System Design, Analysis, and Modeling Activities Supporting the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE)

Final Project Report

Matthew Thornton and Lin Simpson

National Renewable Energy Laboratory

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Milestone Report
NREL/MP-5400-73571
April 2019

System Design, Analysis, and Modeling Activities Supporting the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE)

Final Project Report

Matthew Thornton and Lin Simpson

National Renewable Energy Laboratory

Suggested Citation
Thornton, Matthew and Lin Simpson. 2019. *System Design, Analysis, and Modeling Activities Supporting the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE): Final Project Report*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5400-73571. https://www.nrel.gov/docs/fy19osti/73571.pdf.

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Milestone Report
NREL/MP-5400-73571
April 2019

National Renewable Energy Laboratory
15013 Denver West Parkway
Golden, CO 80401
303-275-3000 • www.nrel.gov

NOTICE

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Fuel Cell Technologies Office. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government.

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via www.OSTI.gov.

Cover Photos by Dennis Schroeder: (clockwise, left to right) NREL 51934, NREL 45897, NREL 42160, NREL 45891, NREL 48097, NREL 46526.

NREL prints on paper that contains recycled content.

Final Report

Project Title

System Design, Analysis, and Modeling Activities Supporting the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE)

Project Period

October 1, 2009 to June 30, 2015

Date of Report

March 5, 2019

Recipient

National Renewable Energy Laboratory (NREL)

Working Partners

HSECoE team: Savannah River National Laboratory (SRNL), Los Alamos National Laboratory (LANL), Pacific Northwest National Laboratory (PNNL), NASA Jet Propulsion Laboratory (JPL), Ford, General Motors (GM), United Technologies Research Center (UTRC), Hexagon-Lincoln, Universite Du Quebec A Trois-Rivieres (UQTR), BASF, University of Michigan, and Oregon State University

Cost-Sharing Partners

None

Contact

Matthew Thornton
National Renewable Energy Laboratory
303-275-4273
matthew.thornton@nrel.gov

DOE Manager

Ned Stetson, Hydrogen Storage Technology Manager
DOE Fuel Cell Technologies Office

Table of Contents

List of Figures

List of Tables

Project Objective

The objective of this project was to identify optimal pathways for successful hydrogen storage system technology through modeling, analysis, and testing support. The National Renewable Energy Laboratory's (NREL's) first objective was to perform vehicle simulations of various system configurations to support the overall systems engineering. The second objective was to lead the storage system energy analysis and provide the Hydrogen Storage Engineering Center of Excellence (HSECoE) with results that will help guide engineering design. Finally, the third objective was to compile and obtain media engineering properties for the HSECoE.

Background

The work described here is an integral component of the U.S. Department of Energy's (DOE's) HSECoE. As part of the National Hydrogen Storage Project it will help meet the overall goals of the Fuel Cell Technologies Office. DOE's program also supports the Advanced Energy Initiative. NREL's work supports DOE's objectives and expected outcomes of the HSECoE.

Vehicle Simulation Modeling

In other efforts under the HSECoE, a number of detailed numerical models were described for different materials-based storage systems. However, those models are restricted to specific storage media and vessel geometries, which include placement and function of heat transfer elements. While useful for evaluating specific storage system designs, the analyses in the literature are not suitable for general systematic assessment of storage vessel/media configurations against a set of performance targets. The detailed models also require time to develop and run. As part of NREL's HSECoE modeling effort, it was found useful to have simplified models that can quickly estimate optimal loading and discharge kinetics, effective hydrogen capacities, system dimensions, and heat removal requirements. Parameters obtained from these models can then be input into the detailed models to obtain an accurate assessment of system performance that includes more complete integration of the physical processes. The following paragraphs in this section (1) describe the methodology developed for conducting such system models across the HSECoE and the integration of those models with full vehicle models, and (2) present some of the performance results from studies using these system models to support and guide the design of materials-based systems for the HSECoE.

To meet the objectives of the HSECoE, there was a need to quickly and efficiently evaluate various materials-based storage systems and to compare their performance against DOE hydrogen storage targets for light-duty vehicles. To accomplish this task, a modeling approach was created that enabled the exchange of one hydrogen storage system for another while keeping the vehicle and fuel cell systems constant [1]. Figure 1 shows a block diagram of the modeling "framework" that was used for system evaluation and comparison by the HSECoE. The framework was used to implement the integrated vehicle, the power plant, and the storage system models. This framework tool was used across the HSECoE to evaluate candidate storage system designs on a common vehicle platform with a consistent set of assumptions.

