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

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Objectives

The overall objective for this project is provide independent analysis to help guide the 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
(K) 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:

- Completed liquid hydrogen carrier (LCH_2) system cost assessments based on Argonne National Laboratory's (ANL) performance assessment of Air Products and Chemicals Inc. (APCI) regenerable organic liquid carrier (n-ethylcarbazole-like material[1]). The high-volume (500,000 units/yr) on-board system factory cost projection is estimated to be \$15.5/kWh useable hydrogen and the mature market (i.e., 250 tonnes/day [TPD] H_2 eq.) refueling cost projection is estimated to be \$4.74/kg H_2 eq. for the base case assumptions. The on-board system weight and volume estimates are 2.2 wt% and 20 g H_2/L for the base case.
  - Updated 5,000 and 10,000 psi compressed hydrogen on-board system factory cost assessments by making slight adjustments to the tank safety factor and carbon fiber requirement

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[1] N-ethylcarbazole is toxic and has a low hydrogen storage capacity (i.e., wt%) making it relatively inappropriate for an actual on-board storage media, however it is being used as a representative material for expected carriers to be developed and allows analysis regarding the system, and delivery to be completed.

  assumptions to be consistent with ANL's updated analysis and results. The high-volume on-board system factory cost projection is estimated to be \$15.6 and \$23/kWh useable H_2 for 5,000 and 10,000 psi, respectively. The on-board system weight and volume estimates are 5.9 and 4.7 wt%, and 18 and 25 g H_2/L for 5,000 and 10,000 psi base cases, respectively.

- Completed review of Rohm & Haas (R&H) ammonia borane (AB) regeneration and first fill cost projections based on R&H plant configuration and performance assessments. The mature market (i.e., 100 TPD H_2 eq.) AB regeneration cost projection was estimated to be \$8/kg H_2 eq. and the mature market (i.e., 10,000 TPY AB) AB first-fill cost projection was estimated to be \$9/kg AB.

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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 for four broad categories of on-board hydrogen storage. The four categories are: reversible on-board (e.g., metal hydrides and alanates), regenerable off-board (e.g., chemical hydrides), 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, system-level conceptual designs are developed for each on-board storage system and required fueling infrastructure. We work closely with ANL to develop a bill of materials consistent with their performance assessment. 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 LCH_2 storage system cost projection was estimated based on APCI's liquid hydrocarbon material and a baseline on-board system design developed by ANL [1]. The LCH_2 material hydrogen capacity is assumed to be 5.8 wt%, but the actual useable hydrogen capacity is just 3.7 wt% assuming a 68% storage efficiency (i.e., some hydrogen is burned to supply the heat for dehydrogenation) and a 95% reactor conversion efficiency. Assuming high manufacturing volumes (~500,000 units/year), we estimated the LCH_2 system cost to be approximately \$2,900 for 5.6 kg of usable hydrogen, or \$15.5/kWh (see Figure 1). The reactor catalyst, palladium, accounts for approximately 32% 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

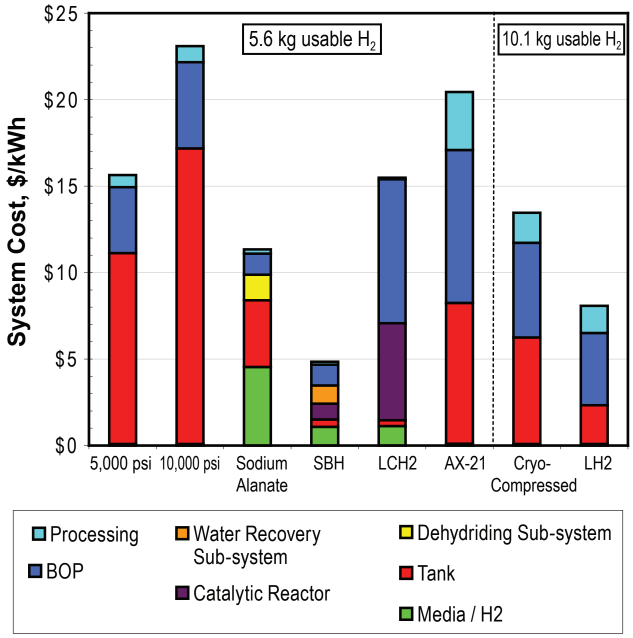

FIGURE 1. Preliminary On-board Storage System Cost Comparison Results

2.2 wt% and 20 g H_2/L, respectively. The palladium, pumps, media, and burner costs were identified as being key sensitivity parameters, along with the assumed conversion efficiency.

