Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements



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DOE Hydrogen and Fuel Cells Program

2020 Annual Merit Review and Peer Evaluation Meeting

May 20, 2020

Project ID # ST008



This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Timeline

- Start: October 1, 2015
- End: September 30, 2021*

Barriers

- A. System Weight and Volume
- B. System Cost
- C. Efficiency
- E. Charging/Discharging Rates
- I. Dispensing Technology
- K. System Life-Cycle Assessment

Budget

- Total Project Funding: \$1,630,000*
 - FY16 Funding: \$336,000
 - FY17 Funding: \$389,000
 - FY18 Funding: \$375,000
 - FY19 Funding: \$275,000
 - FY20 Funding: \$255,000

Partners



*Project continuation and direction determined annually by DOE.

Collaborative effort to manage, update, and enhance hydrogen storage system models developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE)

- Transfer engineering development knowledge from HSECoE on to future materials research.
- Manage the **HSECoE model dissemination** web page.
- Manage, update, enhance, and validate the modeling framework and the specific storage system models developed by the HSECoE.
- Develop models that will accept direct materials property inputs and can be measured by materials researchers.
- <u>Ultimate Goal</u>: Provide validated modeling tools that researchers will use to evaluate the performance of their new materials in engineered systems relative to the DOE Technical Targets.

Relevance – Addressing Barriers with Models

Barriers	Model Addressing Barrier
A. System Weight and Volume	System Estimator
B. System Cost	Tank Volume/Cost Model
C. Efficiency	Framework Model - Onboard Efficiency - Fuel Economy
E. Charging/Discharging Rates	Framework Model - Drive Cycles
I. Dispensing Technology	Framework Model - Initial and Final System Conditions
K. System Life-Cycle Assessment	All Models

Relevance – Improving Model Utilities for Materials Researchers



Modeling Tools Available or In Progress

Framework Model with:

Physical Storage	UTRC/NREL		Estimate performance of light-
Compressed/Cryo-Compressed H ₂	SRNL/NREL	\geq	duty vehicles with four drive
Chemical Hydrogen (CH)	PNNL/NREL		cycles for each storage system
Adsorbent (AD)	SRNL/NREL		
Metal Hydride (MH)	PNNL/NREL		
and-Alone System Design Tools:			
Adsorbent (AD)	SRNL		New MS Excel-based tool
Chemical Hydrogen (CH)	PNNL		New MS Excel-based tool
Metal Hydride (MH)	PNNL		New MS Excel-based tool
Compressed/Cryo-Compressed H ₂	SRNL		
dditional Tools/Models:			
MH Acceptability Envelope (MHAE)	SRNL		
Tank Volume/Cost Model	PNNL		
AD Isotherm Fitting Tool	SRNL		
nite Element Models:			
Metal Hydride (MH) Finite Element (MHFE)	SRNL	Took	post and mass transfer models
Adsorbent (AD) – HexCell and MATI	SRNL		
	Physical Storage Compressed/Cryo-Compressed H ₂ Chemical Hydrogen (CH) Adsorbent (AD) Metal Hydride (MH) tand-Alone System Design Tools: Adsorbent (AD) Chemical Hydrogen (CH) Metal Hydride (MH) Compressed/Cryo-Compressed H ₂ dditional Tools/Models: MH Acceptability Envelope (MHAE) Tank Volume/Cost Model AD Isotherm Fitting Tool inite Element Models: Metal Hydride (MH) Finite Element (MHFE) Adsorbent (AD) – HexCell and MATI	Physical Storage UTRC/NREL Compressed/Cryo-Compressed H2 SRNL/NREL Chemical Hydrogen (CH) PNNL/NREL Adsorbent (AD) SRNL/NREL Metal Hydride (MH) PNNL/NREL tand-Alone System Design Tools: Adsorbent (AD) Adsorbent (AD) SRNL Chemical Hydrogen (CH) PNNL Metal Hydride (MH) PNNL Compressed/Cryo-Compressed H2 SRNL Compressed/Cryo-Compressed H2 SRNL dditional Tools/Models: MH Acceptability Envelope (MHAE) SRNL Tank Volume/Cost Model PNNL SRNL AD Isotherm Fitting Tool SRNL SRNL inite Element Models: Metal Hydride (MH) Finite Element (MHFE) SRNL Adsorbent (AD) – HexCell and MATI SRNL SRNL	Physical Storage UTRC/NREL Compressed/Cryo-Compressed H2 SRNL/NREL Chemical Hydrogen (CH) PNNL/NREL Adsorbent (AD) SRNL/NREL Metal Hydride (MH) PNNL/NREL tand-Alone System Design Tools: Adsorbent (AD) Adsorbent (AD) SRNL tand-Alone System Design Tools: Adsorbent (AD) Adsorbent (AD) SRNL Chemical Hydrogen (CH) PNNL Metal Hydride (MH) PNNL Compressed/Cryo-Compressed H2 SRNL dditional Tools/Models: SRNL MH Acceptability Envelope (MHAE) SRNL AD Isotherm Fitting Tool SRNL inite Element Models: SRNL Metal Hydride (MH) Finite Element (MHFE) SRNL Adsorbent (AD) – HexCell and MATI SRNL