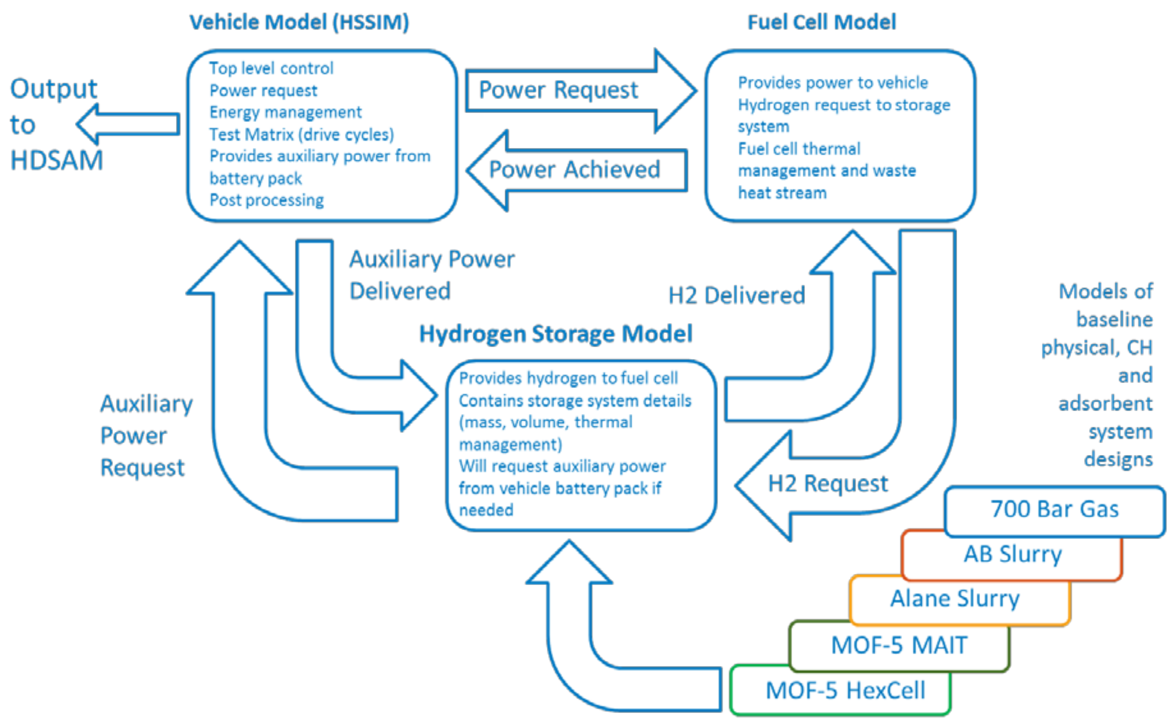

Figure 1. HSECoE framework system model showing main blocks, inputs, outputs, and a sample of storage systems that were implemented

The framework shown in Figure 1 was implemented using a commercial software platform, Simulink. The vehicle-level model was developed by NREL based on its HSSIM (Hydrogen Storage SIMulator) software, which was originally developed to simulate a hydrogen fuel cell vehicle running on compressed gas tanks. The HSSIM vehicle model is designed to evaluate high-level attribute improvements. To accomplish this, the inputs, such as the glider and powertrain components, are also defined at a high level. The vehicle glider is defined with a specific frontal area, drag coefficient, mass, center of gravity, front axle weight fraction, and wheel base. The wheels are defined by inertia, a rolling resistance coefficient, coefficient of friction, and radius. The inputs for the motor are power, peak efficiency, mass per unit of power, cost per unit of power, and time to full power. The battery inputs include power, energy, mass per unit of energy, and round trip efficiency. Auxiliary loads are assumed to be a specified constant plus an amount required for the fuel cell and hydrogen storage systems. These inputs match DOE's technical target units, such as battery kilograms per kilowatt hour, so that the impact of improvements can be evaluated over time as the targets change. For applications for this program, a standard mid-sized vehicle class was selected that included a 100 kW electric motor and a 20 kW/1 kWh battery to capture regenerative braking and provide minor propulsion assistance. The vehicle glider weight (excluding the hydrogen storage system) was 1,610 kg. The fuel cell system was developed by Ford and is based on an 80 kW net stack operating at 80°C. The fuel cell efficiency was consistent with the DOE fuel cell system targets for 50% efficiency at rated power and 60% at quarter power. The fuel cell model included only the essential elements to interface with the vehicle and the hydrogen storage blocks. These included a polarization curve to translate vehicle power to hydrogen required, parasitic power from the compressor, and stack temperature to provide waste heat.

