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

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Objectives

- Identify optimal pathways for successful hydrogen storage system technologies through modeling, analysis, and testing support.
  - Perform vehicle simulations of various system configurations to support the overall systems engineering technology area.
- Support Savanna River National Laboratory (SRNL) and United Technologies Research Center in defining the fuel interface and forecourt energy requirements.
- Lead tank-to-wheels analyses and provide the Hydrogen Storage Engineering Center of Excellence (HSECoE) with results that will help guide engineering design.
- Compile and obtain media engineering properties for the HSECoE through collaboration with the Hydrogen Storage Materials Centers of Excellence (HSMCoE).

Technical Barriers

This project addresses the following technical barriers from the Storage section (3.3.5) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program 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) System Life-Cycle Assessments

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: $2/kWh net
- Specific energy: 1.8 kWh/kg
- Energy density: 1.3 kWh/L
- Charging/discharging rates: 3.3 min

Approach

The work described here is an integral component of DOE's HSECoE and as part of the National Hydrogen Storage Project it will help meet the overall goals of the Hydrogen, Fuel Cells and Infrastructure Technologies Program. DOE's Program supports the Advanced Energy Initiative. NREL's work will support DOE's objectives and expected outcomes of the HSECoE.

The objective of the proposed research is to identify optimal pathways for successful hydrogen storage system technology through modeling, analysis, and testing support. Our first objective will be to perform vehicle simulations of various systems configurations to support the overall systems engineering technology area. The second objective is to support SRNL in defining the fuel interface and forecourt energy requirements. The third objective will be to lead the storage system energy analysis and provide the HSECoE with results that will help guide engineering design. Finally, the fourth objective is to compile and obtain media engineering properties for the HSECoE through collaboration with the HSMCoE.

Accomplishments

In the area of vehicle requirements, NREL has created a vehicle model framework to aid in the development and understanding of hydrogen storage system requirements for light-duty vehicles (Figure 1.). The objective is to take these findings and discover pathways for the successful implementation of hydrogen storage systems that meet DOE performance and cost targets.