Accomplishments and Progress – Design Tools and Framework Estimate Allow Evaluation of Hydrogen Storage Systems

Capabilities:

- Stand-alone design tools now available in Microsoft Excel for adsorbents, metal hydrides, chemical hydrogen storage, and pure hydrogen storage
- Usable-H₂-mass-based and full storage-systemvolume-based capabilities for each design tool
- Multiple kinetics/isotherm expressions available in the stand-alone tools and framework for each storage method
- All models allow material-specific property inputs measured by materials researchers to design materialspecific storage systems

Accomplishments and Progress – Design Tools Flowchart



Accomplishments and Progress – Model Improvements

Original Model	Updated Model							
Adsorbent Model								
Balance of plant (BOP) for cryogenic operation only	BOP options for room temperature, cold, and cryogenic operations							
Insulation thickness hard-coded to 1 inch	Insulation thickness is user controlled							
LN ₂ tank cooling channel always included	LN ₂ tank cooling channels user controlled							
D-A isotherm model used only	D-A and UNILAN isotherm model options							
MOF-5 material properties hard-coded	User-defined adsorbent material properties (with MOF-5 default values)							
Mass of usable H_2 is the starting point of the calculation	Mass of usable H ₂ or maximum total storage system volume starting point							
Metal Hyd	Iride Model							
Single step irreversible reaction	Single step irreversible or two step reversible models selectable							
Hard-coded reaction rate and enthalpy (30 kJ/mol)	Reaction parameters and material properties as inputs							
Mass of usable H_2 is the starting point of the calculation	Mass of usable H ₂ or maximum total storage system volume starting point ⁹							

Excel-Based Chemical Hydrogen Storage Stand-Alone Tool

MS Excel-based tools allow universal availability without cumbersome downloads of MATLAB products

- Usable-H₂-mass-based and system-volume-based tools available
- Downloads available for ammonia borane and alane can be downloaded and modified for other liquid/slurry-based chemical hydrogen storage materials