We also conducted a rough on-board system assessment for a hypothetical autothermal liquid carrier media with similar performance assumptions as the baseline LCH_2 media except we assumed a higher material hydrogen storage capacity and usable hydrogen capacity (i.e., hydrogen does not have to be burned on-board to sustain the dehydrogenation reaction). Based on input from APCI, we assumed the hypothetical autothermal carrier offered a hydrogen material capacity of 6.7 wt% (vs 5.8 wt% in the baseline LCH_2 system) and a 100% storage capacity (vs. 68% storage capacity in the baseline LCH_2 system). We further assumed the autothermal system would require an oxidation reactor that uses a V_2O_5 catalyst, but would not require a heat exchange (HEX) burner[2]. The preliminary estimate indicates that the autothermal carrier could offer weight and volume savings of approximately 25-30% over the baseline LCH_2 system, but that cost savings would be minimal (<5%).

In addition to on-board analysis activities, we conducted a preliminary off-board assessment of the LCH_2 system based on performance information obtained from APCI. The off-board analysis includes an estimate of the cost and energy inputs for LCH_2 regeneration, trucking, and vehicle fueling. We examined the scenario in which hydrogen vehicles were filled with LCH_2, and dehydrogenation occurred on-board the vehicle. We developed base case assumptions and cost estimates for the regeneration system based on feedback from APCI. We also analyzed the capacity limitations for hauling LCH_2 and spent material and developed modified H2A Delivery Component models [2] to analyze trucking, reprocessing and fueling station costs. Our preliminary estimate for the hydrogen selling price based on LCH_2 refueling is \$4.7/kg H_2 eq. (see Figure 2). The costs of hydrogen and the liquid carrier are the two dominant factors having the greatest affect on the hydrogen selling price sensitivity. If the LCH_2 is used as an off-board transportation media only (i.e., fueling station dehydrogenation with compressed gas refueling), the hydrogen selling price would increase to approximately \$6/kg.

Next, we updated our baseline on-board cost, weight and volume assessments for the 5,000 psi and 10,000 psi compressed hydrogen (cH_2) storage systems. The assessment included an independent review of the technical performance by ANL [3], comments received from the FreedomCAR & Fuel Partnership Hydrogen Storage Technical Team, input from Quantum, Toray, Structural Composites Inc., and other tank developers/manufacturers via teleconferences. The key change last year included applying the tank safety factor to the nominal tank pressure (i.e., 5,000 and 10,000 psi) rather than maximum filling over pressure (i.e., 6,250 and 12,500 psi) based on new/contradictory information from industry. We also reduced our carbon fiber tensile strength assumption from 2,940 to 2,550 MPa and modified our end dome shape and thickness assumptions to be consistent with the composite pressure vessel algorithm being used by ANL[3].

