System Level Analysis of Hydrogen Storage Options


2011 DOE Hydrogen Program Review

Washington, DC

May 9-13, 2011

Project ID: ST001

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Overview

Timeline
- Project start date: Oct 2009
- Project end date: Sep 2014
- Percent complete: 40%

Budget
- FY11: $600 K
- FY10: $700 K

Barriers
- H₂ Storage Barriers Addressed:
  - A: System Weight and Volume
  - B: System Cost
  - C: Efficiency
  - E: Charging/Discharging Rates
  - J: Thermal Management
  - K: Life-Cycle Assessments

Partners/Interactions
- Storage Systems Analysis Working Group (SSAWG)
- Hydrogen Storage Engineering Center of Excellence (HSECoE), NREL, SRNL
- BNL, LANL, Ford
- BMW, LLNL, TIAX, and other industry
- FreedomCAR and Fuel Partnership
Objectives and Relevance

- Conduct independent systems analysis for DOE to gauge the performance of H$_2$ storage systems
- Provide results to material developers for assessment against performance targets and goals and help them focus on areas requiring improvements
- Provide inputs for independent analysis of costs of on-board systems.
- Identify interface issues and opportunities, and data needs for technology development
- Perform reverse engineering to define material properties needed to meet the system level targets
Approach

- Develop thermodynamic and kinetic models of processes in physical, complex metal hydride, sorbent, and chemical H₂ storage systems
  - Address all aspects of on-board and off-board storage targets, including capacity, charge/discharge rates, emissions, and efficiencies
  - Assess improvements needed in materials properties and system configurations to achieve storage targets

- Select model fidelity to resolve system-level issues
  - On-board system, off-board spent fuel regeneration, reverse engineering
  - Conduct trade-off analyses, and provide fundamental understanding of system/material behavior
  - Calibrate, validate, and evaluate models

- Work closely with DOE technology developers, HSECoE and others in obtaining data

- Participate in SSAWG meetings and communicate modeling, analysis approach, and results to foster consistency among DOE-sponsored analysis activities
Collaborations

<table>
<thead>
<tr>
<th>Compressed H$_2$ (cH2)</th>
<th>Lincoln Composites, Quantum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cryo-Compressed H$_2$ (CcH2)</td>
<td>BMW, LLNL</td>
</tr>
<tr>
<td>Metal Hydrides</td>
<td>BNL</td>
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<tr>
<td>Chemical Hydrides</td>
<td>LANL</td>
</tr>
<tr>
<td>Sorbents</td>
<td>Ford</td>
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<tr>
<td>GHG Emissions</td>
<td>ANL (GREET)</td>
</tr>
<tr>
<td>Off-Board Spent Fuel Regeneration</td>
<td>BNL, LANL, Dow Chemicals</td>
</tr>
<tr>
<td>Off-Board Cost</td>
<td>ANL (H2A Group), ANL (HDSAM)</td>
</tr>
<tr>
<td>On-Board Cost</td>
<td>TIAX</td>
</tr>
<tr>
<td>SSAWG</td>
<td>HSECoE, DOE, LLNL, OEMs, SNL, Tank Manufactures, TIAX</td>
</tr>
</tbody>
</table>

- Argonne develops the storage system configuration, determines performance, identifies and sizes components, and provides this information to TIAX for manufacturing cost estimation
Summary: FY2011 Technical Accomplishments

- Systems analyzed or updated in FY 2011
  - Physical storage: Two-tank $\text{cH}_2$ system, supercritical $\text{CcH}_2$ system
  - Sorption storage: MOF-5 powder and pellets
  - Chemical storage: Ammonia borane in ionic liquid (AB/IL)
  - Metal hydride: Alane slurry

- Systems are at different stages of development and have been analyzed to different levels of sophistication
  - Results are continually updated
Physical Storage Systems

2-Tank vs. 1-Tank Systems
- Tanks in tight communication (equalized pressures)
- Small loss in capacity and increase in cost

CDS: Charge-Discharge System
Cryogenic Hydrogen Storage in MOF-5
Adiabatic Liquid H₂ Refueling

Key System Requirements

Storage Medium
- 5.6 kg recoverable H₂
- 5-bar minimum delivery pressure
- MOF-5 powder and pellets

