



System Design, Analysis, and Modeling for Hydrogen Storage Systems



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Project ID # ST008

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

Overview

Timeline

Project start date: FY09 Project end date: FY15 Percent complete: 85%

Budget

FY13 DOE funding: \$100K Planned FY14 DOE funding: \$125K Total project value: \$1.8M Cost share percentage: 0%



Barriers

(A) System weight and volume

(B) System cost

(C) Efficiency

(E) Charge/discharge rate

(I) Dispensing technology

(K) System life-cycle assessments

Partners

Savannah River National Lab (SRNL) project lead, Pacific Northwest National Lab (PNNL), United Technologies Research Center (UTRC), Jet Propulsion Lab (JPL), Ford, General Motors (GM), Los Alamos National Lab (LANL), Oregon State University (OSU), University of Michigan (UM), and the DOE Vehicle Technologies Office.

Relevance/Objectives

Support the HSECoE with system design, analysis, modeling, and media engineering properties for materials-based hydrogen storage systems

- Manage Hydrogen Storage Engineering Center of Excellence (HSECoE) vehicle performance, cost, and energy analysis technology area.
- Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance trade-offs at the vehicle system level.
- Energy Analysis: Coordinate hydrogen storage system well-to-wheels (WTW) energy analysis to evaluate off-board energy impacts with a focus on storage system parameters, vehicle performance, and refueling interface sensitivities.
- Media Engineering Properties: Assist center in the identification and characterization of adsorbent materials that have the potential for meeting Department of Energy (DOE) technical targets for onboard systems.
- Lead effort to make select HSECoE wide models available for use by other researchers via Web-based portal.

Objective: Vehicle Performance

- Develop and apply a model for evaluating hydrogen storage requirements, performance and cost tradeoffs at the vehicle system level (e.g., range, fuel economy, cost, efficiency, mass, volume, on-board efficiency)
- Provide high level evaluation (on a common basis) of the performance of materials based systems:
 - Relative to DOE technical targets
 - Relative in class and across class for materials systems
 - Relative to physical storage systems
 - Relative to conventional vehicles

Objective: HSECoE Model Web Access

Coordinate across the HSECoE to make select models developed under this effort available to other researchers and research organizations through Web-based access.

- Assist with model selection
- Coordinate model validation
- Coordinate model documentation
- Manage website and model posting
- Track and record Web activity
- Track and record model downloads



The Hydrogen Storage Engineering Center of Excellence (HSECoE) is working to help reduce our Nation's dependence on foreign energy sources by changing the way we power our cars, homes, and businesses. The HSECoE was selected through a competitive, merit reviewed solicitation process by DOE.



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The Center addresses the significant engineering challenges associated with developing lowerpressure, materials-based, hydrogen storage systems for hydrogen fuel cell and internal combustion engine light-duty vehicles.

This project is incorporated into the DOE's Fuel Cell Technology Program, which consists of applied research and development

activities, conducted through Center of Excellence materials and engineering teams, and independent projects focusing on materials and concepts, testing, and system analysis.



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Approach/Milestones

Date	Milestone	Status
10/13	Participate in the HSECoE face-to-face meeting and present on the status of the modeling efforts and development of GUI interface for the public release of the models.	100%
6/14	Update the chemical system model with Phase II performance data, integrate into the framework; document and release models to the public.	30%
6/14	Present modeling efforts of the HSECoE and the projected status of adsorbent systems to meet the DOE 2017 target of 5.5 wt.%.	50%
8/14	Report on vehicle system modeling of hydrogen storage impacts on vehicle range, acceleration, and fuel economy and associated trade-offs on volume and mass.	50%
8/14	NREL will work with center partners to set up and run vehicle simulations to evaluate the key volumetric, gravimetric, and onboard efficiency trade-offs over three test cases (drive cycles) and progress toward 2017 targets for two chemical hydrogen and two to three adsorbent system designs in support of final design selection for each material class for Phase III work.	25%
9/14	Report on progress of public release of HSECoE models.	0%
9/14	NREL will work with center partners to make enhanced and updated versions of the HSECoE "modeling framework", with four new storage system options, available for public access via the current Web portal.	0%

Approach: Develop HSSIM (Vehicle Model)