Examples of some of the different storage systems evaluated by the HSECoE in the framework model are shown in Figure 1. These included various metal hydride (MH), chemical hydride (CH), and adsorbent storage systems, in addition to compressed gas systems, which were included to benchmark the other systems. Most of the adsorbent storage systems involved metal-organic framework MOF-5 because of its existing material property data and previous modeling studies. The use of a common storage media also allowed for a good comparison of different engineering concepts and configurations on the systems' performance.

In addition to modeling the storage, fuel cell, and vehicle systems, the HSECoE team also developed a standard matrix of test cases to exercise the different hydrogen storage systems against the DOE performance targets. The test cases, which made use of five fuel economy drive cycles from the U.S. Environmental Protection Agency (EPA), are shown in Table 1. Cases 1 through 4 are looped until the storage system can no longer provide the required hydrogen flow rate. Case 1 is used to determine if the storage system can provide its required 5.6 kg of usable hydrogen to the vehicle. It uses a 55%/45% weighting factor between city (urban dynamometer driving schedule, UDDS) versus highway (highway fuel economy test, HWFET) driving. Case 2 uses the US06 (aggressive) drive cycle to confirm the storage system can deliver the DOE peak flow of 1.6 grams of hydrogen per second to the fuel cell. Case 3 (cold case) is used to evaluate the storage system's performance for -20°C cold startup scenarios. Case 4 (hot case) runs the system at 35°C with SC03, the EPA air conditioning test conditions. Case 5 tests the storage system dormancy for cryogenic systems, but it was not used for this reported analysis in the framework.

Table 1. Test Cases for Exercising the Storage Systems Using Various EPA Fuel Efficiency Drive Cycles

Case	Test Schedule	Cycles	Description	Test Temp (° F)	Distance per cycle (miles)	Duration per cycle (minutes)	Top Speed (mph)	Average Speed (mph)	Max. Acc. (mph /sec)	Stops	Idle	Avg. H2 Flow (g/s)*	Peak H2 Flow (g/s)*	Expected Usage
1	**Ambient Drive Cycle** - Repeat the EPA FE cycles from full to empty and adjust for 5 cycle post-2008	UDDS	Low speeds in stop-and-go urban traffic	75 (24 C)	7.5	22.8	56.7	19.6	3.3	17	19%	0.09	0.69	**1. Establish baseline fuel economy (adjust for the 5 cycle based on the average from the cycles) 2. Establish vehicle attributes 3. Utilize for storage sizing**
		HWFET	Free-flow traffic at highway speeds	75 (24 C)	10.26	12.75	60	48.3	3.2	0	0%	0.15	0.56	
2	**Aggressive Drive Cycle** - Repeat from full to empty	US06	Higher speeds; harder acceleration & braking	75 (24 C)	8	9.9	80	48.4	8.46	4	7%	0.20	1.60	**Confirm fast transient response capability – adjust if system does not perform function**
3	**Cold Drive Cycle** - Repeat from full to empty	FTP-75 (cold)	FTP-75 at colder ambient temperature	-4 (-20 C)	11.04	31.2	56	21.1	3.3	23	18%	0.07	0.66	**1. Cold start criteria 2. Confirm cold ambient capability – adjust if system does not perform function**
4	**Hot Drive Cycle** - Repeat from full to empty	SC03	AC use under hot ambient conditions	95 (35 C)	3.6	9.9	54.8	21.2	5.1	5	19%	0.09	0.97	**Confirm hot ambient capability - adjust if system does not perform function**
5	**Dormancy Test**	n/a	Static test to evaluate the stability of the storage system	95 (35 C)	0	31 days	0	0	0	100%	100%			**Confirm loss of useable H2 target**

