VI.F.2 Analyses of Hydrogen Storage Materials and On-Board Systems

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Objective

The overall objective for this project is to help guide DOE and developers toward promising 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 both the near-term and long-term performance 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. Cost
- B. Weight and Volume
- C. Efficiency
- G. System Life-Cycle Assessments

Approach

For each category of on-board hydrogen storage, TIAX will:

- Develop system-level conceptual designs for the on-board storage system and required fueling infrastructure;
- Determine the on-board system cost and performance (e.g., weight and volume) based on process models and activities- or product-based cost models;

- Determine fuel cost and well-to-tank primary energy use and environmental impact (e.g., greenhouse gas emissions) for the required refueling infrastructure by utilizing existing models (e.g., H2A and GREET) with the appropriate inputs and assumptions;
- Determine the overall lifecycle cost and well-to-wheel performance based on well-to-tank results and integration of the on-board storage system in a simulated vehicle drive-cycle; and
- Continually review key assumptions and results with developers, DOE, and stakeholders so that we are providing the most accurate information and so that the DOE and its contractors can increasingly focus their efforts on the most promising technology options.

Accomplishments

We have evaluated a sodium alanate-based hydrogen storage system based on recent literature and developer input, in particular from United Technologies Research Center (UTRC) and Sandia National Laboratory (SNL), who have on-going DOE contracts to develop alanate-based storage systems. Accomplishments include:

- Developed system-level conceptual designs for the on-board storage system;
- Determined the on-board system cost and performance (e.g., weight and volume) based on process models and activities-based cost models;
- Reviewed key assumptions and preliminary results with developers, DOE, and stakeholders including Albemarle, Savanna River National Laboratory, Los Alamos National Laboratory, and FreedomCAR Tech Teams and incorporated their feedback into the final results.

In addition, we have evaluated a sodium borohydride-based hydrogen storage system based on recent literature and developer input, in particular from Millennium Cell, who has an on-going DOE contract to develop chemical hydride-based storage systems. Preliminary results have been generated for the on-board storage system cost, weight and volume and are in the process of being reviewed with developers, DOE, and stakeholders. These preliminary results are not presented here.

Future Directions

In the next fiscal year, we plan to finalize the sodium borohydride on-board system evaluation and complete the off-board (i.e. well-to-tank) assessment for both the sodium alanate and sodium borohydride systems, including the following tasks:

- Review key assumptions and preliminary results for the on-board system with additional developers and stakeholders, and develop final results;
- Develop system-level conceptual designs for the required fueling infrastructure;
- Determine fuel cost and well-to-tank primary energy use and environmental impact for the required refueling infrastructure by utilizing existing models with the appropriate inputs and assumptions;
- Determine the overall lifecycle cost and well-to-wheel performance based on well-to-tank results and integration of the on-board storage system in a simulated vehicle drive-cycle; and
- Continue to work with DOE, H2A, developers, and National Labs throughout the analysis process.

In addition, we will evaluate other storage technology options as directed by DOE. The options will likely include either a base case for the High Surface Area Sorbent (e.g., carbon-based materials) category or an additional Regenerable Off-board (e.g., chemical hydrides) option.

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 research and development (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 system cost and performance, lifecycle cost, primary energy use, and environmental impact for three broad categories of on-board hydrogen storage based on developers' on-going research, input from DOE and key stakeholders, in-house experience, and input from material experts. The three categories of storage are:

- Reversible On-board (e.g., metal hydrides);
- Regenerable Off-board (e.g., chemical hydrides); and
- High Surface Area Sorbents (e.g., carbon-based materials).

We selected a sodium alanate-based ($NaAlH_4$) hydrogen storage system as the base case technology for the Reversible On-board category. We made design assumptions and developed system-level conceptual designs based on literature review, developer feedback and TIAX experience.

Some of the complexities and risks introducing variability into the analyses include the uncertainties surrounding:

- Performance, cost and energy input requirements for alternative hydrogen storage technologies;
- Requirements of the hydrogen vehicle and fueling system (e.g., duration of maximum power requirement over the drive-cycle);
- Future technology developments; and
- Consistency, accuracy, and timeliness of developer input.

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 activities- or product-based cost models will be used to develop preliminary performance and cost results. 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

Sodium alanate desorbs hydrogen (dehydriding) through a reversible, endothermic, two-step reaction. The maximum theoretical reversible hydrogen capacity of sodium alanate is 5.6 wt%, if the reaction goes to completion. For favorable reaction kinetics, relatively high temperatures are required to absorb and desorb hydrogen during refueling and vehicle operation, respectively. In addition, relatively high pressure is required for hydrogen absorption. Therefore, the sodium alanate storage tank was designed to accommodate both rapid heat exchange and high pressure conditions. A conceptual design of the tank only is presented in Figure 1. Additional components and subsystems required to accommodate refueling, provide heat for the dehydriding reaction, and control the flow of hydrogen are represented in Figure 2.