- Fuel economy (mpgge) based on EPA-adjusted five cycle estimate
- Range (miles) from adjusted mpgge
- Onboard efficiency (%)
- Hydrogen flow (moles/s)
- Vehicle performance





Drive Cycles



doi:10.4271/2012-01-1227

ABSTRACT

One of the most critical elements in engineering a hydrogen dired all vision is the design of the colored hydrogen strange system. Because the current compressed-gas hydrogen strange enclosely as a second key challenges, including cott, volumes and capacity, materials-based strange steaked hydrode, thereas hydrode and absorbent materials, encloseling of the system interge technologies in the enclose of the system of the system is the system of the enclose of the system performance and what trade-offs between the hydrogen storage strange strates drawed systems unglet exist that lalow these alternative stranges approaches to babe.

To pain a better understanding of the interactions that exist between virous unstrail-based hydrogen storage systems and the vehicle system as well as the engineering challenges that exist when integrating one of these systems with a vehicle, the Notional Renewable Energy Laboratory (OREL) developed a vehicle-level model designed to be sensitive to these issues. The Hydrogen Storage Simulation Model (MSSLM) was developed under the Hydrogen Storage

Engineering Center of Excellence (HECc20 as a specialized to that could we used to sait in the designed to an early of matrix)-based hydrogen storage systems being counties by the HECC2. This tool is the singled to are only assumes imparison with the HEECc2 in the oil and storade hydrogen storage system models and to exclusive program towards the U.S. Department of Energy's hydrogen storage technical target. This model has been used as the HECC2 cell model developed by Food Meter Company is a HECC2. Technologies, Research Center and other HEECC2 in the Chamber of the HEECC2 in the site of the HEECC2 in the technologies of the HEECC2 in the HEECC2 in the Chamber of the HEECC2 in the site of the HEECC2 in the technologies of the HEECC2 in the HEECC2 in the Chamber of the HEECC2 in the HEECC2 is the HEECC2 in theECC2 in the HEECC2 in the HEECC2 in

This paper focuses on the development, structure, and validation of the vehicle model HSSM and automations in imperious within the formework. HSSM and the framework are then used to obtain trade-offs for various specific matterial-based stronge system designs. This includes hydrogen storage sings analyses, more compositing analyses, range verw volumes studies, and vehicle and composent performance analyses, such as acceleration rates and fuel and lead studies you storage storage storages.

INTRODUCTION

The Hydrogen Storage Engineering Center of Excellence (HSECoE), sponsored by the U.S. Department of Energy

Approach: Modeling Framework



Approach: Model Access Website

http://hsecoe.org



Model Access/Description Sub-Page



Home Mission Partners Approach Technology Areas Progress Technical Gap Models Contact

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Approach: Model Access Website

Model Documentation and Downloads





Accomplishment: Model Posting

•	MH Acceptability Envelope	SRNL	complete
•	MH Finite Element Model	SRNL	complete
•	Physical H2 Framework Mod	es UTRC/NREL	complete
•	MH Framework Model	UTRC/SRNL/NREL	complete
•	Tank Volume/Cost Model	PNNL	complete
•	CH Framework Model	UTRC/PNNL/NREL	6/2014
•	AD Framework Model	UTRC/SRNL/NREL	9/2014
•	AD Finite Element Model	SRNL	3/2015

