IV.B.9 Testing, Modeling, and Evaluation of Innovative Hydrogen Storage System Designs

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Overall Objectives

- Develop and test system simulation models for on-board hydrogen storage systems using adsorbent materials, and determine system compliance with the DOE technical targets
- Design, build, and test an experimental vessel for validation of cryo-adsorption models and determine the fast fill and discharge dynamics of cryo-adsorbent storage systems

Fiscal Year (FY) 2015 Objectives

- Provide support to the modeling group by testing and evaluating new versions of the Framework model and any other models that are to be published on the web
- Participate in Phase III of the program as an original equipment manufacturer (OEM) consultant in face-to-face meetings and in teleconferences of the Coordinating Council, Adsorbent Team, and Modeling Team

Technical Barriers

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

(A) System Weight and Volume

(C) Efficiency

(E) Charging/Discharging Rates

(J) Thermal Management

Technical Targets

In this project, studies are being conducted to develop metal organic framework (MOF)-5 based storage media with optimized engineering properties. This material has the potential to meet the 2020 technical targets for onboard hydrogen storage shown in the following table:

Storage Parameter	2020 Target
System Gravimetric Capacity	0.055 (kg H_2/kg system)
System Volumetric Capacity	0.040 (kg H_2/L system)

FY 2015 Accomplishments

- GM's testing of the Vehicle Simulation Framework provided valuable feedback to the modeling team that led to improvements and refinements being made to the model.
- GM's testing of the "Tankinator" model provided useful input to Pacific Northwest National Laboratory (PNNL) before their release of the model on the web.

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INTRODUCTION

In Phases I and II as part of the Hydrogen Storage Engineering Center of Excellence (HSECoE), the GM team built hydrogen storage system models for sodium alanate, TiCrMn, and cryo-adsorbents that were subsequently tested in the Framework model. GM's role has changed in Phase III, as we have participated in the DOE HSECoE program as an OEM consultant and provided input to the construction of down-selected prototype tanks. GM contributed to the down selection of the HexCell and MATI heat exchange designs for subscale prototype adsorbent systems to be evaluated in Phase III. This selection was made by considering several factors, including the detailed model analyses with experimental validation, the overall system performance projections, the projected costs, and the future direction of adsorbent material research. As an OEM, we are in a unique position to help ensure that the selected designs are based on on-road demands of the fuel cell vehicles. As we transitioned to being an OEM consultant to the program, the deliverables for this phase have been redefined, particularly for our modeling related activities. GM will test and evaluate the Framework model and any other models that are to be published on the web, and provide feedback regarding this testing in support of the modeling group.

APPROACH

The Vehicle Simulation Framework is a MATLAB/Simulink® model that enables users to perform driving simulations for a fuel cell vehicle with a variety of operating conditions and hydrogen storage system options. The Framework is designed so that the performance of different hydrogen storage systems may be compared on a single vehicle, keeping constant the vehicle-level and fuel cell system assumptions. The goal is to be able to separate the differences in performance that arise from the vehicle and fuel cell and those that arise from the storage system [1]. GM's test runs of the Framework were performed on an HP Z800 Workstation with 48 GB of RAM running the 64-bit version of Windows 7. The workstation had an Intel® Xeon® CPU (E5620) with two 2.40 GHz processors. Simulations were run with the 32-bit version of MATLAB® 8.3.0.532 (R2014a), although some were also run with the 64-bit version in order to compare execution times.

In addition to GM's beta testing of the Vehicle Simulation Framework, we evaluated another program that estimates the size and material composition of hydrogen storage tanks. PNNL has developed an Excel program that can be used to cross-compare various hydrogen storage pressure vessel types. The "Tankinator" model can estimate the mass, size, and material cost for cylindrical Type I, III, and IV hydrogen storage tanks [2]. It provides an estimate of basic tank geometry and composition from a limited number of geometric and temperature inputs. PNNL requested that GM perform an evaluation of the model and provide feedback before the model is placed on the HSECoE web site for distribution to the public.

