IV.F.2 Cost Analysis of Hydrogen Storage Systems

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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 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 Storage section (3.3.4.2) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan: (A) Cost

- (B) Weight and Volume
- (C) Efficiency
- (G) System Life Cycle and Efficiency Analyses

Technical Targets

This project evaluates the various on-board hydrogen storage technologies being developed by the DOE Hydrogen Storage Centers of Excellence (CoE) and other developers. 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 evaluated sodium alanate and sodium borohydride hydrogen storage systems based on recent literature and developer input, in particular from United Technologies Research Center (UTRC) and Millennium Cell who have on-going DOE contracts to develop advanced hydrogen storage systems. Accomplishments include:

- Developed system-level conceptual designs for the on-board storage system,
- Projected on-board system performance (e.g., weight and volume) and high-volume manufactured cost,
- Conducted single- and multi-variable sensitivity analyses to determine the most important cost drivers,
- Reviewed key assumptions and results with developers, DOE, and stakeholders (e.g., material suppliers, national labs, FreedomCAR Tech Teams) and incorporated their feedback into the final results, and
- Compared performance and cost results to baseline technologies (5,000 and 10,000 psi storage systems) and DOE targets for the on-board storage system.

In addition, preliminary results have been generated for the off-board (i.e., fuel cycle) cost, energy efficiency, and greenhouse gas emissions from sodium borohydride and magnesium hydride pathways. These preliminary results are in the process of being reviewed by developers, DOE, and stakeholders, so they are not presented here.

Introduction

DOE is funding the development of a number of hydrogen storage technologies as part of its "Grand Challenge" program. This independent analysis project will help 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. Without a consistent and complete comparison of the various technology options, erroneous investment and commercialization decisions could be made, resulting in wasted effort and risk to the development of hydrogen vehicles and a hydrogen infrastructure.

Approach

TIAX is conducting a system-level evaluation of the on-board storage system cost and performance, as well as the well-to-wheel or lifecycle cost, primary energy use, and environmental impact for three broad categories of on-board hydrogen storage. Evaluations are based on developers' on-going research, input from DOE and key stakeholders, in-house experience, and input from material experts. Coordination with Argonne National Labs through DOE's Hydrogen Storage System Analysis Working Group continued to avoid duplication and ensure consistency. The three 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).

This project will utilize an approach that is designed to minimize the risks associated with achieving the project objectives. System-level conceptual designs will be developed for each on-board storage system and required fueling infrastructure. Next, system models and cost models will be used to develop preliminary performance and cost results. We will 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 will be vetted with developers and key stakeholders and refined based on their feedback. This will be an on-going and iterative process so that DOE and its contractors can increasingly focus their efforts on the most promising technology options.

Results

Last year, we projected performance (weight and volume) and high-volume manufactured cost for an on-board sodium alanate hydrogen storage system based on the UTRC technology. This year, we reexamined the overall tank design and assumed media density for the sodium alanate system. We revised the assumed media density from 1.26 g/cc to 1.39 g/cc to account more accurately for the Ti catalyst and by-products from the addition of the catalyst precursor. The result of the media density change was an increase in the overall system volumetric density. However, the change in the overall tank design off-set most of the increase, so that the overall volume only changed from 0.64 to 0.65 kWh/L. The overall system gravimetric density decreased from 0.58 to 0.53 kWh/kg based on changes to the tank design.

In addition, because the balance-of-plant (BOP) makes up a relatively large fraction of the overall cost, we revisited last year's purchased component cost estimates to see if there was room for cost savings. We calculated bottom-up purchased costs using DFMA[®] software based on material, machining, and assembly costs plus 50% markup for component supplier overhead and profit. The overall system factory cost decreased from \$13/kWh to \$11/kWh using this bottom-up method for the BOP purchased component costs.

We also performed detailed single- and multivariable sensitivity analyses for the new sodium alanate base case. We ran single variable sensitivity analyses on the overall sodium alanate system cost, weight, and volume for the top four system parameters: media reversible hydrogen capacity (H_2 wt%), media cost (\$/kg), tank carbon fiber layer thickness (mm), and media relative packing density. The high and low values chosen for media reversible hydrogen capacity had the greatest impact on system cost, weight, and volume. The single-variable sensitivity analysis for the sodium alanate system cost is presented in Figure 1.

DOE selected a sodium borohydride-based (NaBH₄) hydrogen storage system for the initial technology assessment for the regenerable off-board (e.g., chemical hydrides) category of hydrogen storage. We developed sodium borohydride system design parameters,



FIGURE 1. Sodium Alanate Single-Variable Sensitivity Analysis: Factory Cost

conducted a performance (i.e., weight and volume) and cost assessment, and reviewed the results with DOE, developers and stakeholders. We evaluated the Millennium Cell approach to storing and transporting sodium borohydride.