The integrated system model was used to evaluate the performance of various materials-based hydrogen storage systems on a common basis. The test matrix (shown in Table 1) was structured to evaluate the performance of the storage systems against the technical targets under standard and realistic transient driving conditions. The matrix was also designed to exercise a given system from full to empty to provide an understanding of its performance over the entire range of fill conditions. Therefore, the test cases were designed to repeat a drive cycle or set of drive cycles until the storage system being evaluated was empty. Standard drive cycles are typically not long enough to achieve this and would not even deplete a buffer tank in some systems. The important point here is that when evaluating the complex dynamics of hydrogen storage systems, this approach of repeating drive cycles to create test cases is critical to gaining the feedback necessary to refine and improve the systems. As briefly described earlier and shown in Table 1, the test matrix includes five test cases. The first case combines repeats of the UDDS and HWFET cycles until the storage system is depleted. This is used to determine the vehicle-level fuel economy and, from that, to estimate the vehicle range. The fuel economy is calculated using the current EPA five-cycle procedure of adjusting and weighting the UDDS and HWFET figures to provide one fuel economy figure that represents real-world use—it is not the raw figures that come directly from running the cycles. Similarly, the range is then calculated from the adjusted and weighted UDDS and HWFET figure and not simply the cycles' miles achieved until the storage system is empty. The test matrix was found to be a key means of evaluating the fuel economy, range, and other vehicle-level performance features of the storage systems on a common and comparable basis [1]. The following sections show the results for fuel economy, range, and onboard efficiency for the various materials-based storage systems compared with compressed gas systems for HSECoE Phases 1, 2, and 3.

The model outputs from the framework were used to evaluate the status of materials-based systems from all phases of this program. The intent was (1) to use model outputs to evaluate and compare different storage systems and to guide engineering solutions to identify potential solutions to particular barriers; and (2) to develop a platform for evaluating the relative vehicle-level performance of the various materials-based storage systems.

For the following discussion of all simulation results, model applications and results reported are based on Case 1 of the framework exclusively (i.e., UDDS and HWFET combined test cycles). In addition, a mid-size car class was selected as the initial baseline simulation within the framework, as discussed previously. The intent was to be representative of a high-sales-volume mid-size car, such as the Ford Fusion, Chevrolet Malibu, or Toyota Camry. All of the following results are based on the mid-size vehicle configuration described above, but the model is capable of simulating both larger and smaller vehicle classes and configurations. All of the simulation results for range have been normalized to 5.6 kg nominal onboard usable hydrogen mass.

Phase 1 System Results

Simulation results for the Phase 1 systems—an AX-21 system, two MOF-5 adsorbent systems, an ammonia borane (AB) system, and an alane slurry chemical hydride system—are shown in Table 2. In addition, 350-bar and 700-bar compressed gas systems are included for comparison to the materials-based systems.

As shown in Table 2, the fuel economy for materials-based systems ranged from 49 miles per gasoline gallon equivalent (mpgge) for the MOF-5 Press–FCHX system to 43 mpgge for the alane CH system. The alane CH system performed the worst in terms of fuel economy due to its requirement for high temperature conditions to release hydrogen from the material. As a result, the system burns hydrogen to create the needed temperatures for the storage system so that hydrogen can be released for use in the fuel cell. The use of hydrogen for system thermal management results in poor onboard efficiency and, subsequently, poor fuel economy. Alternatively, the AX-21 and MOF-5 Press–FCHX systems performed better due to their high gravimetric efficiency resulting in lower overall system and vehicle mass and therefore better fuel economy. As a result, the AX-21 and MOF-5 Press–FCHX systems also offer the best range results of 274 miles based on the above vehicle configuration and 5.6 kg nominal usable hydrogen storage capacity. All of the other systems in this example were near the 300-mile range target (ranging from 241 to 274 miles). The compressed gas systems demonstrated slightly better but comparable fuel economy and range relative to these example material-based systems.

The MOF-5 Press–FCHX adsorbent system and the AB and alane slurry CH systems all had a gravimetric density of 4.6 weight percent (i.e., the percent of usable hydrogen mass stored to the overall storage system mass; the DOE 2020 technical target for gravimetric density is 5.5 weight percent). These were the best-performing materials-based systems and were comparable to the compressed gas systems, which had gravimetric densities of 4.7–4.8 weight percent. However, the AB and alane slurry systems outperformed the compressed gas systems and all of the other materials-based systems in terms of volumetric density with nearly 40 grams of hydrogen per liter of system. Note that DOE's 2020 technical target for volumetric density is 40 g/L. Out of all the materials-based systems included in Phase 1, the MOF-5 Press–FCHX and AX-21 systems performed the best in terms of fuel economy, range, and gravimetric density, and were comparable to or better than the compressed gas systems. The AB and alane slurry systems performed best in terms of volumetric density; however, it is important to remember that the fluid AB system is an off-board regenerable system that is accompanied by unique refilling challenges, logistics, and costs that are not captured within these simulations (but are discussed later).