Tanks/Volume Cost Model

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Liner uttimate strength (Room Temp.) Liner Thickness [t] total mass (kg) total material cost (kg) total material	liner burst load	bar	118 1	Aluminum liner mass (kg)	26.91	26.9
Line Thickness [t] cm 0.86 exterior L:D Layers of composite (minimum is 3) 10 Upper Bound Wall Thickness Calculation Carbon Fiber Composite Material strength Bar 15306 Safety Factor - 2.25 Wall Radius = R+t cm 23.4 Tank Wall thickness (ideal) cm 1.072949179 Layer thickness increment cm 0.09144 Final Wall thickness cm 1.09728 Minimum layer thickness cm 0.27432 Final Wall thickness cm 1.09728	Liner ultimate strength (Room Temp.)	Bar	3103.0	total mass (kg)	45.34	49.1
extenor LDextenor LD1./420364261./420364261./42036426Layer Bound Wall Thickness CalculationCarbon Fiber Composite Material strengthBarSafety Factor2.25Wall Radius = R+tcmCarbon Fiber Composite (ideal)cmLayer thickness incrementcm0.09144Carbon fiber composite cost (\$/kg)# layers12Rounded up thicknesscm1.09728Carbon fiber composite cost (\$)Minimum layer thicknesscm1.09728Tank Wall total material cost (\$)Final wall thicknesscm1.09728Tank Wall total material cost (\$)	Liner Thickness [t]	cm	0.86			
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Upper Bound Wall Thickness CalculationTank EfficiencyCarbon Fiber Composite Material strengthBar15306Gravimetric (L/kg)2.32Safety Factor-2.25Gravimetric (L/kg)2.32Wall Radius = R+tcm23.4Tank Material CostTank Wall thickness (ideal)cm1.072949179aluminim material cost (\$/kg)4.45Layer thickness incrementcm0.09144Carbon fiber composite cost (\$/kg)30.65# layers12aluminum line cost (\$)119.73Rounded up thicknesscm0.27432Carbon fiber composite cost (\$)565.13Minimum layer thicknesscm0.27432Tank Wall total material cost (\$)684.87Final wall thicknesscm1.09728Tank Wall total material cost (\$)684.87				Layers of composite (minimum is 3)	10	
Carbon Fiber Composite Material strengthBar15306Gravimetric (L/kg)2.32Safety Factor-2.25Wall Radius = R+tcm23.4Tank Material CostTank Wall thickness (ideal)cm1.072949179aluminim material cost (\$/kg)4.45Layer thickness incrementcm0.09144Carbon fiber composite cost (\$/kg)30.65# layers12aluminum line cost (\$)119.73Rounded up thicknesscm0.27432Tank Wall total material cost (\$)565.13Minimum layer thicknesscm1.09728Carbon fiber composite cost (\$)684.87	Upper Bound Wall Thickness Calculation	_		Tank Efficiency		
Safety Factor-2.25Environment (2.6)Wall Radius = R+tcm23.4Tank Material CostTank Wall thickness (ideal)cm1.072949179aluminim material cost (\$/kg)Layer thickness incrementcm0.09144Carbon fiber composite cost (\$/kg)# layers12aluminum line cost (\$)Rounded up thicknesscm1.09728Carbon fiber composite cost (\$)Minimum layer thicknesscm0.27432Tank Wall total material cost (\$)Final wall thicknesscm1.09728	Carbon Fiber Composite Material strength	Bar	15306	Gravimetric (L/kg)	2.32	2.1
Wall Radius = R+tcm23.4Tank Material CostTank Wall thickness (ideal)cm1.072949179aluminim material costLayer thickness incrementcm0.09144Carbon fiber composite cost (\$/kg)# layers12aluminum line cost (\$)Rounded up thicknesscm1.09728Minimum layer thicknesscm0.27432Final wall thicknesscm1.09728	Safety Factor	-	2.25			
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# layers 12 aluminum line cost (\$) Rounded up thickness cm 1.09728 Carbon fiber composite cost (\$) Minimum layer thickness cm 0.27432 Tank Wall total material cost (\$) Final wall thickness cm 1.09728	Layer thickness increment	cm	0.09144	Carbon fiber composite cost (\$/ka)	30.65	30.6
Rounded up thicknesscm1.09728Carbon fiber composite cost (\$)565.13Minimum layer thicknesscm0.27432Tank Wall total material cost (\$)684.87Final wall thicknesscm1.09728684.87	# layers		12	aluminum line cost (\$)	119.73	119.7
Minimum layer thicknesscm0.27432Tank Wall total material cost (\$)684.87Final wall thicknesscm1.09728684.87	Rounded up thickness	cm	1.09728	Carbon fiber composite cost (\$)	565.13	682.2
Final wall thickness cm 1.09728	Minimum layer thickness	cm	0.27432	Tank Wall total material cost (\$)	684.87	802.0
	Final wall thickness	cm	1.09728			

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2.30 575.3

3103 118.125 444.375 0.847629852 0.09144 10 0.9144 0.27432 0.9144 79%

22.5 81.0 0.856529971 1.09728 0.002663 0.001611 24.45380997 84.92744819 23.35652997 82.73288819 128.9213116 115.1036997 105 13817.61194 10103.69967 22.26 26.91 49.17 1.73648704 12