RESULTS

Vehicle Simulation Framework Tests

Two chemical hydride storage systems were first included in the Framework in version v1.1rc5. The chemical hydrogen storage material system is selectable for either an exothermic or endothermic hydrogen release enthalphy. The exothermic and endothermic systems are represented by an ammonia borane slurry and an alane slurry, respectively [3]. The modeling team requested that GM perform Framework simulations using these two storage systems to determine if they run properly with MATLAB® R2014a. In particular, the team had determined that cold test case drive cycle simulations for both material systems had been having issues. Simulations for the alane slurry storage system were crashing after 140–170 seconds, and runs with ammonia borane slurry would hang up at completion before crashing. GM's test simulation using MATLAB® R2014a with the cold case drive cycle and the alane slurry storage system did not crash, but instead ran to completion (74,720.4 seconds). Likewise, a simulation with the ammonia borane slurry and the cold case also ran to completion, and the program ended normally without crashing. Detailed listings of all Simulink® preference settings were sent to the modeling team to help determine if something different in these particular settings was allowing the two cases to run successfully.

Version v1.1rc6 of the Framework contained several updates and was made available for testing. One key change made to this version was the setting of the maximum time step to 0.2 seconds. The value, dtmax, had been lowered to 0.2 seconds in order to avoid spurious trace miss errors and to address issues with the chemical hydride modules. The modeling team requested that GM perform Framework simulations using this version to test the model changes with MATLAB® R2014a. Test runs of the two latest Framework versions, v1.1rc5 and v1.1rc6, were performed for comparison of their performance and execution times. A selection of the simulation results for the two versions are shown in Tables 1 and 2. The default menu options were used for all simulations. Table 1 contains results for the metal hydride storage module. This module had been updated in version v1.1rc6 in order for the thermal conduction model to handle thicker walls. The execution times for v1.1rc6 increased substantially from version v1.1rc5. However, the metal hydride module is still one of the faster executing modules in the Framework. The driving times and, therefore, the distances traveled also are higher for v1.1rc6.

TABLE 1. Metal Hydride Storage Module Results for Both v1.1rc5 and v1.1rc6, Respectively

Drive Cycle	Elapsed Driving Time (s)	Distance Traveled (mi)	Execution Time (h:min)
Fuel Economy	49,649 / 50,926	414 / 424	5:0 / 17:23
Aggressive (US06)	21,400 / 22,442	286 / 299	4:0 / 8:22
Cold Cycle (FTP-75)	79,424 / 82,035	355 / 367	8:0 / 27:50
Hot Cycle (SC03)	57,446 / 59,952	343 / 358	8:0 / 20:04

FTP - Federal Test Procedure

TABLE 2. CH-AB Slurry Storage Module Results for v1.1rc5 and v1.1rc6, Respectively

Drive Cycle	Elapsed Driving Time (s)	Distance Traveled (mi)	Execution Time (h:min)
Fuel Economy	45,164 / 44,926	377 / 373	39:0 / 42:39
Aggressive (US06)	19,813 / 19,623	265 / 263	29:0 / 30:25
Cold Cycle (FTP-75)	72,032 / 71,568	324 / 319	46:0 / 1:00:08
Hot Cycle (SC03)	53,010 / 52,490	318 / 313	38:0 / 44:01

For some versions of MATLAB®, users of the chemical hydride storage modules were experiencing problems in v1.1rc5, and simulations sometimes failed to run to completion. This problem did not occur in our simulations with MATLAB® R2014a, as can be seen in Table 2. Also, simulations using v1.1rc5 with the aggressive cycle were encountering “speed trace miss” messages on completion, including those that were run using MATLAB® R2014a. The new setting of the maximum time step to 0.2 seconds in version v1.1rc6 simulations was successful in preventing these messages from occurring. Execution times for v1.1rc6 (Table 2) showed modest increases for the chemical hydride-ammonia borane (CH-AB) slurry module simulations. These test results were a topic of discussion for the modeling group at subsequent teleconferences. Simulations with the two versions were obtaining somewhat different results for the distance traveled for cases being run with identical input parameters. For the metal hydride and compressed 350 bar storage modules the differences could be as high as 4.5%. For both of the chemical hydride modules, the differences were all below 2%. The differences in distance traveled were determined to be resulting from the change that had been made in the maximum allowable time step for the solver. The value had been lowered to 0.2 seconds in version v1.1rc6 in order to avoid spurious trace miss errors and to address issues with the chemical hydride modules. The modeling team made modifications to the Framework to verify that the model’s computations were converging, and decided to use the 0.2 second time step value as a suitable choice to achieve both convergence and reasonable execution time.

Framework version v1.1rc8 was the first version of the Framework to feature the two cryo-adsorbent storage modules from Savanah River National Laboratory. Testing of these modules (MATI and Hex Cell) was performed. The MATI storage system was tested using lower final temperatures (140 K and 150 K) as well as for the default of 160 K. The module resizes the storage system to take into account the requested final tank temperature. For instance, the storage system mass and usable hydrogen are 158.1 and 5.58 kg, respectively, for the 160 K simulation, but they increase to 163.4 and 5.67 kg for the 140 K simulation. All simulations ran successfully to completion at these temperatures. Varying these and other options should prove to be instructive to end users of the Framework.

