

IV.E.1 Analyses of Hydrogen Storage Materials and On-Board Systems

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Contract Number: DE-FG36-04GO14283

Start Date: June 2004
Projected End Date: September 2009

Objectives

The overall objective for this project is provide independent analysis to help guide the Department of Energy (DOE) and developers toward promising research and development (R&D) and commercialization pathways by evaluating the various on-board hydrogen storage technologies on a consistent basis. Specific objectives include:

- Compare different on-board hydrogen storage approaches in terms of lifecycle costs, energy efficiency and environmental impact;
- Identify and compare other performance aspects that could result in barriers to successful commercialization (e.g., on-board system weight and volume);
- Examine the effects of system-level cost and performance trade-offs for different storage approaches; and
- Project performance and cost relative to DOE targets.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume

(B) System Cost

(F) System Life-Cycle Assessments

Technical Targets

This project evaluates the various on-board hydrogen storage technologies being developed by the DOE Hydrogen Storage Centers of Excellence and independent projects. Insights gained from these evaluations will help guide DOE and developers toward promising hydrogen storage materials and system-level designs and approaches that could meet the DOE targets for storage system cost, specific energy, energy density, fuel cost and efficiency.

Accomplishments

We have performed preliminary and/or updated assessments for several hydrogen storage systems. For each system assessment, we projected on-board system performance and high-volume (~500,000 units/year) manufactured cost, as well as determined the critical cost drivers and conducted single- and multi-variable sensitivity analyses to bound cost results. We also reviewed key assumptions and results with developers, DOE, and stakeholders (e.g., material suppliers, national labs, FreedomCAR and Fuel Partnership Tech Teams) and incorporated their feedback into the final results. Finally we compared performance and cost results to other baseline technologies and DOE targets for the on-board storage system. Specific accomplishments include:

- An updated assessment of the cryo-compressed hydrogen storage system. The baseline design was Lawrence Livermore National Laboratory's (LLNL's) second generation system with design adjustments by Argonne National Laboratory (ANL). We assumed further adjustments for automotive-scale manufacturing based on developer feedback and available literature, and estimated the cost to be \$13.5/kWh for 10.1 kg of usable hydrogen stored.
- A preliminary assessment of a liquid hydrogen storage system based on a typical design derived from available literature. The preliminary cost estimate was \$8/kWh for 10.1 kg of stored hydrogen.
- An updated evaluation of 5,000 psi and 10,000 psi compressed hydrogen (cH₂) storage systems incorporating updated system design and carbon fiber cost assumptions. The updated cost estimates for 5,000 psi and 10,000 psi systems were \$17/kWh and \$27/kWh, respectively, for 5.6 kg of usable hydrogen.

- A preliminary assessment of a liquid hydrocarbon-based chemical hydrogen storage system based on Air Products' liquid hydrogen carrier (LCH₂) material. For a system storing 5.6 kg of usable hydrogen, model results indicate a cost of \$15.5/kWh, a gravimetric capacity of 2.1 wt%, and a volumetric capacity of 18 g H₂/L.
- An updated evaluation of the sodium borohydride (SBH)-based chemical hydrogen storage system incorporating updated system design assumptions using the latest information from Millennium Cell (MCell) and ANL. For a system storing 5.6 kg of usable H₂, model results were \$4.8/kWh, 3.3 wt%, and 0.9 kWh/L. These results are very similar to our original assessment.

In addition, preliminary results have been generated for the off-board (i.e., refueling) cost, energy efficiency, and greenhouse gas emissions for the LCH₂ pathway. We also reported updated off-board results for the SBH pathway.

- Preliminary results indicate that the cost of LCH₂ refueling is lower than refueling via cH₂ pipeline and liquid hydrogen (LH₂) truck delivery pathways. These preliminary results are in the process of being reviewed by developers, DOE, and stakeholders.
- The updated cost of SBH refueling based on advanced regeneration processes being investigated by Rohm & Hass, are significantly cheaper than the previous process evaluated, but are still more expensive than refueling via cH₂ pipeline and LH₂ truck delivery pathways.