2.14

4.45 30.65 119.73

682.27 802.01

Framework Model GUI



Framework Model GUI



Framework Model GUI—Inputs



Framework Model GUI—Model Results

Select storage syste	em T	st system	Types 1 Which consistion framework
est system with no internal dyna ell, and this amount can be tuned	nics. It d to under	vers exactly the flow rate requested by the fuel cell at 6 bar. Once it has delivered 0.5kg of H2 the delivery pressure drops rapidly. The system demands a con and the effect on system efficiency.	Hydrogen Vehicle Simulation Framework
			Select storage system is the request of the net expected by the data of all second bias detended bigs 112 the detency present driver query. The system detencies a constant and/ery present from the form of a with second and a to host in obtaining the term of a system driver of the system detencies a constant and/ery present from the form
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Run simulation			Results (at end of simulation) Dataset tatwale mile 37 14 daviet Na 50 DhA ford eccomp miggs 60 Usavir 2 Na 50 DhA ford eccomp miggs 60 Usavir 2 Na 50 DhA ford eccomp miggs 60 Disrupt system class 10 0
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12 delivered	kg	0.50 Distance traveled miles 37 Vehicle enced (moh)	
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Jsable H2	kg	0.49 EPA Range miles 25 60 Miles 1	Mark 1
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Gravimetric capacity	%		
/olumetric capacity	g/L		
On-board efficiency	%	98.0 generate MATLAB plots 20 finite finite	
emperature	С	30.0	
Pressure	bar	6 🖌	
Chan ainsulation		Save results Generate all plots	2500 3000 3500 4000 4500 \$] plots

Framework—Model Results



Site Visits



New versus Return Visits



User Flows



Visitor Locations



87.50%

50 00%

100.00%

100.00%

100.00%

100.00%

8 (5.30%)

4 (2.65%)

2 (1.32%)

2 (1.32%)

2 (1.32%)

2 (1.32%)

5. Germany

6. Australia

8

10 Egypt

Bangladesh

Belgiur

China

7 (7.14%)

2 (2.04%)

2 (2.04%)

2 (2.04%)

2 (2.04%)

2 (2.04%)

12.50%

25 00%

100.00%

0.00%

100.00%

50.00%

4.88

4 00

1.00

6.00

1.00

1.50

00:03:20

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00:00:00

00:13:57

00:00:00

00:00:18

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0 (0.00%)

6. Sydney

7. Sao Paulo

8. Aiken

9. Richland

10. Stuttgart

114

7 (6.14%)

5 (4.39%)

4 (3.51%)

4 (3.51%)

4 (3.51%)

3 (2.63%)

3 (2.63%)

3 (2.63%)

3 (2.63%)

2 (1.75%)

% of Total: 75.50% (151)

Accomplishments: Response to Reviewers' Comments

- Comment: There is a lack of variation in powertrain configurations. The project team should add range extender powertrain sensitivity analysis.
 - Response: The powertrain and vehicle platforms included in the vehicle performance modeling task were limited by design due to project budget and time constraints.
- Comment: It would be instructive to redo the analyses on a fixed volume basis. FCEVs will have a fixed packaging volume for fitting the storage system on board the vehicle. Greater discrimination between the various storage concepts could result from a fixed-volume analysis.
 - Response: The focus of the vehicle level analysis for this project was to perform simulations on a fixed usable H2 mass basis. As such, most of the analyses used a 5.6 kg usable H2 assumption and the storage models were designed and coded to be consistent with this assumption. That said, a fixed volume analysis was performed in FY12. A summary table of the results from this study is presented on the following slide.

Results: Fixed Volumetric Effects on Range Analysis

Example simulated volume effects on vehicle range and onboard usable H2 (from framework) for various adsorbent system designs