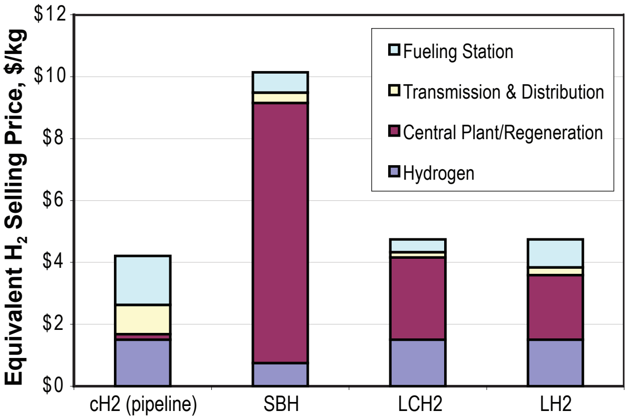

FIGURE 2. Preliminary Off-board Refueling Cost Comparison Results

Using these updated assumptions, we estimated the cH_2 system factory costs to be approximately \$2,900 (\$15.6/kWh) for 5,000 psi and \$4,300 (\$23.1/kWh) for 10,000 psi systems storing 5.6 kg of usable hydrogen (see Figure 1). This represents a decrease in cost of 9% for 5,000 psi and 13% for 10,000 psi systems compared to those reported last year. The carbon fiber composite accounts for approximately 70% and 75% of the overall system cost for the 5,000 psi and 10,000 psi tanks, respectively. The range of uncertainty for the tank's carbon fiber purchased cost and safety factor assumptions have the biggest impact on the base case cost estimate (roughly 15-20% each). The updated system gravimetric and volumetric capacities are estimated to be 5.9 wt% and 18 g H_2/L for 5,000 psi and 4.7 wt% and 25 g H_2/L for 10,000 psi systems.

We also evaluated ownership cost (i.e., combination of hydrogen storage system purchased cost and refueling cost) for both the LCH_2 and cH_2 storage systems to compare the combined off-board and on-board costs with other infrastructure options (see Figure 3). Combining the base case on-board system costs (i.e., \$15.4/kWh for LCH_2, \$15.6/kWh for 5,000 psi, and \$23.1/kWh for 10,000 psi), with the projected base case off-board refueling costs (i.e., \$4.74/kg for LCH_2, \$4.21/kg for

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[2] Based on feedback from APCI, our rough estimate assumes there would be no net change in cost, weight, and volume resulting from swapping the HEX burner for an oxidation reactor.

[3] The resulting pressure vessel design calls for both hoop and helical fiber windings in the cylindrical portion of the vessel, with a 1.8 hoop to helical winding ratio. The end domes consist of only helical windings, and the composite thickness is non-uniform and thickest near the vessel exit hole.

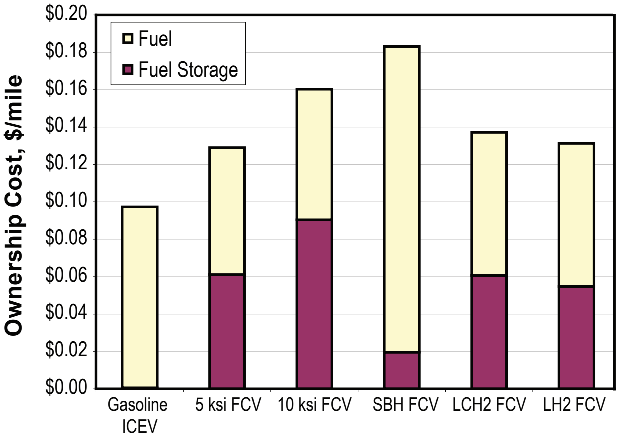

FIGURE 3. Preliminary Fuel System Ownership Cost Comparison Results

5,000 psi, and $4.32/kg for 10,000 psi) resulted in an ownership costs of roughly $0.14, $0.13 and $0.16 per mile, respectively, based on the assumptions presented in Table 1. The implicit assumption in this ownership cost assessment is that each fuel system and vehicle performs equally well and has the same operating lifetime.

Finally, TIAX completed a high-level review of R&H's cost assessment of the regeneration [4] and first fill production [5] of AB. TIAX reviewed two confidential AB reports generated by R&H in February as well as other relevant reports and evaluated all the process equipment and assumptions in addition to the implementation of these assumptions into the H2A Delivery Components Model supplied by R&H. Overall, we believe that R&H did an appropriate assessment of the AB first-fill and regeneration costs. The review was partially based on proprietary information received from R&H via the aforementioned reports as well as several conference calls. The AB regeneration pathway was based on a process being evaluated by Los Alamos National Laboratory (LANL).

The estimated baseline AB regeneration cost is projected to be slightly cheaper than the previously analyzed regeneration cost for sodium borohydride (SBH), but more expensive than regeneration cost projection for a liquid hydrocarbon (LCH_2) based on an n-ethylcarbazole-like hydrogen storage media. We expect AB delivery and fueling station costs to be much lower than cH_2 or LH_2 options, but the overall equivalent hydrogen selling price would still likely be more than twice as expensive as these more conventional options. Key cost reduction opportunities include reducing utility and feedstock costs (i.e., electricity, natural gas, hydrogen) which represent over 60% of the regeneration cost. Reducing overall energy use will reduce utility costs as well as improve the primary energy use and greenhouse gas (GHG) emissions results.