Introduction

DOE is funding the development of a number of hydrogen storage technologies as part of its "Grand Challenge" applied R&D program. This independent analysis project helps guide the DOE and Grand Challenge participants toward promising R&D and commercialization pathways by evaluating the various hydrogen storage technologies on a consistent basis. Using this consistent and complete comparison of various technology options, R&D can be focused and accelerated. Without such an approach, erroneous investment and commercialization decisions could be made, resulting in wasted effort and risk to the development of hydrogen vehicles and a hydrogen infrastructure.

TIAX is conducting system-level evaluations of the on-board storage systems cost and performance, as well as the well-to-wheel (or lifecycle) cost, primary energy use, and environmental impact for four broad categories of on-board hydrogen storage. The four categories of

storage are: Reversible On-Board (e.g., metal hydrides and alanates), Regenerable Off-Board (e.g., chemical hydrides); and High Surface Area Sorbents (e.g., carbon-based materials), and Advanced Physical Storage (e.g., cryo-compressed hydrogen, liquid hydrogen). Evaluations are based on developers' on-going research, input from DOE and key stakeholders, and in-house expertise.

Approach

This project utilizes an approach that is designed to minimize the risks associated with achieving the project objectives. In coordination with ANL developers, system-level conceptual designs are developed for each on-board storage system and required fueling infrastructure. Next, system models and cost models are used to develop preliminary performance and cost results. We utilize in-house activities- and product-based cost models to determine high-volume manufactured cost projections for the on-board storage system, and H2A-based discounted cash flow models to estimate hydrogen selling prices based on the required off-board hydrogen infrastructure. Subsequently, these results are vetted with developers and key stakeholders and refined based on their feedback. Coordination with DOE's Hydrogen Storage System Analysis Working Group avoids duplication and ensures consistency. This is an on-going and iterative process so that DOE and its contractors can increasingly focus their efforts on the most promising storage technology options.

Results

Our cryo-compressed system cost estimate was based on the LLNL second generation cryo-compressed tank design [1]. The 151 liter, 5,000 psi, multi-layer vacuum insulated tank allows for a maximum 10.7 kg of liquid hydrogen storage, and 10.1 kg of "usable" hydrogen based on a 94% drive cycle utilization calculated by ANL [2]¹. A detailed bill of materials (BOM) and operating conditions were obtained from LLNL and ANL analysis [1,2], and, based on tank developer feedback, we made several design adjustments to more closely model a system suitable for high manufacturing volumes. For example, we assume electronic control valves (rather than manual); and an electronic control system which would communicate with hydrogen dispensers at fueling stations, interpret temperature and pressure measurements, and control the system valves.

¹ Storing super-critical (i.e., high-pressure) liquid hydrogen would allow for more hydrogen to be stored in the same size tank, thereby increasing the tank's storage capacity and reducing the overall cost on a \$/kWh basis. Storing high-pressure compressed hydrogen or a two-phase mixture instead of pure LH₂ would have the opposite effect.

We used netting analyses to estimate the tank's carbon fiber requirement, and obtained information and feedback from cryogenic tank developers, cryogenic component vendors, and patent literature to derive system cost estimates for the on-board cryogenic compressed hydrogen storage system. Our cost model indicates that the system cost of the cryo-compressed system would be approximately \$4,500 at high production volumes, or \$13.5/kWh based on 10.1 kg of usable hydrogen. The carbon fiber and cryogenic control valves combined account for 50% of the total system cost. We also estimated that a system designed for 5.6 kg of usable hydrogen would cost approximately \$20/kWh. Note that cost per kWh is expected to be less for the larger tank capacities mainly because balance of plant (BOP) costs are not significantly increased for larger tank sizes.