Type-3 Containment Vessel
- 2.25 safety factor
- 5,500 P and T cycles
- Toray 2550 MPa CF
- Al 6061-T6 alloy liner

Heat Transfer System
- 1.5 kg/min H₂ refueling rate
- 1.6 g/s H₂ min flow rate
- 5 W heat in-leakage
Modeled Adsorption Isotherms: MOF-5 Powder and Pellets

- Sudik et al (2010 Annual AIChE Meeting)
  - MOF-5 (Basolite Z100-H) loose powder, 130 kg.m\(^{-3}\) bulk density
  - 6 wt% surface excess at 77 K, 55 bar
  - Pelletization causes ~12% loss in excess gravimetric but ~300% gain in volumetric capacity at 77 K

- Sorption fitted to Dubinin-Astakhov (D-A) isotherm, solution thermodynamics for integral enthalpy of adsorption

\[
\Delta H_a = H_a - n_a h_0 = n_a (h_x - h_0) - T^2 \frac{\partial}{\partial T} \left[ \frac{\Phi}{T} \right]
\]
Optimum Pressures and Temperatures: MOF-5 Pellets

All results for LH₂ refueling

- Optimum P and T for maximum gravimetric capacity are 100-120 atm and ~60 K for powder and 310 kg.m⁻³ bulk density, higher for 510 kg.m⁻³ bulk density
- Optimum T lower than the T at which recoverable excess uptake is maximum
- System volumetric capacity increases with P for 130-310 kg.m⁻³ bulk densities, but does not reach the 40-g.L⁻¹ target
Discharge Dynamics: MOF-5 Powder and Pellets

All results for LH₂ refueling

- Required bed permeability for 1 psi in-bed pressure drop and 20 charge and discharge tubes: \(10^{-14} - 10^{-13} \text{ m}^2\)
  - Initial measurement: \(5.4 \times 10^{-13} \text{ m}^2\) for 360 kg.m\(^{-3}\) density pellet
- Required conductivity for 10 U tubes: \(0.04 - 0.5 \text{ W.m}^{-1}.\text{K}^{-1}\)
  - Measured conductivity for powder and pellets: \(0.088 \text{ W.m}^{-1}.\text{K}^{-1}\)
  - Measured conductivity for 500 kg.m\(^{-3}\) pellets with 10 wt% graphite flakes: \(~0.6 \text{ W.m}^{-1}.\text{K}^{-1}\)
Dormancy and H$_2$ Loss: MOF-5 Powder and Pellets

- Dormancy: Function of amount of H$_2$ stored and P/T at start of the event
  - Minimum dormancy is 6 W.d (1.2 days at 5 W in-leakage rate)
  - Peak H$_2$ vent rate is 0.3-1.9 g.h$^{-1}$.kg$^{-1}$ for 5 W in-leakage rate, 25-100% initially full tank
  - Average loss rate below the 0.05 g.h$^{-1}$.kg$^{-1}$ DOE target if the tank less than one-third full
  - No H$_2$ loss if tank is <15% full, or with minimal daily driving
H₂ Storage using Ammonia Borane in Ionic Liquids

- Volume exchange tank design for storing fresh and spent fuel
- Adiabatic vs. non-adiabatic dehydrogenation reactor
- Buffer hydrogen tank
- Heat transfer system (FCS HT and LT coolants)
- Gas liquid separator (coalescing filter)
- Startup reactor (electrically heated)
Reactor Operating Temperatures

- All results for 100% conversion (2.35 H₂-equiv released)
- Increasing recycle leads to lower peak and higher reactor inlet T
  - Stability of ionic liquid related to peak T; inlet T affects choice of pump materials
- Reactor peak and inlet T are insensitive to LHSV and outlet T
- Low recycle ratio is preferred because pumping power increases nonlinearly with R
- Reactor heat transfer decreases as the outlet T is allowed to rise
AB Stability

- All results obtained with kinetic constants derived using 75-110°C data
  - H$_2$ loss rate $>>$ 0.05 g/h/kg at $\geq$50°C ambient temperature,
    15 W.m$^{-2}$.K$^{-1}$ heat transfer coefficient for natural convection
  - Loss rate target met at <30°C ambient temperature (full tank)
  - Loss rate proportionately lower with partially full tank
  - Maximum cumulative loss limited to 1 H$_2$-equiv
Stationary Loss Rates (AB)