This category of chemical hydride releases hydrogen through a simple exothermic hydrolysis reaction onboard the vehicle to produce hydrogen and spent chemical hydride (note that hydrogen evolves from both the chemical hydride and reacted water). In the Millennium Cell approach, sodium borohydride is stored as a solution with water so that additional water is not carried separately to release hydrogen during the hydrolysis reaction. Sodium hydroxide (NaOH) is used to stabilize the sodium borohydride solution by raising the solution pH to greater than 13. To generate hydrogen on demand, the solution is sent to a catalytic reactor after which humidified hydrogen is separated from the excess water and spent sodium borohydride (i.e., sodium metaborate). The reaction consumes and vaporizes water driving up the concentration of the metaborate in solution. Water must be recovered from the humidified hydrogen stream to purge system components and dilute the metaborate solution to prevent precipitation. The overall system configuration is represented in Figure 2.

We assume the sodium borohydride material can achieve 21.3 wt% hydrogen storage capacity (weight of water not included) based on the hydrolysis of one mole of sodium borohydride with four moles of water. We further assume the concentration of sodium borohydride in a solution of water and NaOH is 26 wt% based on Millennium Cell results and near-term projections. The resulting media hydrogen storage capacity for the sodium borohydride solution would be 5.5 wt% (maximum) based on these assumptions. Precipitation of the sodium metaborate solution after hydrolysis is the limiting factor for the sodium borohydride concentration specification.

A Millennium Cell design is assumed for the catalytic reactor, which consists of a flow-through reactor using 1 wt% ruthenium (Ru) catalyst supported on a nickel (Ni) foam substrate. Sodium borohydride/ metaborate solutions are highly caustic (> pH 13) and corrosive requiring that high temperature/pressure $(>50^{\circ}C / >2 bar)$ components be stainless steel and the reactor catalyst substrate be durable. The reactor operates at 145°C and the temperature is maintained by regulating the pressure at which steam is generated (maximum of 6 bar). We assume the reactor can achieve an average conversion efficiency of 92% at 40% of peak demand flow based on Millennium Cell data. Note that the reactor can deliver 100% of peak demand flow (0.02 g/s/kW), but at a lower conversion efficiency (~80%).

After conversion in the reactor, the hydrogen stream, saturated with water vapor at ~145°C, enters a



**Additional safety and start-up components maybe required

FIGURE 2. Sodium Borohydride Components Conceptual Designs (5.6 kg hydrogen stored)

liquid separator followed by an air-cooled condenser that cools the stream to ~70°C and returns water to the sodium metaborate solution. We estimate the concentration of the (mostly) sodium metaborate solution will be about 60 wt% at the liquid separator under peak demand flow conditions assuming 80% conversion efficiency. Water from the condenser can be added to the solution to reduce its concentration to around 40 wt%. At this concentration, the solution would still have to be maintained above 35°C in order to prevent precipitation. Higher conversion efficiencies (e.g., 92% for 40% of peak demand flow) will result in even higher sodium metaborate concentrations and temperatures required to prevent precipitation.

Next, we assume the metaborate solution is sent to a separate section of the main storage tank, separated from the sodium borohydride solution via a movable partition or bladder system. While this single-tank volume exchange design has not been demonstrated at automotive scale, Millennium Cell has demonstrated smaller tanks with this space-saving design feature. Conceptual designs of the key system components are presented in Figure 3. Detailed design assumptions can be found in this year's DOE Annual Merit Review presentation (Lasher et al, 2006).

We found that the current status of the sodium borohydride system will likely be about twice as heavy as a 5,000 psi compressed hydrogen storage system, but, if technically feasible, the sodium borohydride system with a single-tank volume exchange design will be smaller than even a 10,000 psi system. Results for the 5,000 psi and 10,000 psi hydrogen storage systems are based on results from a previous TIAX analysis (Carlson et al, 2004) adjusted for <100% carbon fiber translational strength. As can be seen in Figures 4-5, the sodium borohydride system weight and volume are driven primarily by the media and tank. The sodium borohydride system evaluated here will not likely meet the DOE 2007 system weight and volume targets, but it can exceed the system cost target (see Figure 6) based on the high-volume manufactured cost assessment (excluding regeneration costs). However, preliminary results indicate that refueling costs will be higher than those projected for compressed hydrogen (results are not presented here).

