IV.D.1e System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage

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Objectives

- Perform vehicle simulations of various systems configurations.
- Provide support in defining the fuel interface and forecourt requirements.
- Lead the storage system energy analysis and provide results.
- Compile and obtain media engineering properties through collaboration with the Hydrogen Storage Material Center of Excellence (HSMCoE).

Technical Barriers

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

(A) System Weight and Volume
(B) System Cost
(C) Efficiency
(E) Charging/Discharging Rates
(I) Dispensing Technology
(K) Systems Life-Cycle Assessments

Technical Targets

This project is conducting simulation and modeling studies of advanced onboard solid state hydrogen storage technologies. Insights gained from these studies will be applied toward the design and synthesis of hydrogen storage vessels that meet the following DOE 2015 hydrogen storage for light-duty vehicles targets:

- Cost: to be determined
- Specific energy: 0.055 kg H_2/kg system
- Energy density: 0.040 kg H_2/L system
- Charging/discharging rates: 3.3 min

Accomplishments

- Developed a vehicle model framework to aid in the development and understanding of hydrogen storage system requirements for light-duty vehicles.
- Devised a methodology to assess onboard hydrogen storage technical target sensitivity in a light-duty vehicle context.
- Obtained preliminary greenhouse gas emissions and well-to-wheels (WTW) efficiency figures for baseline physical storage systems.
- Identified potential materials for analysis and provided storage system design guidance to help meet DOE storage targets with sorption materials.

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Introduction

Overcoming challenges associated with onboard hydrogen storage is critical for the widespread adoption of hydrogen-fueled vehicles to occur. The overarching challenge is identifying a means to store enough hydrogen onboard to enable a driving range greater than 300 miles within vehicle-related packaging, cost, safety, and performance constraints. By means of systems analysis and modeling, hydrogen storage system requirements for light-duty vehicles can be assessed. With these findings and through collaboration with our Hydrogen Storage Engineering Center of Excellence (HSECoE) partners pathways for successful hydrogen storage system technology can be identified thus enabling future commercialization of hydrogen-fueled vehicles.

Approach

An array of tools and experience at NREL is being used to meet the objectives of the HSECoE. Specifically, extensive knowledge of multiple vehicle simulation, WTW analysis, and vehicle performance tools are being employed and integrated with fuel cell and material-based hydrogen storage system models developed by our

HSECoE partners. This integrated model framework allows for the evaluation of various hydrogen storage options. Engineering requirements are defined from these studies thus enabling the design of hydrogen storage vessels that could potentially meet DOE performance and cost targets in a vehicle system context.

In the area of media engineering, attaining the objectives of the HSECoE relies on NREL's leadership in developing custom analytical instrumentation for hydrogen sorption analysis. These tools are used to thoroughly characterize hydrogen storage sorbents so that an optimized storage vessel specific to the sorption material may be efficiently engineered. NREL will use these methods to analyze sorption materials identified by the HSECoE as holding promise for application in commercial on-vehicle refuelable hydrogen storage systems capable of meeting DOE targets.

Results

An approach to evaluate hydrogen storage system characteristic trade-offs across several vehicle configurations was demonstrated. Evaluating trade-offs between storage system characteristics – including gravimetric capacity, transient response time, cost, and full flow rate – and understanding their sensitivity to overall vehicle system viability can assist in prioritizing research areas of onboard hydrogen storage.

Initial analysis involved two parts. In Part 1, a fuel cell vehicle (FCV) configuration was assumed. Each of the four hydrogen storage system characteristics considered was swept in a parametric study and the vehicle viability, a normalized measure of the vehicle cost and performance, was recorded. Holding all other vehicle components – including the fuel cell, motor, and energy storage system (ESS) – constant through this exercise helped identify vehicle viability sensitivity to varying levels of certain hydrogen storage characteristics as shown in Figure 1.