We used similar resources and knowledge gained from the cryo-compressed system evaluation to conduct a preliminary assessment of a LH₂ on-board storage system. The main cost difference between the two tanks stems from the fact that the lower pressure LH₂ tank does not require a carbon fiber composite layer. In addition, BOP components may be de-rated for lower pressure operation. Our preliminary high-volume cost estimate for the LH₂ system was \$8/kWh, based on 10.1 kg of usable hydrogen. Cryogenic control and relief valves accounted for 30% of the total cost. We also estimated that a system designed to store 5.6 kg of usable hydrogen would cost \$14/kWh.

As with previous storage technology assessments, we captured the uncertainty of key system costs by conducting single- and multi-variable sensitivity analyses. Additionally, we analyzed the effect of replacing the specified stainless steel vacuum shell with an aluminum shell. We estimate that the total cost of the cryo-compressed system and the liquid system could be reduced by 5% and 8%, respectively, by using an aluminum vacuum shell. Further cost reductions may be possible by replacing other stainless steel components with aluminum. Using an aluminum shell also improves the gravimetric capacity of the cryo-compressed system from 5.5 wt% to 7.2 wt%, as well as the gravimetric capacity of the liquid system from 6.5 wt% to 9 wt%.

We estimated the volumetric capacity of both cryogenic hydrogen storage systems to be 33 g H₂/L. Many of the components are estimated to require the same volume for the two systems. The extra volume required by the carbon fiber and high pressure control valves on the cryo-compressed system is balanced by the tank ullage requirement for the liquid system.

A preliminary LCH₂ storage system cost was estimated based on Air Products' liquid hydrocarbon material and a baseline on-board system design developed by ANL [3]. We worked closely with ANL to develop a BOM consistent with their performance

assessment. Assuming high manufacturing volumes (~500,000 units/year), we estimated the LCH₂ system cost to be approximately \$2,900 for 5.6 kg of usable hydrogen, or \$15.5/kWh. The usable hydrogen capacity was calculated assuming a 67% storage efficiency (i.e., some hydrogen is burned to supply the heat for dehydrogenation) and a 95% conversion efficiency. The reactor catalyst, palladium, accounts for approximately 30% of the overall system cost, and the burner and pumps account for approximately 20% each. We calculated the system's gravimetric and volumetric capacities to be 2.1 wt% and 18 g H₂/L. Key sensitivity parameters are currently being reviewed.

We updated our assessment of the SBH-based chemical hydrogen storage system incorporating the latest design information from MCell and ANL. Along with dimensional changes to system components, the new design includes a condensate tank, a hydrogen ballast tank, and an accumulator; and eliminates the primary separator from the previous design. The system reactor design incorporated several changes, including an increase in conversion efficiency from 92% to 100%, an increase in operating pressure from 6 bar to 12 bar, and the integration of an active water/glycol cooling loop. Finally, wetted tank parts that were previously polypropylene were updated to 316 stainless steel, as per MCell suggestion, due to increased operating temperatures.

We ran our cost model for three scenarios, varying the H₂ storage capacity and the SBH concentration. For our primary scenario, we evaluated a 5.6 kg H₂ system, and assumed a SBH concentration of 24 wt% based on TIAX/ANL analysis. Our updated model indicated a cost of \$4.8/kWh, a gravimetric capacity of 3.3 wt%, and a volumetric capacity of 26 g H₂/L.

Finally, we updated the baseline assessments for the 5,000 psi and 10,000 psi cH₂ on-board storage systems. Key changes included updating the maximum operating pressure of the tanks to account for a 25% overpressure during filling and updating the carbon fiber cost assumption from \$10/lb of fiber to \$13/lb of fiber. Using these updated assumptions, we estimated the 5,000 psi cH₂ system to cost \$17/kWh for 5.6 kg of usable hydrogen. We calculated the gravimetric and volumetric capacities to be 5.6 wt% and 17 g H₂/L, respectively. For the updated 10,000 psi cH₂ system, we calculated the system cost to be \$27/kWh, the gravimetric capacity to be 4.2 wt%, and the volumetric capacity to be 23 gH₂/L. The carbon fiber composite cost accounts for 75% and 80% of the 5,000 psi system and 10,000 psi system cost, respectively.