Table 2. Adsorbent System Phase 1 System Results for Case 1 (UDDS/HWFET Cycles)

Case 1	Adjusted Fuel Economy (mpgge)	Range 5.6 kg H_2 (mi)	Onboard Efficiency (%)	Volumetric Density (g/L)	Gravimetric Density (wt%)
AX21 Press–FCHX	49	274	97.0	25.2	4.3
MOF-5 Comp–FCHX	48	269	97.0	24.1	3.5
MOF-5 Press–FCHX	49	274	98.0	25.3	4.6
AB Slurry—Exothermic	45	252	96.0	38.9	4.6
Alane Slurry—Endothermic	43	241	88.0	38.9	4.6
350 bar Compressed Gas	50	280	100.0	17.0	4.8
700 bar Compressed Gas	50	280	100.0	25.0	4.7

Phase 2 System Results

For the Phase 2 adsorbent system, the focus was on improving the thermal management systems for the MOF-5 material. These systems were designed around the HexCell and MATI heat exchangers and the material density appropriate for each of these respective systems (i.e., MOF-5 powered for the HexCell and compressed puck for the MATI). Concurrent with the Phase 2 design changes for the adsorbent systems, improvements were also made to the CH slurry systems.

For the Phase 2 systems shown in Table 3, the new designs did not result in any significant changes to the vehicle-level performance. This provided a reality check on these system designs, confirming that design changes that resulted in better system performance in terms of weight, volume, and cost did not result in any degradation in the vehicle-level performance. The fuel economy for Phase 2 materials-based systems ranged from 49/48 mpgge for the MOF-5 systems to 44 mpgge for the alane slurry system. As with the Phase 1 designs, the alane slurry system performed the worst in terms of fuel economy due its onboard endothermic nature. As mentioned above, the system burns hydrogen to create the needed temperatures for the storage system hydrogen release and storage system thermal management. The use of hydrogen for system thermal management results in poor onboard efficiency and, subsequently, poor fuel economy. Alternatively, the AB slurry and MOF-5 systems performed better in this example due to their high gravimetric efficiency, resulting in lower overall system and vehicle mass and therefore better fuel economy. As a result, the MOF-5 systems also showed the best range results of 274/269 miles based on the above vehicle configuration and 5.6 kg nominal usable hydrogen storage capacity. The compressed gas systems demonstrated slightly better but comparable fuel economy and range relative to these example material-based systems.

The AB slurry chemical hydrogen storage material system had a gravimetric density of 4.2 weight percent (i.e., the percent of usable hydrogen mass to the overall storage system mass; the DOE 2020 technical target for gravimetric density is 5.5 weight percent). This was the best performing materials-based system and was comparable to the compressed gas system, which had a gravimetric density of 4.7 weight percent. As with the Phase 1 systems, the AB slurry system outperformed the compressed gas systems and all of the other materials-based systems in terms of volumetric density with nearly 37 grams of hydrogen per liter of system. DOE's 2020 technical target for volumetric density is 40 g/L. For all of the materials-based systems included in Phase 2, the HexCell powder MOF-5 system performed the best in terms of fuel economy and range, and was comparable to the compressed gas systems. As noted, the AB slurry system performed best in terms of volumetric density, but the AB slurry system is an off-board regenerable system that is accompanied by unique refilling challenges, logistics, and costs that are not captured in these simulations.

Table 3. Adsorbent System Phase 2 System Results for Case 1 (UDDS/HWFET Cycles)

Case 1	Adjusted Fuel Economy (mpgge)	Range 5.6 kg H_2 (mi)	Onboard Efficiency (%)	Volumetric Density (g/L)	Gravimetric Density (wt%)
MOF-5 HexCell	49	274	92.0	17.5	3.5
MOF-5 MATI	48	269	97.0	20.7	3.4
AB Slurry—Exothermic	47	263	97.0	36.8	4.2
Alane Slurry—Endothermic	44	246	93.0	34.3	3.4
350 bar Compressed Gas	50	280	100.0	17.0	4.8
700 bar Compressed Gas	50	280	100.0	25.0	4.7

Phase 3 System Results

For the Phase 3 adsorbent systems, the focus was on final design refinements for the HexCell and MATI systems. The simulation results for these systems are shown in Table 4 and Table 5. In addition to changes made within the storage system models, the base vehicle model was also changed between Phase 2 and Phase 3 in order to improve the vehicle-level modeling based on new validation information. Specifically, changes were made to the vehicle model to include more aggressive controls for assist, more regen recapture, and higher efficiencies within the vehicle. As a result, the fuel economy and related range improved for all of the systems, but the relative performance across the Phase 3 systems remained constant with that of past phases. That is, the adsorbent systems showed marginal improvement over the CH systems and the physical storage systems performed best in terms of fuel economy and range. These enhancements were performed in order to improve the overall robustness of the framework model as it will be made available to the broader research community and become a research tool that will be used beyond the life of the HSECoE. The framework model, as well as many of the other models developed under the HSECoE, is available through NREL at the HSECoE website (www.hsecoe.org) [2].