Tank Mass Estimator (Tankinator)

The Type I tank model can be used for any of four metals: 6061-T6 aluminum, 316 stainless steel, 4130 chromoly steel, and 4340 steel. The tank design must meet two criteria: a proof load of 1.5 times the operating pressure, under which the tank wall must not yield, and a burst load of 2.25 times the operating pressure, for which the tank must not exceed the peak von Mises stress. Initially, all four metals are compared using a thin wall stress relationship that calculates an estimate that is useful for low pressures. A thick-walled calculation is then performed for the chosen metal. Higher pressures and weak aluminum must be considered thick-walled even in the moderate pressure range. A series of three von Mises stress calculations are done to further refine the wall thickness. The design ratio, which is the calculated stress divided by the allowable stress limit, is used to correct the wall thickness estimate in these three iterative steps. The design ratio indicates how close the estimated wall thickness is to the ideal thickness and should converge to 1.0, otherwise additional refinements would be necessary [2].

For example, a case was run for a 6061-T6 aluminum tank with operating temperature of 22°C, pressure of 250 bar, inner radius of 22.5 cm, and inner length of 81 cm. The outer radius estimate undergoes the series of refinements from 26.53, 26.95, 27.05, to 27.08 cm, resulting in a final wall thickness estimate of 4.58 cm and a tank mass of 162.9 kg. A final design ratio of 1.001 and von Mises error of 0.14% confirm that the calculation has converged. Raw materials for the tank are estimated to be $725 based on 2007 commodity costs that are used for comparison purposes. Several other geometry, temperature, and pressure combinations were input for test runs, and the program always converged and obtained reasonable results. Suggestions for minor additions to the model’s parameter descriptions were made to help clarify the use of the design ratios in refining the wall thickness estimates.

The Type III tank model is designed for cryogenic operating conditions. The tank is composed of an aluminum liner with a carbon fiber overwrap. The aluminum liner is sized to withstand 21% of the burst pressure, and the carbon fiber overwrap is sized to withstand the remaining 79% of the burst pressure. The thicknesses are calculated using the thin-walled pressure vessel hoop stress formula. Both low-bound and high-bound estimates are calculated. The low-bound value represents the best estimate value, and the high-bound value provides a conservative estimate that doesn’t take credit for the support of the liner. This gives an idea of how large of a contribution the aluminum liner provides. As with the Type I tank model, testing was performed with a range of input parameters. Tank designs were calculated for an internal radius up to 30 cm and operating pressures as high as 300 bar, the limits suggested in the documentation. All results passed the built-in accuracy checks. The variations seen in the relative masses of the aluminum and carbon fiber composite were quite instructive, and they provided useful information for comparing tank designs.

The Type IV tank model is based on the assumption that the high-density polyethylene (HDPE) liner carries no load. However, the HDPE liner thickness is a required input parameter. The model description states that a thin-walled pressure vessel approximation is used; therefore, the estimates have a limited range of accuracy. As with the Type III model, this model provides fast, accurate estimates of the carbon fiber composite mass, thickness, and cost for comparison purposes.

CONCLUSIONS

- GM continued to participate in Phase III as an OEM consultant to the HSECoE team. GM contributed to the down selection of the HexCell and MATI heat exchange designs for subscale prototype adsorbent systems that were evaluated in Phase III.
- The Vehicle Simulation Framework has been thoroughly tested and will prove to be a valuable tool to the user community.

REFERENCES

1. H_2 Vehicle Simulation Framework: MODEL DESCRIPTION AND USER MANUAL, J.M. Pasini, J. Cosgrove.

2. PNNL Tank Mass Estimator for Cross Comparison of Type 1, Type 3, and Type 4 Pressure Vessels, Nicholas Klymyshyn, PNNL.

3. Slurry Model for Chemical Hydrogen Storage in Fuel Cell Vehicle Applications," Brooks, Kriston P., Richard P. Pires, and Kevin L. Simmons.

FY 2015 PUBLICATIONS/PRESENTATIONS

1. M. Cai, et al. (2015), Testing, Modeling, and Evaluation of Innovative Hydrogen Storage System Designs, presented at the 2015 DOE Hydrogen Program Annual Merit Review Meeting, Washington, D.C.