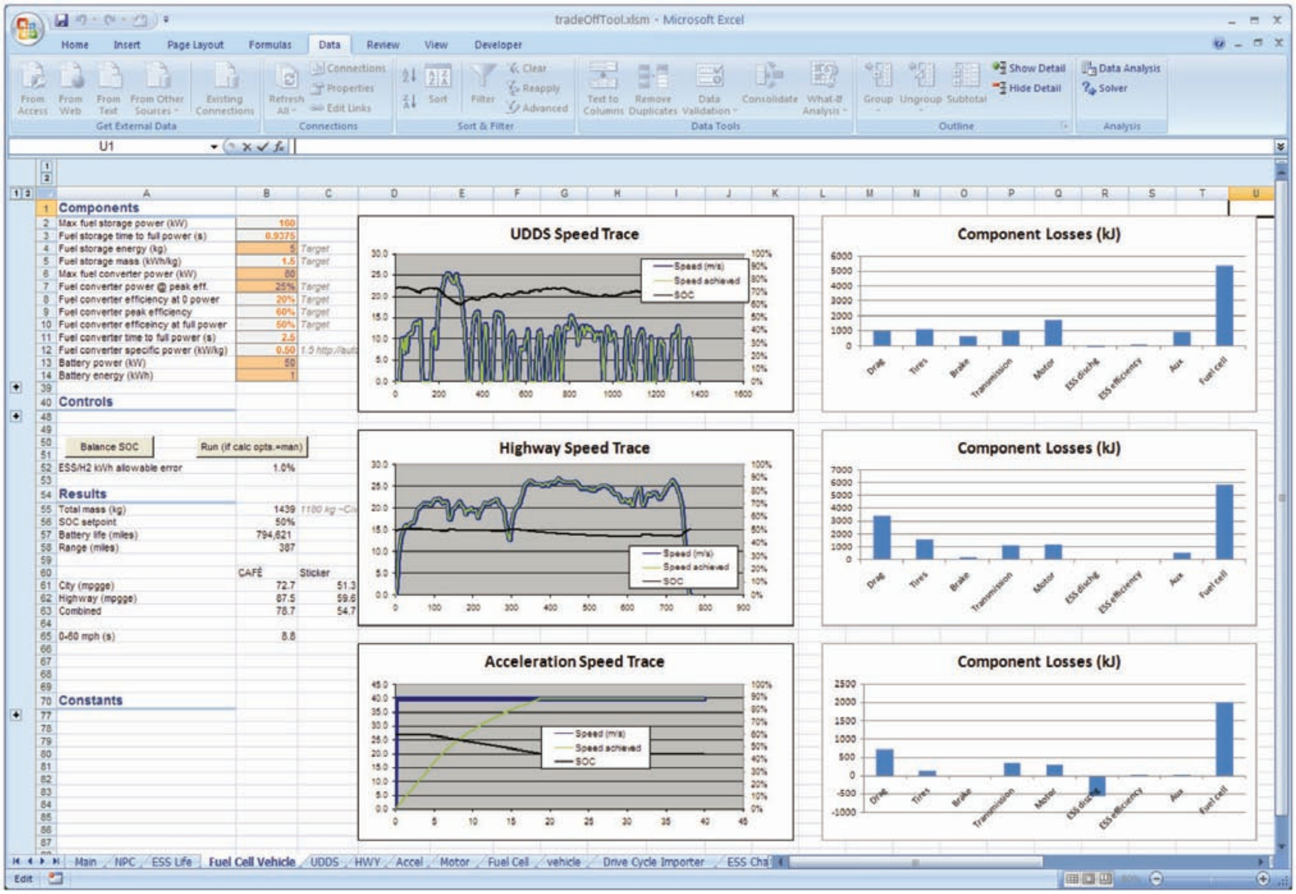

FIGURE 1. Hydrogen Storage Vehicle Modeling Evaluation Framework

Hydrogen storage response surfaces specific to a particular hydrogen storage technology are to be integrated with the vehicle model. With the characteristics of each technology embedded within the vehicle model, NREL will be able to analyze vehicle performance as a whole across numerous drive cycles and acceleration tests for each technology. Making trade-offs between various system components and vehicle configurations in the process will help to explore each storage technology's viability in a vehicle system context.

Currently, the tool models hydrogen fuel cell vehicles employing compressed hydrogen storage technologies and includes sensitivity to key powertrain components (e.g. motor, fuel cell, engine, energy storage, hydrogen storage) and all DOE technical targets. NREL has been able to assess the base model accuracy by validating model outputs against compressed hydrogen fuel cell vehicles currently in operation. Specific vehicle parameters of interest were collected for the 2008 Ford Focus FCV, 2008 Honda FCX Clarity and the 2008 Chevrolet Equinox fuel cell vehicle. Published vehicle performance data was also obtained including range, acceleration and fuel economy figures. Each vehicle was modeled with acceleration and fuel economy tests. The model outputs were then compared to the published data. An error of no more than 6% was observed between published and modeled acceleration performance. Furthermore, the greatest error in combined fuel economy was 2%. The range calculation however yielded a spread in error between 3-30%. It can be speculated that this error is due perhaps to the difference between reporting total hydrogen on-board verses total usable hydrogen on-board.

In cooperation with the integrated power plant/storage system technology team, the compressed hydrogen and fuel models currently serving as place holders will be replaced with detailed fuel cell and storage system response surfaces. These response surfaces will simulate the characteristics for each storage type. This will allow the vehicle model to confirm that the virtual storage system design can provide the hydrogen flow demand within constraints while meeting the imposed targets and vehicle performance goals.

In parallel to the vehicle modeling the NREL team is working on a tank-to-wheel analysis. NREL will be incorporating this analysis into the Greenhouse gases, Regulated Emissions and Energy use in Transportation (GREET) model with fuel and vehicle cycle results to create a total energy-cycle analysis for each hydrogen storage technology. The vehicle fuel use inputs for this analysis will come from the vehicle performance modeling discussed above. In preparation for the overall life cycle analysis for the center, NREL has coordinated with Argonne National Laboratory and the Storage Systems Analysis Work Group to develop a method for ensuring consistency of assumptions throughout the total well-to-wheels analysis.

Finally, as lead of the DOE Hydrogen Sorption Center of Excellence (HSCoE), NREL is working with our partners and the pertinent scientific community to make sorption material recommendations for future HSCoE materials development efforts and for further analysis by groups assigned by DOE including the HSECoE. NREL identified several materials within four material classes that could meet DOE hydrogen storage system targets. These material classes include: (1) cryocompressed sorbents, (2) substituted materials, (3) multiple hydrogen binding metal centers, and (4) weak chemisorption/spillover. Within each material class, the HSCoE has selected materials for development based on established selection criteria. For each of the selected materials, roadmaps have been constructed to guide development. In addition, NREL has applied selection criteria from the HSECoE to choose a set of materials for further hydrogen storage systems analyses. In the near term, to help calibrate system analysis/design models, the material properties from a standard activated carbon (i.e. AX-21) will be used. However, the HSCoE has identified a short list of materials to begin assembling the requisite properties needed for hydrogen storage system analysis and design. This includes: (a) class 1 cryocompressed materials that have uniform ~1 nm pore sizes that can have very good bulk densities; (b) class 2 BCx materials with high boron concentrations and high surface areas that will enable near ambient temperature storage temperatures; and (c) class 4 spillover materials that enable ambient temperature storage. Longer term materials development and characterization efforts will be performed as new materials are created with promising hydrogen storage properties. NREL will perform the measurements/characterization needed to provide the HSECoE the requisite material properties for their analysis and design efforts.

Future Directions

- Continue work on system configuration modeling, vehicle simulations, cost analysis, fuel interface requirements, and collaboration with the HSMCoE.
- Identify the hydrogen storage and vehicle applications with the highest value.
- Use experimental investigations and modeling to collect the data necessary to support HSECoE Go/No-Go decisions.
- Work with HSECoE partners to model storage system requirements.
- Work with Pacific Northwest National Laboratory to perform cost analyses.
- Collaborate with HSECoE partners to determine storage system requirements and down-select system design concepts.
- Perform tank-to-wheels analyses and initial energy requirements assessments with HSECoE partners.
- Compile/obtain media engineering properties with HSMCoE.

FY 2009 Publications/Presentations

1. FY 2009 DOE Annual Merit Review Meeting, May 20, 2009, Washington, D.C.