- Stationary rate defined as state at which rates of heat generation and heat loss to the ambient are equal
  - True steady state does not exist because $\alpha$ changes continuously
  - No stationary state at $>50^\circ$C ambient temperature (full tank)
  - Results consistent with dynamic simulations
  - Desirable activation energy $>142$ kJ/mol for acceptable loss rates
Preliminary Summary: AB System Analysis

- Product stream recycle is needed to control the reactor peak temperature and AB conversion
- Recycle between 0.6 and 0.95 for complete AB conversion
  - Very difficult to control the peak temperature with heat transfer
  - Lower peak temperatures with higher recycle, but pumping power increases non-linearly
- The reactor can also be operated adiabatically while controlling peak T and AB conversion
  - The reactor peak temperature can be lower if operated adiabatically but the recycle ratio is high

Weight Distribution

- Medium: 63%
- Tank: 19%
- CDS: 12%
- BOP: 6%

Volume Distribution

- Medium: 79%
- Tank: 13%
- CDS: 5%
- BOP: 3%

4.9 wt%

49.5 g.L\(^{-1}\)
LANL has developed a one-pot process for regenerating spent AB using hydrazine (N₂H₄) as the limiting reagent in liquid ammonia:

\[ \text{BNH}_2 + \text{N}_2\text{H}_4 \rightarrow \text{BH}_3\text{NH}_3 + \text{N}_2 \]

Currently hydrazine is produced by the Bayer Ketazine or PCUK Peroxide process:

- **Bayer Ketazine process feed materials**: Cl₂, NaOH, and NH₃
- **PCUK process feed materials**: H₂O₂ and NH₃

FCHtool analysis: energy to produce N₂H₄ dominates the overall energy consumed in AB regeneration.

![AB Regeneration Using Hydrazine](image)

**PCUK Pathway** (per kg H₂ Regenerated in AB):
- NH₃ Production: 263 MJ
- N₂H₄ Production: 227 MJ
- H₂O₂ Production: 331 MJ
- Regeneration: 149 MJ

**Bayer Ketazine Pathway** (per kg H₂ Regenerated in AB):
- NH₃ Production: 174 MJ
- N₂H₄ Production: 246 MJ
- NaOH/Cl₂ Production: 929 MJ
- Regeneration: 149 MJ

WTT Efficiency = 12%  
WTT Efficiency = 8%
H₂ Storage in Alane Slurry: Decomposition Kinetics

- Analyzing new BNL data for micron-sized particles in dibutyl ether (slurry with 60-wt% solids)
- Faster kinetics than previous nano-sized dry powder
- Fitted to Avrami-Erofeev equation with $n = 4.5$, $E = 93.1$ kJ/mol
- Induction time correlated with $T$

\[
d\alpha/dt = nk(1 - \alpha)(-\ln(1 - \alpha))^{(n-1)/n}
\]
Regeneration of Alane

Three-step process

- Formation of a first tertiary amine alane adduct (TMAA or DMEAA)
- Transamination of TMAA or DMEAA to form triethylamine alane adduct (TEAA)
- Decompose TEAA to recover alane

FCHtool analysis: 85% thermal efficiency, 73% SMR efficiency

- Molar ratio: ether/Al = 4, TEA/DMEA = 4, TEA/TMAA = 4

WT T Efficiency = 24-43%
Summary and Status

- Results given as single data points, consult references for range, sensitivity and background
- Metrics cover all DOE targets for on-board and off-board storage
- Some results vetted, others for developmental materials and processes
- Completed analyses of multi-tank systems, MOF-5, and AB systems
  - AlH\textsubscript{3} slurry ongoing
  - Reversible metal hydride: 2LiNH\textsubscript{2}/MgH\textsubscript{2} and LiNH\textsubscript{2}/MgH\textsubscript{2}
  - Physical storage systems: CcH\textsubscript{2} storage issues