The results for system cost, weight, and volume described above are compared in Figure 1, Figure 2, and Figure 3, respectively. For each storage system, we conducted single- and multi-variable sensitivity analyses to evaluate the effects of the uncertainties of critical cost

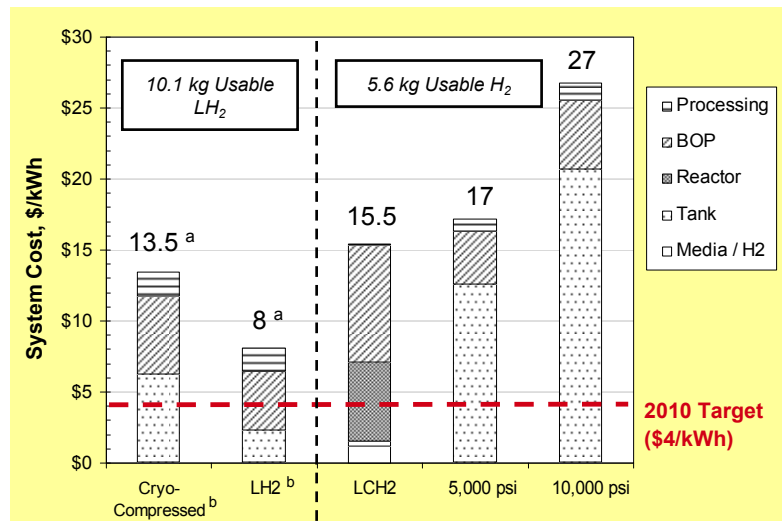
variables. These variables are the focus of on-going discussions with developers and stakeholders.

In addition to on-board analysis activities, we conducted a preliminary off-board assessment of the LCH₂ system based on performance information obtained from Air Products. The off-board analysis includes an estimate of the cost and energy inputs for LCH₂ regeneration, trucking, and vehicle fueling. We examined the scenario in which dehydrogenation of the liquid carrier occurred at the fueling station (and vehicles are filled with compressed gas), as well as the scenario in which vehicles were filled with LCH₂, and dehydrogenation occurred on-board the vehicle. We developed base case assumptions and cost estimates for the regeneration system. We also analyzed the capacity limitations for hauling LCH₂ and spent material and developed modified H2A Delivery Component models to analyze trucking, reprocessing and fueling station costs.

We also updated our off-board SBH cost models. TIAX received detailed cost estimates for two advanced SBH reprocessing pathways from Rohm & Hass. The process assumptions that served as the foundation for these cost estimates were reviewed by ANL. TIAX used H2A-based spreadsheet tools to evaluate the cost of reprocessing and SBH transport. As with previous SBH analyses (using a hydrogen-assisted Schlessinger process), it was determined that the reprocessing portion of the delivery process had the largest effect on the overall cost. Using the TIAX-modified H2A spreadsheet and inputs provided by Rohm & Haas and ANL, the costs for reprocessing was estimated to be \$9.8/kg H₂ and \$5.1/kg H₂ for the two advanced processes. In both cases the primary cost drivers are capital costs and electricity costs. Significant alterations to either of these parameters could lead to significant changes in the overall price of SBH reprocessing.