ExoEndo	1	Exothermic/Endotheric Flag (Exo = 1, Endo = 0)			Out	but
Kinetic_Model	1	Kinetic Model Flag (Avrami Kinetics = 1, nth Order Kinetics = 2)		JUT		
MW_CH	30.8 g/mol	molecular weight Chemical Hydrogen Material		•••		
slurry	1	Fluid Properties Flag (Slurry (1) or Liquid (0))				
x_H2	0.152	Wt Fraction H2 in the CHS Material				
n_rxn	1	Number of Reactions to Model (1 or 2) Run				
DH_rxn_1	-17981 J/mol H2	Reaction Enthalpy Rxn 1 (negative=exothermic)				
Beta1	2.355 mol H2/mol CH	Molar Ratio H2 maximum for CH material Rxn 1				
A1	244 sec-1	Pre-exponential factor for Rxn 1	Name	Value	Unite	Description
E1	29900 J/mol H2	Activation Energy for Rxn 1	Name	value	Units	Description
n1	3.1	Exponent for Avrami or Reaction Order for Rxn 1	System Mass and Volume			
DH_rxn_2	0 J/mol H2	Reaction Enthalpy Rxn 2 (negative=exothermic)	TotalMass	131,7338405	kg	Total Estimated System Mass
beta2	0 mol H2/mol CH	Niolar Ratio H2 maximum for CH material RXN 2	Total//aluma	144	1	Total Estimated System Valuma
F2	0 J/mol H2	Activation Energy for Pyn 2	Totalvolume	144	L	Total Estimated System volume
n2	1	Exponent for Avrami or Reaction Order for Rxn 2	Usable H2	5.63829624	kg	Estimated Usable H2 for System
x_inert	0.5	Weight fraction inert with CHS Material to Slurry	DOE Mass Target	0.042800667	kg H2/kg sys	DOE Gravimetric Target 2020
Cp_CH	2694 J/kg/K	Heat Capacity CHS Material	DOF Vol Target	0 039154835	kg H2/L svs	DOF Volumetric Target 2020
Cp_i	1846 J/kg/K	Heat Capacity inert slurrying agent		0.033134033	Kg 112/ L 393	DOE Volumetrie ranget 2020
Cp_p	774 J/kg/K	Heat Capacity CHS Material Product	Design Parameters			
rho_CH	780 kg/m3	Density CHS Material	ReactorLength	0.403	m	Reactor Length
rho_i	1000 kg/m3	Density inert slurrying agent	Vhallast	0.01/0677/5	m2	Ballast Tank Volume
rho_P	1640 kg/m3	Density CHS Material Product	Vballast	0.014007745		
ppm_imp	500 ppm	Concentration of impurity 1	MFeed	78.09274571	kg	Mass Chemical Hydride Required
A_Imp MW_imp	0.1 g impurity/g adsorbent	Adsorbent maximum loading impurity 1	LiqRadLength	1.534666617	m	Slurry Radiator Length
ppm_imp2	2000 ppm	Concentration of impurity 2	GasRadLength	0.708811328	m	Hydrogen Gas Radiator Length
A_imp2	0.35 g impurity/g adsorbent	Adsorbent maximum loading impurity 2	Recuplength	0	m	Recuperator Length (if endothermic)
MW_imp2	80.5 g/mol	molecular weight impurity 2	Recupterigin	0		Recuperator Length (il endotherninc)
Usable H2	0 kg	Mass of usable hydrogen required	Startup Time	75.96206604	sec	Time to Reach 30% Conversion
Total Volume	0.144 m3	Total system volume required	Target Temperature	148.9828824	°C	Temperature to Reach 30% Conversion
Max Power	25 kW	Maximum Hydrogen Storage H2 Production Required		246 2200427	°C	Maximum Deceter Terrenerature
Ave Power	15 kW	Average Hydrogen Storage H2 Production Required	Maximum Temperature	240.3299437	L	Maximum Reactor Temperature
Pset	25	Ballast Tank Pressure Initial Condition and Setpoint	End of Parameters			
Q_heater	8000	Reactor heater per length				
I max	400 °C	Maximum acceptable reactor temperature	1- 112			
voi_tiag	1	Flag for either volume or usable H2 constrained design: 1 = volume, 0 = usa	DIE HZ			