In Part 2 of the analysis, each of the hydrogen storage characteristics was swept while allowing specific vehicle component power and energy levels to vary. These components included the fuel cell, motor, and ESS. By allowing the vehicle components to vary with changes in the hydrogen storage system, the "Most Viable" FCV configuration could be identified for a particular system.

The results in Figure 2 suggest that allowing the fuel cell, motor, and ESS power and energy levels to vary as

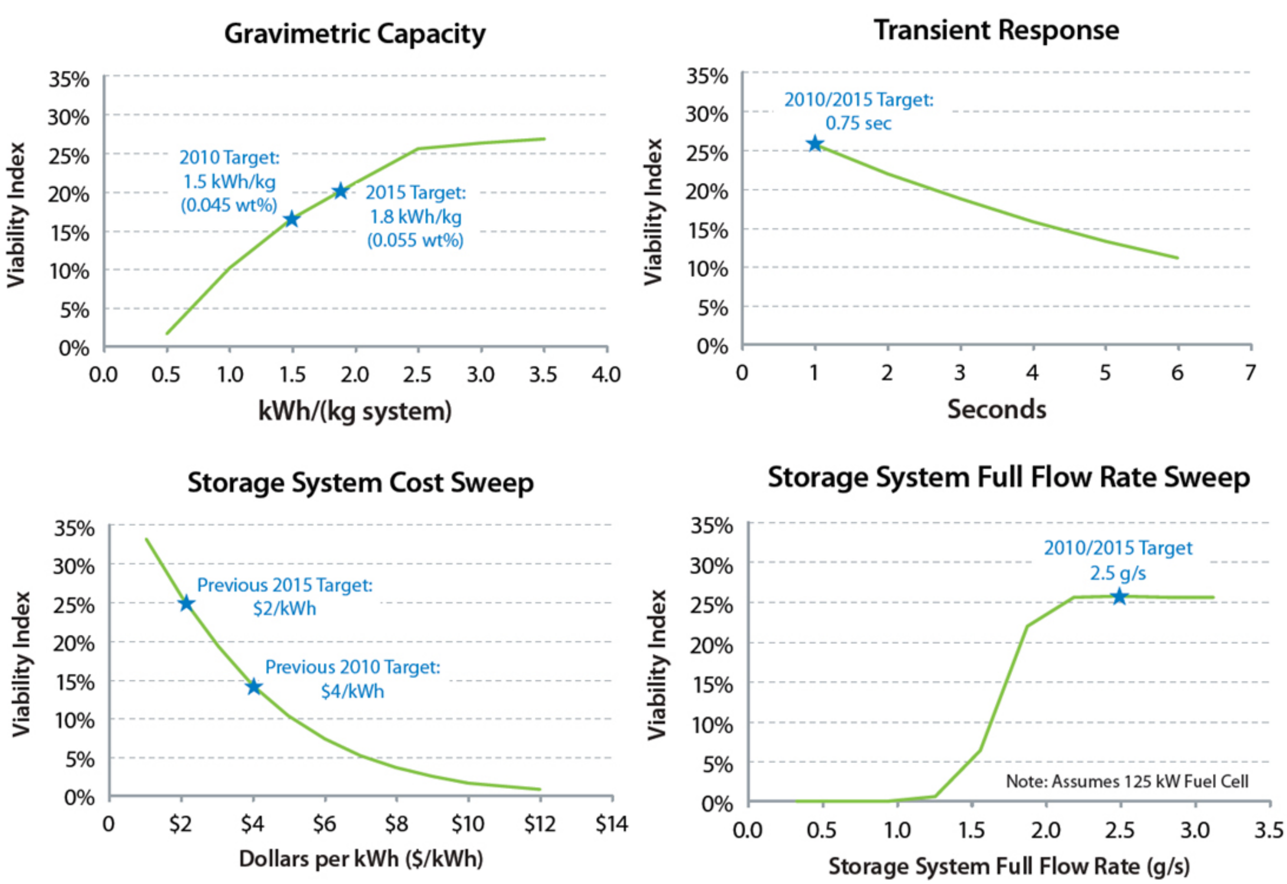

FIGURE 1. Onboard Hydrogen Storage Technical Target Sensitivity in a Light-Duty Vehicle Context - Part 1 Results