Table 4. Adsorbent System Phase 3 System Results for Case 1 (UDDS/HWFET Cycles)

Case 1	Adjusted Fuel Economy (mpgge)	Range 5.6 kg H_2 (mi)	Onboard Efficiency (%)	Volumetric Density (g/L)	Gravimetric Density (wt%)
MOF-5 HexCell	54	302	97.0	20.5	4.1
MOF-5 MATI	53	297	96.1	23.2	3.5
AB Slurry—Exothermic	54	302	96.5	36.9	3.9
Alane Slurry—Endothermic	48	269	82.5	33.1	2.9
350 bar Compressed Gas	55	308	100.0	17.1	4.8
700 bar Compressed Gas	55	308	100.0	25.3	4.8

Table 5. Adsorbent System Phase 3 Results for Case 2 (US66 Drive Cycle—Aggressive Driving)

Case 2	Unadjusted Fuel Economy (mpgge)	Range 5.6 kg H_2 (mi)	Onboard Efficiency (%)	Volumetric Density (g/L)	Gravimetric Density (wt%)
MOF-5 HexCell	57	319	97.1	20.8	4.2
MOF-5 MATI	56	314	96.2	23.1	3.5
AB Slurry—Exothermic	57	319	97.8	37.4	4.0
Alane Slurry—Endothermic	49	274	84.1	32.0	2.8
350 bar Compressed Gas	58	325	100.0	17.1	4.8
700 bar Compressed Gas	58	325	100.0	25.3	4.8

Trade-Off Study Results

In addition to providing high-level feedback on the performance and design of a given materials-based system, trade-off studies quantifying the relative range impacts resulting from changes to the storage system capacity and volume were also performed. Table 6 shows results of the volume study based on the Phase 2 adsorbent storage systems. In this application, modelers worked with HSECoE system architects to provide high-level feedback on the performance and design of their given material systems. The focus of this activity was an example of a trade-off study quantifying the relative range impacts resulting from a fixed-volume study.

In this fixed-volume study, four different adsorbent system designs were evaluated in conjunction with three different volume levels. The four adsorbent systems included powdered MOF-5 operating at 60 bar and 80 K full tank conditions with an assumed aluminum tank, powdered MOF-5 operating at 60 bar and 40 K full tank conditions with an assumed carbon-fiber tank, compacted MOF-5 0.52 g/cc operating at 200 bar and 80 K full tank conditions with an assumed aluminum tank, and compacted MOF-5 0.52 g/cc MOF-5 operating at 200 bar and 40 K full tank conditions with an assumed carbon-fiber tank. Each system was simulated in a mid-size passenger vehicle using the modeling framework for Case 1 to provide range and fuel economy for three volume assumptions: 140 L, 205 L, and 253 L. These three volume levels were based on assumptions from the DOE 2020 hydrogen storage technical targets and represent the high, medium, and low range of practical storage system volume for passenger vehicles. For comparison, the usable capacity in the 350 bar compressed gas storage system for the Ford Focus fuel cell vehicle was 4 kg with an external volume of about 230 L.

This study shows that the volumetric target is much more sensitive to range than the gravimetric target is. That is, storage systems that had high mass but allowed for more onboard hydrogen storage through compaction or low-temperature operation had small fuel economy penalties but were accompanied by much higher ranges due to their ability to store more hydrogen onboard for a given volume. This information was used by the adsorbent system architects and modelers to help refine their system designs for Phase 3.