R&H calculated the baseline AB first-fill cost to be $9/kg AB. Approximately 75% of the first-fill cost comes from the cost of SBH, which is assumed to be $5/kg SBH for the baseline analysis. The first-fill cost has a relatively minor impact on the costs at the regeneration plant (impacting plant storage and material replacement costs),

TABLE 1. Ownership Cost Assumptions

Preliminary Ownership Cost Assumptions	Gasoline ICEV	cH2 FCV	cH2 FCV	SBH FCV	LCH2 FCV	LH2 FCV	Basis/Comment
Annual Discount Factor on Capital	15%	15%	15%	15%	15%	15%	Input assumption
Manufacturer + Dealer Markup	1.74	1.74	1.74	1.74	1.74	1.74	Assumed mark-up from factory cost estimates
Annual Mileage (mi/yr)	12,427	12,427	12,427	12,427	12,427	12,427	Car vehicle miles traveled divided by total registrations for 2006
Vehicle Energy Efficiency Ratio	1.0	2.0	2.0	2.0	2.0	2.0	Based on ANL drive-cycle modeling
Fuel Economy (mpgge)	31.0	62.0	62.0	62.0	62.0	62.0	ICEV: Car combined CAFE sales weighted FE estimate for MY 2007
H_2 Storage Requirement (kg H_2)	NA	5.6	5.6	5.6	5.6	5.6	Design assumption based on ANL drive-cycle modeling
Fuel Price ($/eq. gal)	3.00	4.21	4.21	10.14	4.74	4.74	FCV: Equivalent H_2 price from Off-board Assessment
H_2 Storage System Factory Cost ($/kWh)	NA	15.6	15.6	5.0	15.5	14.0	H_2 storage cost from On-board Assessment

ICEV - internal combustion engine vehicle
FCV - fuel cell vehicle
FE - fuel economy
MY - model year

but it can have a bigger impact on the on-board storage system cost. If we assume the AB hydrogen storage capacity is 16.3 wt%, 34 kg of AB would be required to provide the targeted 5.6 kg H_2 on-board the vehicle, resulting in an on-board storage system cost contribution of approximately $300 or $1.60/kWh of stored hydrogen. The DOE 2010 and 2015 cost targets for the complete on-board storage system (inclusive of first-fill, storage tanks, reactors, balance of plant, etc.) are $4/kWh and $2/kWh H_2, respectively.

All of the results reported above should be considered in the context of meeting both on-board and off-board cost targets as well as other DOE targets, including on-board system weight, volume, durability/operability, charging/discharging rates; and off-board primary energy use/GHG emissions and fuel purity.

Conclusions and Future Directions

The cost assessments conducted this year allow direct comparison with prior cost assessments and DOE targets. Our models allow us to identify critical cost components, which enables focused discussion with tank developers and manufacturers.