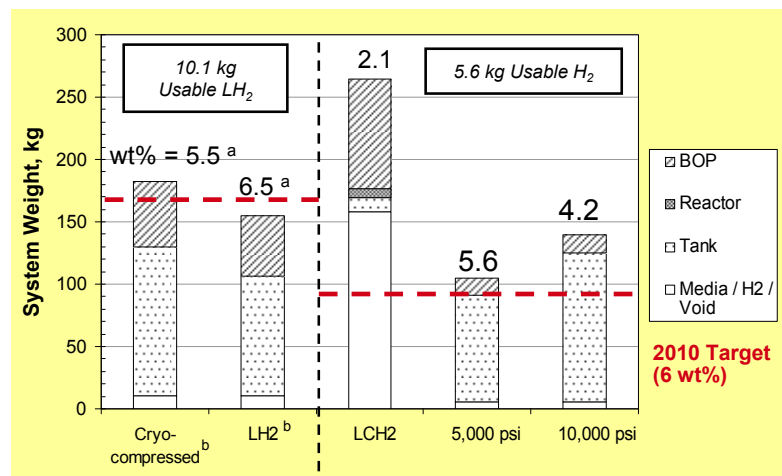
Conclusions and Future Directions

The cost assessments conducted this year allow direct comparison with prior cost assessments. Our models allow us to identify critical cost components,



^a Normalizing the cryo-compressed and liquid H₂ systems for 5.6 kg of usable hydrogen results in system costs of ~\$20/kWh and ~\$14/kWh, respectively.
^b An aluminum shell (rather than SS) offers approximately 5% and 8% cost savings for the cryo-compressed and liquid H₂ systems, respectively.

FIGURE 1. Preliminary On-board Storage System Cost Comparison Results



^a Normalizing the cryo-compressed and liquid H₂ systems for 5.6 kg of usable hydrogen results in system gravimetric capacities of ~4.0 wt% and ~4.4 wt%, respectively.
^b An aluminum shell (rather than SS) increases gravimetric capacities to 7wt% and 9 wt% for the cryo-compressed and liquid H₂ systems, respectively.

FIGURE 2. Preliminary On-board Storage System Weight Comparison Results

which enables focused discussion with tank developers and manufacturers.

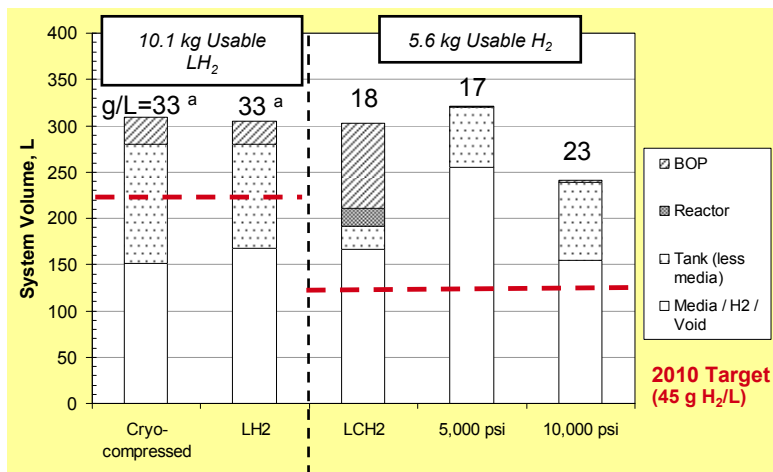
- The baseline cryo-compressed system and liquid system, each storing 10.1 kg of usable hydrogen, offer improved gravimetric and volumetric storage capacities compared with other storage systems evaluated to date. Additionally, the cryo-compressed and LH₂ systems are estimated to be lower cost on a per kilowatt hour basis than

compressed systems. However, when normalized to 5.6 kg of usable storage, the cryogenic systems lose their cost advantage compared with 5,000 psi compressed systems.