For three fixed volume scenarios: 140/205/253 liters

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Usable H2 (kg)	Range (mi) Usable H2	Gravimetric Capacity (weight percent)	Volumetric Capacity (g/L)	Volume (L)
Powder MOF-5 60 bar 80k Al	51.11	2.00	102.20	2.80	12.86	140 ¹
Powder MOF-5 60 bar 40k CF	51.30	4.20	215.50	6.61	29.84	140
0.52 g/cc MOF-5 200 bar 80k Al	50.47	3.35	169.10	2.68	23.94	140
0.52 g/cc MOF-5 200 bar 40k CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60 bar 80k Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60 bar 40k CF	50.97	6.70	341.50	7.97	32.64	205
0.52 g/cc MOF-5 200 bar 80k Al	49.93	5.35	267.10	2.92	26.11	205
0.52 g/cc MOF-5 200 bar 40k CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60 bar 80k Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60 bar 40k CF	50.89	8.60	437.60	8.68	33.96	253
0.52 g/cc MOF-5 200 bar 80k Al	49.32	6.85	337.90	3.02	27.05	253
0.52 g/cc MOF-5 200 bar 40k CF	49.71	9.30	462.30	4.77	39.56	253

¹ Actual volume used = 155.56 L, which represents the lowest value in the data set available.

Response to Reviewers Comments, Cont.

- Comment: The progress in MOF-5 isotherm measurement appears to be slow, perhaps due to limited funding.
 - Response: The "material characterization" component of this effort was only involved with sorbents, and leveraged the vast amount of information generated by the Hydrogen Sorption Center of Excellence. This part of the effort provided guidance for identifying potential sorbents for the Engineering Center and providing the specific engineering properties needed to make down-selections and to improve model confidence. Most of this activity in the past focused on nonmetal organic framework materials (MOFs), and ultimately, since MOFs were selected for Phase II and Phase III activities, the vast majority of the work and information provided was down selected. At this time, the main focus of the NREL "material characterization" effort is involved with model validation, especially for temperatures below 75 K.

Collaboration and Coordination: Web Model Team Roles and Responsibilities

- Storage system model development, coding and documentation—convert models to appropriate format for use in framework (Simulink[®]). PNNL and SRNL
- Framework management—GUI development and storage system model integration. UTRC





- BASF

- Vehicle model development and validation—framework output management and validation. Storage system model integration and framework update posting. NREL
 - Fuel cell model development and validation. Ford
- Framework model and standalone model posting and Web portal management, NREL
 - Model documentation. NREL, PNNL, Ford, SRNL, UTRC



Management of collaboration efforts across organizations is done through monthly and ondemand modeling team telecons, bi-annual face-to face-meetings, and through SharePoint

















UQTA

Proposed Future Work

- Focus on model validation and model Web access
 - Add CH models to Framework (June)
 - Add Adsorbent models to Framework (September)
 - Post Adsorbent finite element model similar to MH FE Model
- Continue to run vehicle simulations to:
 - Evaluate the impact of changes to Phase III storage system designs and refinements
- Energy analysis
 - Work complete
- Media engineering properties
 - Work complete

Summary

- Manage HSECoE vehicle performance, cost, and energy analysis technology area.
- Lead effort to make models developed by HSECoE available to other researchers via Web-based portal.
- Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance trade-offs at the vehicle system level.



Technical Back-Up Slides

Results: Fixed Volumetric Effects on Range Analysis

Example simulated volume effects on vehicle range and onboard usable H2 (from framework) for various adsorbent system designs 14

For three fixed volume scenarios: 140/205/253 liters

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Usable H2 (kg)	Range (mi) Usable H2	Gravimetric Capacity (weight percent)	Volumetric Capacity (g/L)	Volume (L)
Powder MOF-5 60 bar 80k Al	51.11	2.00	102.20	2.80	12.86	140 ¹
Powder MOF-5 60 bar 40k CF	51.30	4.20	215.50	6.61	29.84	140
0.52 g/cc MOF-5 200 bar 80k Al	50.47	3.35	169.10	2.68	23.94	140
0.52 g/cc MOF-5 200 bar 40k CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60 bar 80k Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60 bar 40k CF	50.97	6.70	341.50	7.97	32.64	205
0.52 g/cc MOF-5 200 bar 80k Al	49.93	5.35	267.10	2.92	26.11	205
0.52 g/cc MOF-5 200 bar 40k CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60 bar 80k Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60 bar 40k CF	50.89	8.60	437.60	8.68	33.96	253
0.52g/cc MOF-5 200 bar 80k Al	49.32	6.85	337.90	3.02	27.05	253
0.52 g/cc MOF-5 200 bar 40k CF	49.71	9.30	462.30	4.77	39.56	253

¹ Actual volume used = 155.56 L, which represents the lowest value in the data set available.