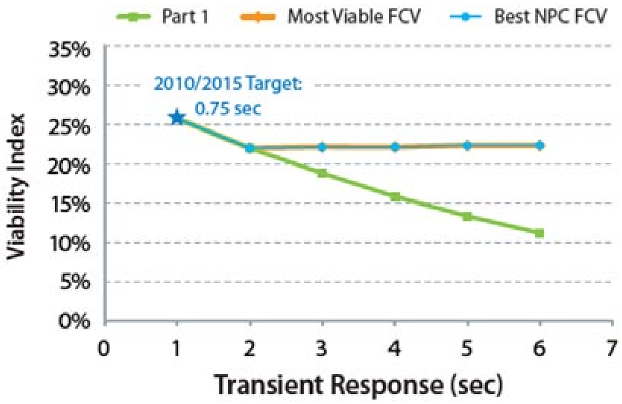

FIGURE 2. Onboard Hydrogen Storage Technical Target Sensitivity in a Light-Duty Vehicle Context - Part 2 Results

the transient response of the hydrogen storage system increases assists in maintaining a higher viability index than if the vehicle component sizing remained fixed.

In the area of media engineering, NREL worked with our HSECoE partners to compile engineering properties for selected sorbents. Initially, the commercially viable sorbents AX-21 (i.e. MSC-30) and MOF-5 were selected as model sorbents to provide the basic information needed to construct accurate hydrogen storage system models. However, the materials will probably not be sufficient to meet the HSECoE goals or the DOE 2015 targets. Thus, NREL led the sorption materials team to develop detailed sorbent selection criteria and to identify potential sorbent materials that may improve the hydrogen storage system designs. As part of this work, additional metal-organic framework, high specific surface area carbon, and weak-chemisorption sorbents were identified. With most of these novel sorbents, most of the engineering properties are unknown and thus need to be measured to feed into the storage system designs. As part of this work, the Engineering Center specifically removed from further consideration MOF-177, but identified four other materials to more fully characterize.

With NREL's unique sorption materials perspective, our initial assessment of the state of sorbent materials for hydrogen storage was refined based on recent modeling results from the Storage System Working Analysis Group (SSWAG) led by Argonne National Laboratory (ANL), and TIAX. The initial conclusion by NREL is that while confirmation of many of the specifics still needs to be made, sorbents should meet the vast majority of DOE targets. The main issues are cost, volumetric and gravimetric capacities, and depending upon the hydrogen storage conditions used, the well to fuel cell efficiency. Based on an initial assessment of the SSAWG using MOF-177, an optimized adiabatic storage system filled with liquid hydrogen would operate at ~250 bar and 80 K with a gravimetric capacity of >5 wt% and a volumetric capacity of ~35 g/L. However, this hydrogen storage system will be almost an order of magnitude higher than DOE present 2015 targets. Based on these results, NREL developed several recommendations for improving the hydrogen storage system including increasing the overall capacity of the system to ~13 Kg, decrease the storage maximum pressure to ~40 bar, and enable larger temperature swings to increase the amount of delivered hydrogen. With these changes, it may be possible to meet DOE 2010 capacity targets, and be within a factor of 2 or DOE 2010 cost targets (Figure 3).