<table>
<thead>
<tr>
<th>Performance and Cost Metric</th>
<th>Units</th>
<th>chH\textsubscript{2} 350-T4</th>
<th>chH\textsubscript{2} 700-T4</th>
<th>LH2</th>
<th>CcH\textsubscript{2}</th>
<th>MOF-5</th>
<th>AB</th>
<th>2010 Targets</th>
<th>2015 Targets</th>
<th>Ultimate Targets</th>
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<tbody>
<tr>
<td>Comment</td>
<td></td>
<td>1-Tank</td>
<td>1-Tank</td>
<td>Powder</td>
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<td>Usable Storage Capacity (Nominal)</td>
<td>kg-H\textsubscript{2}</td>
<td>5.6</td>
<td>5.6</td>
<td>5.6</td>
<td>5.6</td>
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<tr>
<td>Usable Storage Capacity (Maximum)</td>
<td>kg-H\textsubscript{2}</td>
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<td>5.6</td>
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<tr>
<td>System Gravimetric Capacity</td>
<td>wt%</td>
<td>5.5</td>
<td>5.2</td>
<td>5.6</td>
<td>5.5-9.2</td>
<td>6.5</td>
<td>4.9</td>
<td>4.5</td>
<td>5.5</td>
<td>7.5</td>
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<td>System Volumetric Capacity</td>
<td>kg-H\textsubscript{2}/m\textsuperscript{3}</td>
<td>17.6</td>
<td>26.3</td>
<td>23.5</td>
<td>41.8-44.7</td>
<td>34.9</td>
<td>49.5</td>
<td>28</td>
<td>40</td>
<td>70</td>
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<tr>
<td>Storage System Cost</td>
<td>$/kg-H\textsubscript{2}/m\textsuperscript{3}</td>
<td>17.6</td>
<td>26.3</td>
<td>23.5</td>
<td>41.8-44.7</td>
<td>34.9</td>
<td>49.5</td>
<td>28</td>
<td>40</td>
<td>70</td>
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<tr>
<td>Fuel Cost</td>
<td>$/gge</td>
<td>4.2</td>
<td>4.3</td>
<td>TBD</td>
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<tr>
<td>Cycle Life (1/4 tank to Full)</td>
<td>Cycles</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>5500</td>
<td>5500</td>
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<td>1000</td>
<td>1500</td>
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<tr>
<td>Minimum Delivery Pressure, FC/ICE</td>
<td>bar(abs)</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>3-4</td>
<td>5</td>
<td>5</td>
<td>5/35</td>
<td>5/35</td>
<td>3/35</td>
</tr>
<tr>
<td>System Fill Rate</td>
<td>kg-H\textsubscript{2}/min</td>
<td>1.5-2</td>
<td>1.5-2</td>
<td>1.5-2</td>
<td>1.5-2</td>
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<td>Minimum Dormancy (Full Tank)</td>
<td>W-d</td>
<td>NA</td>
<td>NA</td>
<td>2</td>
<td>4-30</td>
<td>6</td>
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<tr>
<td>H\textsubscript{2} Loss Rate (Maximum)</td>
<td>g/h/kg-H\textsubscript{2}</td>
<td>NA</td>
<td>NA</td>
<td>8</td>
<td>0.2-1.6</td>
<td>1.9</td>
<td>0.75</td>
<td>0.1</td>
<td>0.05</td>
<td>0.05</td>
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<tr>
<td>WTE Efficiency</td>
<td>%</td>
<td>56.5</td>
<td>54.2</td>
<td>22.3</td>
<td>41.1</td>
<td>41.1</td>
<td>12.0</td>
<td>60</td>
<td>60</td>
<td>60</td>
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<tr>
<td>GHG Emissions (CO\textsubscript{2} eq)</td>
<td>kg/kg-H\textsubscript{2}</td>
<td>14.0</td>
<td>14.8</td>
<td>TBD</td>
<td>19.7</td>
<td>19.7</td>
<td>62.9</td>
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<tr>
<td>Ownership Cost</td>
<td>$/mile</td>
<td>0.13</td>
<td>0.14</td>
<td>TBD</td>
<td>0.12</td>
<td>TBD</td>
<td>TBD</td>
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</tbody>
</table>
Future Work

As lead for Storage System Analysis Working Group, continue to work with DOE contractors to model, validate, and analyze various developmental hydrogen storage systems.