- The base case on-board LCH_2 system evaluated was nearly 4 times more expensive, 2.5 times heavier, and 2 times larger than DOE 2010 targets. The LCH_2 media itself narrowly contains enough hydrogen to meet the DOE on-board system gravimetric target (5.8 wt% vs. 5.5 wt% target). Also, substantial cost reductions and/or performance improvements are needed for the on-board reactor and balance-of-plant (BOP) components to meet targets.
- Although improvements to the LCH_2 material and storage capacities increases system-level weight and volume in the hypothetical autothermal carrier system, they do little to decrease the on-board system cost because the dehydrogenation reactor and BOP account for over 90% of the system cost, and are unaffected by storage capacity. Also, even with the weight and volume improvements, additional material and BOP improvements would be required to meet the 2010 weight and volume targets.
- The off-board LCH_2 hydrogen selling price is approximately 1.6 to 2.4 times the DOE target of $2-3/kg hydrogen, but is only about 13% more expensive than the 5,000 psi compressed hydrogen delivery option. Additional LCH_2 off-board cost reductions are possible if the carrier material cost is at the low end of the assumed range ($2-12/gal) or if carrier losses are lower than the assumed 2.75% of media throughput.
- When base case on-board and off-board costs are combined, we see that the LCH_2 fuel system has potential to have roughly the same ownership cost as a gasoline ICEV when gasoline is assumed to be $4.25/gal ($0.14/mile), but 40% higher ownership cost when gasoline is $3.00/gal[4].
- The base case 5,000 psi cH_2 system meets the DOE 2010 on-board system gravimetric target, but there is currently no clear path to achieving on-board storage system cost or volume targets as currently configured. The base case 5,000 and 10,000 psi systems evaluated here were 4 and 6 times more expensive, and 2.2 and 1.6 times larger than DOE 2010 targets, respectively. The 10,000 psi system is also 20% above the 2010 target weight.
- When base case on-board and off-board costs are combined, we see that the 5,000 psi cH_2 fuel system has potential to have roughly the same ownership cost as a gasoline ICEV when gasoline is assumed to be $4.00/gal ($0.13/mile), but 30% higher ownership cost when gasoline is $3.00/gal[4]. However, the 10,000 psi fuel system ownership cost will likely be 60% (6¢/mi or ~$740/yr) higher than a conventional gasoline ICEV for the base case when gasoline is $3.00/gal.
- An initial AB regeneration cost projection was estimated to be $8/kg H_2 eq., which is 2.7-4 times more expensive than the total target delivery cost of $2-3/kg H_2.

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 and evaluate other storage technology options as necessary based on discussions with DOE.

- LCH_2 – update and finalize assumptions and results based on feedback, and complete sensitivity analysis.
- Activated carbon – update and finalize assumptions and results based on updated design and new carbon fiber requirement calculations.
- Cryo-compressed – update based on Lawrence Livermore National Laboratory's Generation 3 Design and new carbon fiber requirement calculations.
- Liquid – incorporate feedback from developers and stakeholders and incorporate relevant updates from the cryo-compressed system assessment.
- New technologies – to be determined by DOE (one or two of the following: AB, adsorbent, alane, MOF177, spillover material, others).
- Update all hydrogen storage systems as necessary to ensure a consistent comparison of storage technologies.

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[4] Different assumptions for annual discount factor, markups, annual mileage and fuel economy would yield slightly different results.

FY 2009 Publications/Presentations

1. Lasher, S. et al, "Hydrogen Storage Using a Liquid Carrier: Off-board System Cost Assessment," Report for Joule Milestone, June, 2008.

2. Lasher, S. et al, "Hydrogen Storage Using a Liquid Carrier: On-board System Cost Assessment," Report for Joule Milestone, June, 2008.

3. Lasher, S. et al, "Hydrogen Storage using a Liquid Carrier: Off-board and On-board System Cost Assessments," Final Report, October 29, 2008.

4. Lasher, S. et al, "Activated Carbon System Cost Assessment," Draft Report, February 26, 2009.

5. Lasher, S. et al, "Hydrogen Storage Using Compressed Hydrogen: On-board System Cost Updates," Final Report, March 24, 2009.

6. Lasher, S. et al, "Compressed and Liquid Hydrogen Carrier System Cost Assessments," DOE Annual Hydrogen Merit Review, May 19, 2009, Crystal City, VA.

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1. Ahluwalia, R.K., Hua, T.Q., Peng, J.K., 2007, "System Level Analysis of Hydrogen Storage Options," 2007 DOE Hydrogen Program Review, May 15–18, Arlington, VA.

2. TIAX, 2008, H2A Delivery Components Carrier Model v34.

3. Hua, T.Q., Peng, J.K., Ahluwalia, R.K., "Analysis of Compressed Hydrogen Storage Systems," Argonne National Laboratory, Feb. 2009.

4. Rohm and Haas Company, 2009, "1st-Fill Ammonia Borane Manufacturing Cost Estimate," 1Q 2009 Milestone Report, February 9.

5. Rohm and Haas Company, 2009, "Ammonia Borane Regeneration – LANL Process: Baseline manufacturing Cost Estimate," 1Q 2009 Milestone Report, February 16.