Table 6. Constant Volume Range Impact Study

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Usable H_2 (kg)	Range Usable H_2 (mi)	Gravimetric Capacity (wt%)	Volumetric Capacity (g/L)	Volume (L)
Powder MOF-5 60 bar 80 K Al	51.11	2.00	102.20	2.80	12.86	140
Powder MOF-5 60 bar 40 K CF	51.30	4.20	215.50	6.61	29.84	140
0.52 g/cc MOF-5 200 bar 80 K Al	50.47	3.35	169.10	2.68	23.94	140
0.52 g/cc MOF-5 200 bar 40 K CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60 bar 80 K Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60 bar 40 K CF	50.97	6.70	341.50	7.97	32.64	205
0.52 g/cc MOF-5 200 bar 80 K Al	49.93	5.35	267.10	2.92	26.11	205
0.52 g/cc MOF-5 200 bar 40 K CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60 bar 80 K Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60 bar 40 K CF	50.89	8.60	437.60	8.68	33.96	253
0.52 g/cc MOF-5 200 bar 80 K Al	49.32	6.85	337.90	3.02	27.05	253
0.52 g/cc MOF-5 200 bar 40 K CF	49.71	9.30	462.30	4.77	39.56	253

Al: aluminum tank
CF: carbon-fiber tank

Storage System Energy Analysis

In support of the engineering and design of the materials-based systems under the HSECoE, energy analyses on the various storage system designs were performed to provide high-level estimates on the overall energy inputs required by a given system, including well-to-power-plant (WTPP) efficiency (%), hydrogen cost ($/kg), and greenhouse gas (GHG) emissions (carbon dioxide equivalent) on a gram per mile basis for future 2020 scenarios. Results of some of these analyses obtained from running the H2A Hydrogen Delivery Scenario Analysis Model (HDSAM) are shown in Table 7 and Table 8. The HDSAM model was run for several adsorbent systems (the HexCell powder MOF-5, the MATI compacted puck MOF-5 [0.32 g/cc], and a 60 bar 80 K gas adsorbent) and for the AB slurry and alane slurry chemical hydrogen storage material systems to produce preliminary WTPP efficiency, GHG emissions, and hydrogen cost figures. In addition, model runs were performed on a 700-bar compressed gas system and a cryogenic-compressed liquid hydrogen system (CcH_2 <200 K) for comparison to the materials-based systems. The well-to-wheel (WTW) GHG emissions breakdowns by category for this analysis are shown in Figure 2.

The AB system offers several onboard advantages over the alane system—being an exothermic onboard reaction leads to higher onboard efficiency (96% vs. 88%). The alane system has higher regeneration cycle costs, and higher energy inputs. Both chemical hydrogen materials systems showed a higher cost and lower efficiency than the adsorbent systems and the two physical storage systems. This indicates a need for advancements and cost reductions for chemical hydrogen storage material systems in general. This analysis supports the need for additional research focused on reducing the cost of chemical hydrogen storage material off-board regeneration cycles in order for these systems to be viable. The adsorbent systems performed better than the chemical hydrogen storage material systems in terms of cost, energy, and GHG emissions, but they were still higher in all of these areas than the physical storage systems were. The adsorbent systems also require additional advancements in order to compete with the incumbent systems. In general, the results from Table 7 and Table 8 shows that the adsorbent systems investigated do not outperform compressed gas systems.

Table 7. Vehicle WTW Results for Adsorbent and CH Systems Compared to Compressed Gas and Liquid Hydrogen Systems

	WTW H_2 Cost ($/kg-$H_2$)	WTW Energy Efficiency	WTW GHG Emissions (g/mile)	Volumetric Efficiency (g-H_2/L)
2020 700 bar Gas—T520[a]	$3.91	56.4%	230	25.6
2020 CcH_2—Liquid Hydrogen Truck	$4.49	46.5%	289	41.8
2020 Liquid AB	$13.96	16.5%	915	41.4
2020 Liquid Alane	$7.89	24.7%	642	32.2
2020 Adsorbent 1 60 bar 80 K Gas—T340[b]	$5.92	40.4%	401	24.1
2020 Adsorbent HexCell 100 bar 80 K Gas—T340[b]	$6.16	39.2%	412	17.5
2020 Adsorbent MATI 100 bar 80 K Gas—T340[b]	$5.69	42.1%	391	20.7

[a] T520: 520 bar insulated tube truck; [b] T340: 340 bar insulated tube truck

Table 8. Vehicle WTW GHG Breakdown for Adsorbent and CH Systems Compared to Compressed Gas and Liquid Hydrogen Systems