Physical Storage
- Multi-tank compressed H₂ tank systems representative of current designs
- Supercritical cryo-compressed storage concepts

Metal Hydrides
- Update of alane slurry storage system analysis (BNL collaboration)
- Regeneration of alane/other off-board regenerable metal hydrides
- Reversible metal-hydride storage system

Sorbent Storage
- Analysis of generic sorbent system with arbitrary heat of adsorption

Chemical Hydrogen
- On-board system for AB/IL class of materials (LANL collaboration)
- Fuel cycle efficiency of AB regeneration (LANL collaboration)
Supplemental Slides
## MOF-5 On-Board Performance: Key Assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference Values</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sorbent</strong></td>
<td>MOF-5 (Basolite Z100-H)</td>
</tr>
<tr>
<td></td>
<td>Skeletal density</td>
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<tr>
<td></td>
<td>Crystallographic density</td>
</tr>
<tr>
<td></td>
<td>Bulk density</td>
</tr>
<tr>
<td></td>
<td>Thermal conductivity</td>
</tr>
<tr>
<td><strong>Insulation</strong></td>
<td>Multi-Layer Vac. Super Insulation</td>
</tr>
<tr>
<td></td>
<td>Layer density</td>
</tr>
<tr>
<td></td>
<td>Density</td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
</tr>
<tr>
<td></td>
<td>Effective conductivity</td>
</tr>
<tr>
<td><strong>Tank</strong></td>
<td>T700S Carbon Fiber</td>
</tr>
<tr>
<td></td>
<td>Tensile strength</td>
</tr>
<tr>
<td></td>
<td>Density</td>
</tr>
<tr>
<td></td>
<td>L/D</td>
</tr>
<tr>
<td></td>
<td>Liner</td>
</tr>
<tr>
<td></td>
<td>Shell</td>
</tr>
<tr>
<td><strong>Refueling</strong></td>
<td>Adiabatic Refueling with LH₂</td>
</tr>
<tr>
<td></td>
<td>LH₂ pump efficiency</td>
</tr>
<tr>
<td></td>
<td>Storage temperature</td>
</tr>
<tr>
<td></td>
<td>Temperature swing</td>
</tr>
<tr>
<td><strong>Discharge</strong></td>
<td>H₂ Recirculation</td>
</tr>
<tr>
<td></td>
<td>Temperature</td>
</tr>
<tr>
<td></td>
<td>Recirculation rate</td>
</tr>
<tr>
<td><strong>Balance of System</strong></td>
<td>Miscellaneous weight</td>
</tr>
<tr>
<td></td>
<td>Miscellaneous volume</td>
</tr>
</tbody>
</table>
Weight and Volume Distribution

- 6.5-wt% gravimetric and 34.9 kg.m\(^{-3}\) volumetric capacities with MOF-5 powder at 60-K storage T and 150-atm storage P
  - Medium and liner account for ~50% of the overall weight
  - 69% volumetric efficiency
Discharge Dynamics: Temperature and Sorption Fields

- Effect of bed thermal conductivity on temperature and sorption fields after discharge at full flow rate (1.6 g.s\(^{-1}\))
  - MOF-5 powder, storage P: 150 atm, storage T: 60 K

\[ \lambda_e = 0.088 \text{ W.m}^{-1}\text{.K}^{-1} \]

\[ 0.2 \text{ W.m}^{-1}\text{.K}^{-1} \]

\[ 0.4 \text{ W.m}^{-1}\text{.K}^{-1} \]

\[ T_{\text{mean}} = 92.2 \text{ K} \]

\[ T_{\text{mean}} = 87.5 \text{ K} \]

\[ T_{\text{mean}} = 84.5 \text{ K} \]

\[ n_e = 53.4 \text{ g.kg}^{-1} \]

\[ n_e = 25.8 \text{ g.kg}^{-1} \]

\[ n_e = 27.1 \text{ g.kg}^{-1} \]

\[ P_{\text{initial}} : 150 \text{ atm} \]

\[ P_{\text{final}} : 5 \text{ atm} \]

\[ T_{\text{initial}} : 60 \text{ K} \]

\[ k : 5.4 \times 10^{-14} \text{ m}^2 \]
## AB/bmimCl as H₂ Carrier

- Work at UPenn has shown that 1.1 H₂-equiv are released in 5 min and 2.2 H₂-equiv in 20 min from 50:50 wt% AB/bmimCl at 110°C