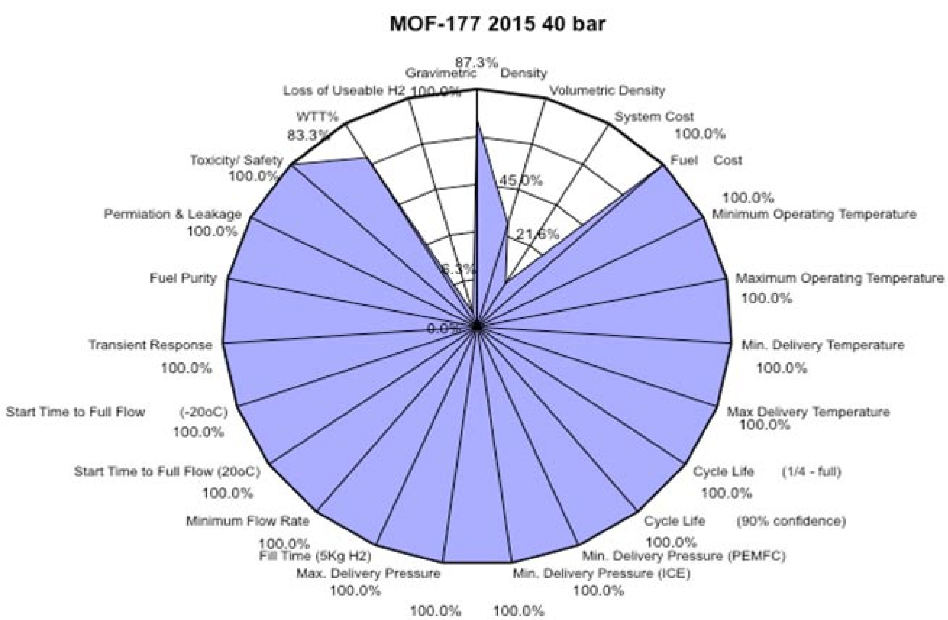

FIGURE 3. Spider Chart for MOF-177 based on ANL SSWAG Analysis at 40 bar for DOE 2015 Targets

NREL also recommended using improved and less expensive optimized pore size sorbents that more than double the volumetric capacities, and that enable lower operating pressures and operating at lower storage temperatures with larger temperature swings. This would enable sorbents to be used to potentially meet the HSECoE Phase II and perhaps the DOE 2015 targets, including cost and capacities. However, recent emphasis by DOE on overall well to fuel cell hydrogen efficiencies still need to be fully evaluated for this scenario.

Conclusions and Future Direction

- FCV viability sensitivity to onboard hydrogen storage system improvements can be estimated.
- Improved volumetric capacity by way of optimized materials is needed as well as the inclusion of system cost and efficiency for sorbent based system analysis.
- In collaboration with our HSECoE partners, sub-system models will be refined and fully integrated into the vehicle model framework.
- Working with our vehicle manufacturer partners, the Hydrogen Storage Simulation model vehicle viability index estimation methodology will be further reviewed and validated and sensitivity analysis repeated as necessary.
- NREL will investigate data and WTW model integration requirements.
- Systematic compaction measurements to determine maximum attainable sorbent material densities while maintaining the inherent capacities will take place.

FY 2010 Publications/Presentations

1. Fall MRS Conference, Boston MA, November 30 – December 3, 2009, Invited Presentation, "Hydrogen Sorption Material," A.C. Dillon, J.L. Blackburn, J. Bult, C.J. Curtis, M. Davis, T. Elko-Hanson, C. Engtrakul, T. Gennett, A. Groves, M.J. Heben, A. Herwadkar, K.M. Jones, Y.H. Kim, K.J. O'Neil, P.A. Parilla, J.D. Rocha, L.J. Simpson, E. Whitney, S.B. Zhang, Y. Zhao.

2. M. Thornton, K. Day, and A. Brooker, "Evaluation of Hydrogen Storage System Characteristics for Light-Duty Vehicle Applications" SAE Congress (oral only) April 14th 2010, Detroit, MI.

3. Hydrogen Storage Engineering Center of Excellence Face-to-Face Meeting, March 2–4, 2010, Invited, "MOR Team Lead Technical Update," L.J. Simpson

4. FY 2010 DOE Annual Merit Review Meeting, June 8, 2010, Washington, D.C.