WTW GHG Breakdown ($g\ CO_2$ eq/mile)	**700 bar Gas 2020**	**CcH_2 Liq. H_2 2020**	**Liquid AB 2020**	**Liquid Alane 2020**	**Adsorbent 2020**
Plant Gate	186	186	206	218	218
Regen	0	0	670	344	0
Liquefaction	0	91	0	0	0
Terminal	23	12	1	1	62
Transport (Trailer)	3	1	2	2	2
Station	19	3	0	0	79
Vehicle Storage Parasitics	0	0	37	77	46
Total	**230**	**292**	**915**	**643**	**407**

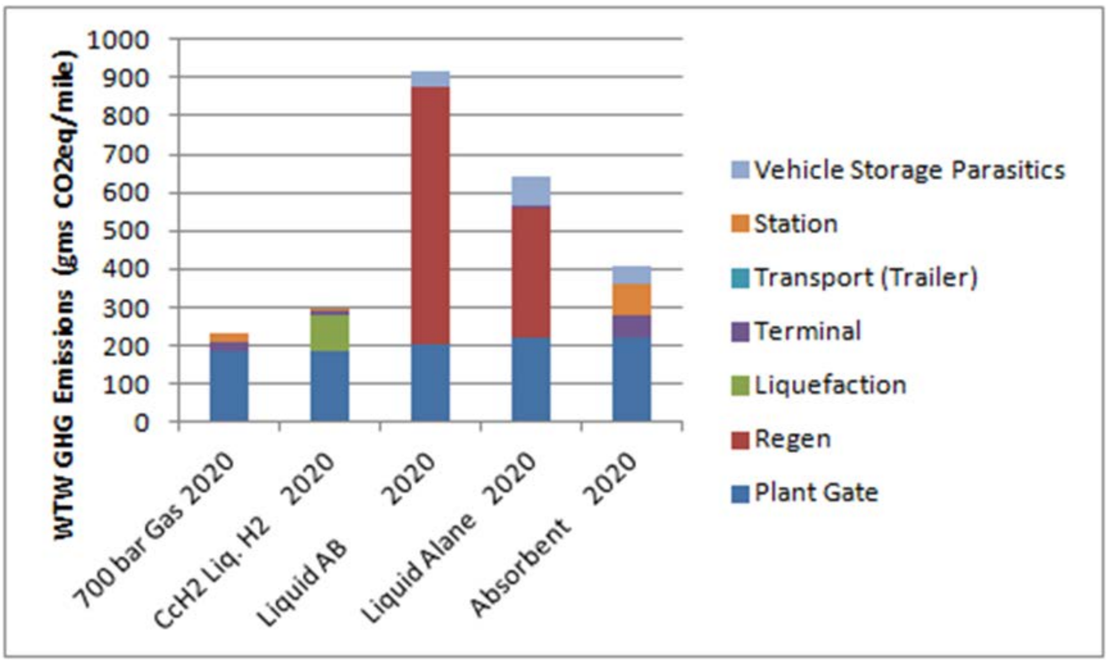

Figure 2. WTW GHG emissions breakdown

Use of HDSAM requires a specific hydrogen delivery scenario as well as specific information for each storage system. Table 9 and Table 10 show the specific delivery and storage system information used for these analyses.

Table 9. HSECoE Base Assumptions for HDSAM

Base Assumptions	
Production	Steam methane reforming
Market: Sacramento	Sacramento, 15% market penetration
Plant (and Regeneration)	62 miles (100 km) from city gate
Electricity	U.S. grid
Large Scale Storage—Geologic	Liquid hydrogen
Transport	Plant to city gate terminal
Gaseous Hydrogen	Pipeline
Liquid Hydrogen	Liquid carrier—truck
Distribution	City gate terminal to refueling stations—truck
Refueling Station Size	1,000 kg/day max. (may be limited by one delivery per day or 9% coverage)

Table 10. Storage System Information Required for HDSAM Analysis

System Information
System weight, wt%, density, and volume
Total and usable H_2 (5.6 kg)
Venting rate and dormancy time
System temperature and pressure at full and ¼ tank
Energy used to release H_2
System cost
Cooling load at refueling station
Fill time
Fuel economy (from HSSIM)

References

1. M. Thornton, A. Brooker, J. Cosgrove, M. Veenstra, and J.M. Pasini, "Development of a Vehicle-Level Simulation Model for Evaluating the Trade-Off between Various Advanced On-Board Hydrogen Storage Technologies for Fuel Cell Vehicles," *SAE Technical Paper* 2012-01-1227 (2012), doi:10.4271/2012-01-1227.

2. U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office Hydrogen Storage Engineering Center of Excellence, http://hsecoe.org/models.html.