- Cryogenic storage system estimates (e.g., cryo-compressed and LH₂) have considerable uncertainty associated with the high-volume cost of cryogenic BOP components (e.g., valves). We will continue to work with tank developers understand these costs.
- High-pressure on-board systems are generally governed by carbon fiber tank related variables including fiber and matrix costs, translation strength, and safety factor. Continual validation of these critical assumptions will be essential during this project.
- Preliminary results indicate that the LCH₂ on-board storage system would have similar cost and volume metrics, but an inferior weight metric when compared to the 5,000 psi cH₂ system. For the LCH₂ on-board system, the cost of the palladium catalyst, as well as the pumps and the burner are key system costs, and along with the LCH₂ media, are key contributors to the system cost uncertainty.
- If LCH₂ dehydrogenation occurs on-board vehicles, the off-board delivery cost of LCH₂ is dominated by regeneration costs at the central plant. The preliminary results indicate that the hydrogen selling price for the LCH₂ delivery infrastructure is less than that of cH₂ pipeline or LH₂ truck delivery. Along with the cost of hydrogen, the cost of the liquid carrier media and the conversion efficiency are key sources of uncertainty.
- Consistent with the previous results, the updated SBH on-board storage system cost estimate looks attractive compared to other storage technologies. The updated off-board reprocessing pathways show improvement over past results, but still remain high compared with baseline cH₂ pipeline and LH₂ truck delivery pathways.

The rest of this fiscal year, we plan to continue to work with developers and stakeholders to improve the accuracy of the analyzed on-board and off-board system models to date.

- Work with Air Liquide and other developers to finalize results for the LH₂ storage system.
- Incorporate developer feedback and generate final results for the on-board and off-board LCH₂ system assessments.



Note: Volume results do not include void spaces between components (i.e., no packing factor was applied).

^a Normalizing the cryo-compressed and liquid H₂ systems for 5.6 kg of usable hydrogen results in system volumetric capacities of ~28 g H₂/L system volume each.

FIGURE 3. Preliminary On-board Storage System Volume Comparison Results

- Review the updated compressed storage results with tank developers and manufacturers and incorporate feedback.
- Update all hydrogen storage systems as necessary to ensure an accurate comparison of storage technologies.

In the next fiscal year, we will evaluate other storage technology options based on discussions with DOE.

FY 2008 Publications/Presentations

Presentations made under the title: Lasher, S. et al; "Analyses of Hydrogen Storage Materials and On-Board Systems" since last year, unless otherwise noted:

1. DOE Annual Hydrogen Merit Review; June, 2008, Crystal City, VA.
2. DOE Cryo-compressed Hydrogen Sidebar Meeting, June, 2008, Crystal City, VA.
3. FreedomCAR and Fuel Partnership Hydrogen Storage Tech Team Meeting; April, 2008, Detroit, MI.
4. Unnasch, S. et al; "H2A Hydrogen Carrier Analysis"; NHA Conference, March, 2008, Sacramento, CA.
5. Ringer, M. et al; "H2A Delivery Models Update: Improvements and Advanced Carrier Inclusion"; Storage System Analysis Working Group Meeting, December, 2007, Washington, DC.
6. SBH Review Meeting, September, 2007, Argonne, IL.
7. DOD Hydrogen Storage New Project Kickoff Meeting, August, 2007, via teleconference.

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2. Ahluwalia, R.K. et al., 2008, "Independent Review of Cryo-compressed Storage of Hydrogen: Interim Report," Argonne National Laboratory, Hydrogen Storage Tech Team Meeting, Aug., 2006, Revised Feb., 2008.
3. Ahluwalia, R. et al., 2007, "Systems Level Analysis of Hydrogen Storage Options," Argonne National Laboratory, DOE Hydrogen Program Review, May 15-18, 2007.
4. Lasher, S. et al, 2008, "Analyses of Hydrogen Storage Materials and On-Board Systems – Cryo-compressed and Liquid Hydrogen System Cost Assessments"; DOE Annual Hydrogen Merit Review; June 10, 2008.
5. Moreno, O., 2007, "Development of an Advanced Chemical Hydrogen Storage and Generation System: On-board Fueling System Based on Sodium Borohydride," July 13, 2007.