<table>
<thead>
<tr>
<th>AB</th>
<th>Unit</th>
<th>Value</th>
<th>Comments/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>kg/mol</td>
<td>30.9</td>
<td></td>
</tr>
<tr>
<td>H₂ content</td>
<td>wt. %</td>
<td>19.6</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>kg/m³</td>
<td>780</td>
<td></td>
</tr>
<tr>
<td>Thermal stability and decomposition</td>
<td>°C</td>
<td>90 - 110</td>
<td>1st H₂-equiv released, &gt;1 h induction period for release at 85°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>150°C</td>
<td>2nd H₂-equiv released</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&gt;450°C</td>
<td>3rd H₂-equiv released</td>
</tr>
<tr>
<td>ΔH</td>
<td>kJ/mol-H₂</td>
<td>21</td>
<td>Exothermic reaction</td>
</tr>
</tbody>
</table>

### Solvent: 1-butyl-3-methylimidazolium chloride (bmimCl)

<table>
<thead>
<tr>
<th>Solvent: 1-butyl-3-methylimidazolium chloride (bmimCl)</th>
<th>Unit</th>
<th>Value</th>
<th>Comments/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>kg/mol</td>
<td>174.7</td>
<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>°C</td>
<td>70</td>
<td>BASF</td>
</tr>
<tr>
<td>Flash point</td>
<td>°C</td>
<td>192</td>
<td>BASF</td>
</tr>
<tr>
<td>Density</td>
<td>kg/m³</td>
<td>1050</td>
<td>at 80°C, BASF</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Pa-s</td>
<td>0.147</td>
<td>at 80°C, BASF</td>
</tr>
<tr>
<td>Specific heat</td>
<td>kJ/kg-K</td>
<td>1.81</td>
<td>at 80°C, BASF</td>
</tr>
<tr>
<td>Thermal stability</td>
<td>°C</td>
<td>NA</td>
<td></td>
</tr>
</tbody>
</table>

### 50:50 wt% AB/bmimCl

| Melting point | °C | NA | Liquid at room temperature |
| Density | kg/m³ | NA | |
| Viscosity | Pa-s | NA | Stirrable liquid at room temperature |
| Specific heat | kJ/kg-K | NA | |
| Thermal stability and decomposition | °C | NA | Foams once H₂ is released; foam begins to convert to white solid after releasing 1 H₂-equiv; entire mixture becomes solid after releasing 2 H₂-equiv; no induction period for H₂ release. |
| ΔH | kJ/mol-H₂ | 33 | Exothermic reaction |
Storage Capacity

- Of all the systems built, Gen3 CcH₂ has the highest demonstrated gravimetric and volumetric capacity
- Alane slurry shows high volumetric capacity but stable 70-wt% slurry not formulated, volume-exchange tank not developed
- On-going studies to find AB/IL formulations that remain liquid under all conditions, volume-exchange tank not developed
- CcH₂ model capacities in agreement with Tech Val data

Diagram to be regarded as a snapshot in time
Different systems not analyzed to same level of sophistication
Advanced materials not ready for deployment
Some component concepts require further development

Consult ANL reports for complete details, assumptions and background
Weight Distribution

- 350-bar cH₂, LH₂ & CcH₂ systems may meet 2015 gravimetric target
- CcH₂ system with Al shell approaches the ultimate gravimetric target
- CF is the main contributor to the overall weight in cH₂ systems
- Metal liner is a heavy component in all Type-3 pressure vessels
- Medium weight dominates in metal hydride and chemical H₂ systems

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cH₂: Compressed H₂
350b: 350 bar
700b: 700 bar
LH₂: Liquid H₂
CcH₂: Cryo-compressed H₂
MOF: MOF-177
SA: TiCl₃ catalyzed NaAlH₄
LCH₂: Organic liquid carrier
SBH: Alkaline NaBH₄ solution
AB: Ammonia borane

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ANL Analysis
5.6 kg Usable H₂

<table>
<thead>
<tr>
<th>Type 3</th>
<th>Type 3</th>
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<tbody>
<tr>
<td>1-Tank</td>
<td>2-Tank</td>
<td>1-Tank</td>
<td>2-Tank</td>
</tr>
</tbody>
</table>