We assume the sodium alanate can achieve 4 wt% reversible hydrogen storage capacity under the

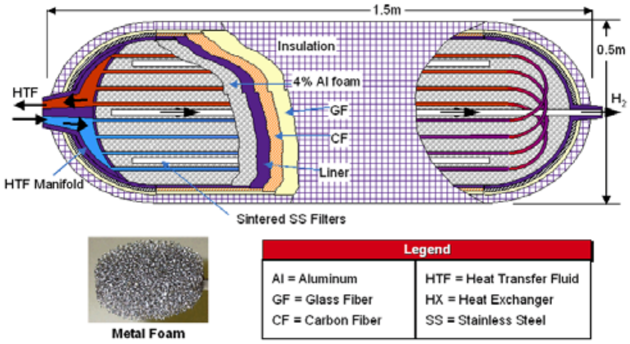

Figure 1. Sodium Alanate Tank Conceptual Design (5.6 kg hydrogen stored)

design conditions of 100 bar/100°C absorption and 2 bar/120°C desorption based on demonstrated performance of the catalyzed material. We further assume a titanium trichloride catalyst precursor (4 mol%) that results in a slightly lower overall material hydrogen storage capacity of 3.2 wt% due to the weight of the catalyst itself (Ti) and the unreactive salt that forms (NaCl). Detailed design assumptions can be found in this year's Merit Review presentation (Lasher et al., 2005).

Based on our detailed design and high-volume cost assessment of the tank, dehydriding subsystem, and balance of plant components, we found that the current status of the sodium alanate system will not meet the DOE cost, volume or weight targets (see Figure 3). The sodium alanate system weight and volume are driven primarily by the assumed media hydrogen storage capacity (4 wt%) and media packing density (60%), respectively. The system cost is driven in large part by the cost of the catalyzed media, assumed to be $5.20/kg for the base case, and balance of plant components (e.g., valves, sensors) in the overall system and dehydriding subsystem. Assuming a very optimistic media cost of $3/kg (equal to raw material costs only) reduces the overall cost of the system by about 15%.

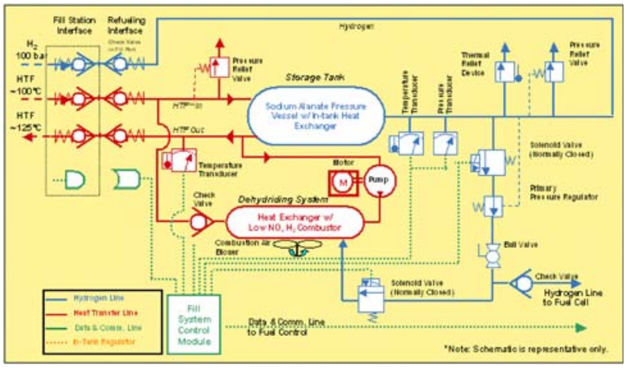

Figure 2. Sodium Alanate On-board Storage System Schematic

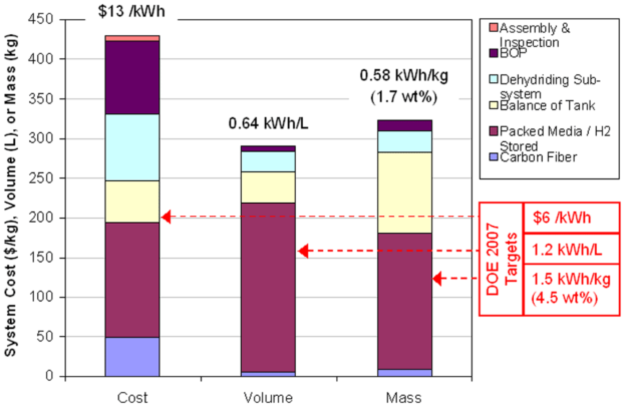

Figure 3. Sodium Alanate Cost, Volume, and Mass Results Compared to DOE Targets

Comparison to our previous analysis (Carlson et al., 2004) of compressed hydrogen storage systems designed to hold the same amount of hydrogen (5.6 kg) showed the sodium alanate system was about the same cost and volume as the 5,000 or 10,000 psi systems, but three times heavier. The sodium alanate tank weight and volume results will also be compared to the measured results soon to be completed by UTRC on their prototype system.

Conclusions

- Materials with much higher (perhaps >7 wt%) reversible hydrogen storage capacity are required to meet even the DOE 2007 targets. However, materials with higher reversible hydrogen storage capacity may have more challenging thermal requirements.
- Thermal integration with the power unit is critical for system efficiency and meeting cost, weight, and volume targets. If none of the desorption heat can be supplied by the power unit, 24% of the stored hydrogen may have to be burned to supply the necessary heat.
- Many other challenges remain, including:
  - Long refueling times and slow transient response based on current system design;
  - Unknown or unfavorable effects of cycling and poisoning on system life;
  - Additional start-up systems may be required that could increase system size/cost and reduce drive-cycle efficiency (e.g., 33 MJ heat required to heat media from 0 to 100°C); and
  - Unknown safety requirements (i.e., powder can be explosive, reacts with water or air).

FY 2005 Publications/Presentations

1. Lasher, S. et al.; "Analyses of Hydrogen Storage Materials and On-Board Systems"; Hydrogen Storage Tech Team Meeting; April 21, 2005; Detroit, MI
2. Lasher, S. et al.; "Comparison of Hydrogen Storage Options"; NHA Annual Hydrogen Conference; March 30, 2005; Washington, DC
3. Lasher, S. et al.; "Analyses of Hydrogen Storage Materials and On-Board Systems"; Storage System Analysis Meeting; March 29, 2005; Washington, DC
4. Lasher, S. et al.; "Analyses of Hydrogen Storage Materials and On-Board Systems"; Hydrogen Storage Tech Team Meeting; August 19, 2004; Detroit, MI

References

1. Lasher, S. et al.; "Analyses of Hydrogen Storage Materials and On-Board Systems"; DOE Annual Hydrogen Program Merit Review; May 25, 2005; Crystal City, VA
2. Carlson, E. et al.; "Cost Assessment of PEM Fuel Cells for Transportation Application"; DOE Annual Hydrogen Program Merit Review; May 2004; Washington, DC