Refueling costs are being evaluated based on transporting the spent sodium metaborate solution back to a central plant for regeneration of sodium borohydride. We are in the process of finalizing the sodium borohydride off-board assessment based on information published by Millennium Cell, Rohm & Haas and others. We are working with the developers, Argonne National Labs, and DOE to define a process configuration for sodium borohydride regeneration that would represent today's technology, but suitable for large scale production. We have also analyzed the capacity limitations for hauling sodium borohydride/metaborate and developed an H2A Delivery Components model



FIGURE 3. Sodium Borohydride System Schematic





FIGURE 4. Storage System Mass Results



FIGURE 5. Storage System Volume Results



FIGURE 6. Storage System Factory Cost Results

spreadsheet to analyze trucking costs. We are currently developing additional H2A model spreadsheets for the regeneration system and forecourt station.

Conclusions and Future Directions

A few general conclusions can be drawn from the results of the sodium borohydride-based hydrogen storage system design evaluated here. Note that not all of these comments will apply to other chemical hydridebased systems.

- Media with much higher (perhaps >9 wt%) hydrogen storage capacity may be required to meet the DOE 2007 weight and volume targets based on the chemical hydride system design evaluated here. However, materials with higher hydrogen storage capacity may have more challenging and costly regeneration requirements.
- Design and demonstration of a single-tank volume exchange design for an automotive-scale system is critical to the on-board storage volumetric density. A two-tank system would increase the overall system volume by almost 80%. Note that the volume exchange design may also be critical for the delivery and storage of the sodium borohydride/ metaborate off-board the vehicle.
- Water and thermal management required to avoid sodium metaborate precipitation (and in some cases freezing) are the most critical processes to the proper operation of the sodium borohydride system evaluated here. The conceptual system design will likely require tank heating to prevent sodium metaborate precipitation, which will reduce on-board system efficiency.
- Water addition from the fuel cell exhaust would also help to prevent solution precipitation, but detailed fuel cell water balances have shown that little or no water will likely be available for this purpose.
- At high production volumes, almost one-fourth of the factory cost of the on-board sodium borohydride storage system will be the media cost. Low-cost regeneration processes are required so that replacement of this media during refueling will not result in exorbitant operating costs.
- Despite the challenges, sodium borohydride-based hydrogen storage offers the following potential advantages:
 - Low purchased cost for the on-board hydrogen storage system
 - Low-pressure storage and delivery
 - Better system-level volumetric storage density than 10,000 psi compressed hydrogen (automotive-scale single-tank volume exchange design must be demonstrated)
 - Potential for conformable tank design (must be proven)
 - "Pumpable" nature of the sodium borohydride solution should make off-board material handling easier

In the next fiscal year, we will evaluate other storage technology options as directed by DOE. The option will likely be an additional regenerable off-board technology, such as organic liquids. In addition, we plan to finalize the off-board (i.e., well-to-tank) assessment for all the technologies evaluated to date. The off-board assessment includes:

- Develop system-level conceptual designs for the required fueling infrastructure,
- Determine refueling cost and well-to-tank primary energy use and environmental impact for the required infrastructure by utilizing the H2A model format with the appropriate inputs and assumptions, and
- Continue to work with DOE, H2A, developers, National Labs, other stakeholders, and the Hydrogen Storage System Analysis Working Group throughout the analysis process.

FY 2006 Publications/Presentations

1. Lasher, S. et al; "Comparison of On-board Hydrogen Storage Options"; Fuel Cell Seminar, November 2005, Palm Springs, CA.

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

2. FreedomCAR and Fuel Partnership Hydrogen Delivery Tech Team Meeting; July 2005, Columbia, MD.

3. FreedomCAR and Fuel Partnership Hydrogen Storage Tech Team Meeting; September 2005, Washington, D.C./ Detroit, MI.

4. Metal Hydride CoE System Analysis Meeting; September 2005, Washington, D.C.

5. Chemical Hydride CoE System Analysis Meeting; October 2005, Argonne, IL.

6. DOE Storage System Analysis Working Group Meeting; November 2005, Palm Springs, CA.

7. DOE Hydrogen Transition Analysis Meeting; January 2006, Washington, D.C.

8. FreedomCAR and Fuel Partnership Hydrogen Storage Tech Team Meeting; April 2006, Detroit, MI.

9. DOE Annual Hydrogen Merit Review; May 2006; Crystal City, VA.

10. DOE Storage System Analysis Working Group Meeting; May 2006, Crystal City, VA.

References

1. Carlson, E. et al.; "Cost Assessment of PEM Fuel Cells for Transportation Application"; DOE Annual Hydrogen Merit Review, May 2004, Washington, DC.

2. Lasher, S. et al.; "Analyses of Hydrogen Storage Materials and On-Board Systems"; DOE Annual Hydrogen Merit Review; May 17, 2006, Crystal City, VA.