- 438 kg
- 5.5% 4.5 wt%
- 7.5%
Volume Distribution

- CcH₂ system meets 2015 volumetric target but not ultimate target
- Medium volume significant in all options and, by itself, exceeds the 2015 system target in cH₂ systems
- Insulation volume important in cryogenic systems
- CDS in LCH₂ is bulky because of highly endothermic reaction
- BOP in SBH (adiabatic reactor, exothermic release) is bulky because of condensers

BOP: Balance of Plant
CDS: Charge-Discharge System
Hydrogen Loss During Extended Parking

- 40% of H₂ stored in LH₂ tank vented to ambient in a typical use cycle
- Negligible H₂ loss from insulated cryogenic pressure vessels with some daily driving
- H₂ loss from alane determined by kinetics and ambient temperature, not by heat transfer
- H₂ loss from AB/IL determined by kinetics, ambient temperature, and heat transfer coefficient

![Graph showing peak H₂ loss (g/h/kg) for different materials and temperatures.](image)

- ANL Analysis
  - 5.6 kg Usable H₂
- 2015 Target
  - 0.05 g/h/kg
- Materials: 350b, 700b, LH₂, CcH₂, MOF, AX-21, Alane, SA, LCH₂, SBH, AB
- Temperatures: 25°C, 50°C
- Full Tank, 50°C
- Full Tank
- Half Tank
- NA

Image omitted for clarity.
Dormancy

- Shorter dormancy in LH$_2$ system if the fuel tank is partially full
- Longer dormancy in CcH$_2$ system with partially-full tank, no stranded driver syndrome
- Longer dormancy in cryogenic sorbent systems than CcH$_2$ because of heat of desorption
- Dormancy definition not meaningful for alane and AB storage
Cost of On-Board Systems at High-Volume Manufacturing

- Cost data from TIAAX studies with ANL inputs, 500,000 units/year
- Fiber cost dominates in cH₂ systems, less expensive in cryogenic sorption systems
- Material cost important in sorption systems and in SA system
- Dehydrogenation catalyst cost important in LCH₂ system

Consult TIAAX reports for complete details, assumptions and background.
Efficiency of On-Board Systems

- Venting loss accounts for inefficiency of LH\(_2\) system
- 10-30\% H\(_2\) consumed in alane, SA and LCH\(_2\) systems to sustain high-temperature endothermic reactions
- ~1\% loss in AB system efficiency because of fuel pump, additional FCS coolant and radiator fan power
- DOE target for on-board system efficiency is 90\%
Well-to-Tank Efficiency

- 350- and 700-bar $\text{ch}_2$ options have $<60\%$ WTT efficiency
- Reversible metal hydrides may have higher WTT efficiency than $\text{ch}_2$
- LCH2 regeneration is exothermic and can reach 60% efficiency
- High uncertainty in alane regeneration efficiency because of vacuum distillation steps and low-grade waste heat requirement
- Options involving cryogenic $\text{H}_2$ have $< 41\%$ WTT efficiencies
- Low efficiencies for AB and SBH regeneration

Note: No-go decision was made on hydrolysis of SBH for on-board applications
Well-to-Engine Efficiency

- Only $c\text{H}_2$ and $Cc\text{H}_2$ have same WTT and WTE efficiencies
- Sorbent systems have nearly same WTT and WTE efficiencies
- Low WTE efficiencies for exothermic AB and SBH options because of off-board losses in regeneration
- Low WTE efficiencies for cryogenic options because of off-board losses in liquefaction
- WTE efficiencies <50% for endothermic SA and LCH2 options because of on-board losses

Note: No-go decision was made on hydrolysis of SBH for on-board applications
Greenhouse Gas Emissions

- Values given in kg of CO$_2$ equivalent per kg of H$_2$ delivered to the vehicle or per mile driven
  - 63.4 mpgge assumed fuel economy for 2015 advanced FC vehicle
- As reference, GHG emissions for 2015 mid-size ICE vehicle with 31 mpgge fuel economy is 0.35 kg-CO$_2$/mile
Refueling Cost

- H2A data for cost of unit operations, natural gas at $0.22/Nm³
- Liquefaction contributes significantly to the fuel cost in options requiring LH₂
- Regeneration is the main component of fuel cost in SBH option
- No storage option can meet the $2-3/kg cost target (untaxed)

Consult ANL and TIAAX reports for complete details, assumptions and background.