</th>
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<td>2015</td>
<td>FAIL</td>
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</tbody>
</table>
Results: Target Goals at Elevated Temperature

Assumptions: 6x hydrogen storage efficiency (hydrogen density is 6x gaseous density at given temperature and pressure). Tank shell material strength or material cost is based on low temperature. Perfect insulation is assumed such that the tank shell temperature peak is only 100C. Additional weight of insulation system is not included.

<table>
<thead>
<tr>
<th>System</th>
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<th>kWh/kg</th>
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<th>$/kWh net</th>
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</table>
Results Compared to DOE Target Potentials

- Carbon fiber, steel, titanium, and aluminum tanks all have some potential to meet the 2015 Gravimetric, Volumetric, and Cost goals.
  - However, adding realistic hydride system components could eliminate any or all of the designs from serious contention.
- Only carbon fiber tanks have the potential to meet the Ultimate Gravimetric goal.
  - It would take a change in the basic assumptions to allow steel, titanium, or aluminum to meet this target goal.
  - Again, adding realistic hydride system components could eliminate any or all of the designs from serious contention.
- None of the tanks have the potential to meet the Ultimate Volumetric goal.
  - Increasing the hydride efficiency (above a 6x factor) or increasing pressure (above 200 Bar) is necessary.
- The Ultimate cost goal has not been set by DOE, but all tank shells under consideration could exceed the 2015 goals.
Hydride System Requirements

- The Tank Shell calculations give us some minimum requirements for the Hydride System.
- To meet Ultimate gravimetric goal the hydride must have an effective weight percent of:
  - At least 8.6 wt% $\text{H}_2$ [ hydrogen wt./(system wt.-tank shell wt.) ]
- To meet the Ultimate volumetric goal the effective hydrogen density must be:
  - At least 74.4 g $\text{H}_2$/l
  - This is greater than 6x density of $\text{H}_2$ @ 100C, 200 Bar
- To meet the 2015 cost goal the hydride system cost (full system excluding tank shell) must be:
  - Less than $1$/kWh
  - Ultimate DOE goal is not yet established
Cost Modeling & Manufacturing Analysis
Accomplishments

Spreadsheet of On-Board Storage Cost
- Provides some details on the manufactured costs of specific components
- Provides costs of purchased items
- Manufacturing cost for system
- Use of preexisting data including TIAX analysis results
  - Sodium Borohydride
  - Sodium Alanate (Both UTRC [more detail], TIAX [less detail but probably 2005$])
  - AX-21 (Not much detail)
Accomplishments (cont’d)

- Received conceptual designs
  - Ammonia Borane
    - No clear specifications, but BOM list
  - Metal Hydride
    - Going to revisit their previous estimate
  - Adsorbent

- Clear from analysis of TIAX values that previous targets were unobtainable
  - Exception 2010 cost target met by Sodium Borohydride
  - Progress formulas applied appear to have provided best possible numbers

- Cost of hydrogen media carrier alone: hydride, AX-21
  - TIAX estimates close to previous cost targets
  - UTRC example for NaAlNH4 was higher
## Previous Cost Estimates

### Table 1 - TIAx and UTRC Cost Estimates for AX-21 and Metal Hydrides

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<td>Hydrogen $</td>
<td>18</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>$2,918</td>
<td>$2,112</td>
<td>$2,043</td>
<td>$3,956</td>
</tr>
</tbody>
</table>

### Targets

<table>
<thead>
<tr>
<th></th>
<th>$/kWh</th>
<th>$/kg</th>
<th>$/kWh</th>
<th>$/kg</th>
<th>$/kWh</th>
<th>$/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Media Cost</td>
<td>3.43</td>
<td>6.19</td>
<td>7.51</td>
<td>15.02</td>
<td>15.65</td>
<td>11.33</td>
</tr>
<tr>
<td>Total</td>
<td>521.07</td>
<td>377.14</td>
<td>408.60</td>
<td>791.20</td>
<td>11.33</td>
<td>12.27</td>
</tr>
<tr>
<td>Total</td>
<td>15.65</td>
<td>11.33</td>
<td>12.27</td>
<td>23.76</td>
<td>11.33</td>
<td>12.27</td>
</tr>
</tbody>
</table>
Cost Model Requirements & Assumptions

- Engineered Cost Model
  - Allows user to change variables and see where most improvement can come
  - Cost Targets TBD
    - Storage System cost -- discounted 2003$
    - (fuel cost) – discounted 2005$
      - with GDP Implicit Price Deflator
  - Only on-board storage – not off-board regeneration
- High degree of transparency
  - Needs to provide estimated cost currently
    - Include a Bill of Materials (BOM) cost database
  - Apply progress ratios
Cost Model Requirements (cont’d)

- Provide predicted future price with high production
  - Provide an ability to change progress values
  - Provide estimates based on assumed units per year?
    - Previous results used 500,000 units per year as high volume
    - UTRC used 1,000,000 units
  - Manufacturing costs of the storage material (not trivial)
    - No clear path to commercialization

- Provide an ability to transform on-board storage estimates
  - From one size to a slightly different sized on board storage system

- Issue: How much flexibility in the model to estimate systems
  - Three very different versions of Ammonia Borane
Bill of Materials

- Detailed component specifications being defined
  - Quantity and specification
    - The more details on the specification, the better the estimate
      - For example, the type of carbon steel (SAE No. 1005 through 1095?)
      - Ammonia Borane
        - Fill-tank bladder specifications
        - Tubing – specifications, material, welded, connection specifications
  - Specifics on ambient temperature each component must operate, specific duty item is undertake.
    - Example, valves
      - Electronic, input size, output size, specific brand could give required specifications
    - Example, Step motor
      - Input condition (voltage, current); Drive Condition, Full step, Dynamic torque, Unipolar or Bipoloar, any ramp up/acceleration; Environmental Condition (humidity, Ambient temperature, pressure, condensation)
      - Motor Life(# of motor shaft revolutions)
Cost Modeling Next Steps

- Complete detailed estimates for each system
- Determine the scope of ultimate change for each system
- Develop scaling functions for main manufactured components
- Develop manufacturing cost estimate for manufactured costs
- Develop approach for instituting progress ratios to develop high output costs
- Determine approach for valuing high production estimates for carrier media