Flag for volume- or usable-H₂-constrained design

Excel-Based Metal Hydride Stand-Alone Design Tools

Hyd	rogen Mass-Based I	Metal Hydride	e Storage Design Tool Input Sheet				
		Material Pro	operties				
Name	Value	Units	Description				
f_H2	0.1	decimal fraction	Hydride Carrying capacity of metal hydride		Bun		
f_inert	0	decimal fraction	Fraction of inert in metal hydride bed (Enter 0 if f	_H2 accour	Kuli		
kbed	8	W/m-K	Thermal Conductivty of hydride bed				
rho_cry	1000	kg/m^3	Crystalline Density of metal hydride				
f_void	0	decimal fraction	Fraction of voids in metal hydride bed (Enter 0 if r	ho_cry = rho_bed)			
rho_inert	0	kg/m^3	Density of inert material in hydride bed (Enter 0 if	f rho_cry = rho_bed)		Innut	
dH_rxn1	37000	J/mol	Enthalpy per mole H2 rxn 1 (Endothermic +)			_ input	
dS_rxn1	125	J/mol-K	Entropy per mole H2 rxn 1				
dH_rxn2	0	J/mol	Enthalpy per mole H2 rxn 2 (set to zero if single st	ep rxn)			
dS_rxn2	0	J/mol-K	Entropy per mole H2 rxn 2 (set to zero if single ste	p rxn)			
beta_rxn1	1	mol/mol	Moles H2 produced per mole feed, Reaction 1 (En	ter 0 if no rxn 2)			
beta_rxn2	0	mol/mol	Moles H2 produced per mole feed, Reaction 2 (Ent	ter 0 if no rxn 2)			
		System Para	imeters				
Name	Value	Units	Description				
dmH2	5.6	kg	Mass of useable H2 available in the tank				
r	0.005	m	Coolant tube external radius				
th_tube	0.00089	m	Coolant tube thickness			Output	
	45	к	acceptable hydride temperature rise during refue	ling		• dip di	
PH2hi	100	atm	Upper Hydrogen Operating Pressure			_	
PH2IO	5	atm	Lower Hydrogen Operating Pressure				
HemObi	1	option	Hemispherical endcap option				
-			Material Option $1 = 6061 - 162 = 316 SS 3 = Composi$	te Type III (AL liner) 4 =			
Type	2	option	Composite Type IV (plastic liner)				
L/d	4	decimal fraction	Desired exterior Ltank over dtank Enter Zero to Ca	liculate		•	-
L_tank	0	m 	Desired tank exterior length Enter 0 to calculate	C t			
D_tank	0	m	Desired tank exterior diameter Enter 0 to Calculat	System mas	ss (kg)		225.5053
ot	300	seconas	Target Refueling time (300 s = DOE 2020 target)	System yolu	mo(m2)		0 112207
en_comb	0.8	decimal fraction	Combustion Efficiency in required	System volu		0.112207	
				Combustor	y>0/n=0		1
Separate mo	dels for ma	ss-of-us	able-H	Mass H2 Bu	ırned (kg)		1.321687
 constrained and system-volume- constrained design tools Models based on thermodynamics and heat transfer only: no kinetics or mass 				Tank Outer Diameter (m) Tank Length (m)			0.32275
							1.249055
				Number of		101	
				Total Hydride Mass (kg)			69.21687
				Tank Mass	117.0723		

Maximum Temperature (°C)

Percentage of DOE 2025 Gravimetric Target (%)

transfer included

153.45

45.13911

Excel-Based Cryo-Adsorbent Stand-Alone Design Tools

	VOLU	ME		DUN	Clear			
	Values	Units	Comments	KUN	Results	Description	Name	Units
Pi	1.00E+07	Pa	Initial/Full tank pressure	UNILAN				Output values
Pf	5.00E+05	Pa	Final/Empty tank pressure			Total hydrogen stored	H2stored	kg_H2
Ti	80	К	Initial/Full tank temperature			Usable hydrogen	H2usable	kg_H2
Tf	160	K	Final/Empty tank temperature			Total H2 Storage System Mass	System_mass	kg
ystem_Vol	267.6779	L	Target system total volume			Total Projected H2 Storage System Cost	System_Cost	\$
ype_Ads	2		Type of adsorbent/HX: 1) None (compressed H2)?, 2) Powe	der/HexCell, 3) Compact/MATI		System-based gravimetric capacity	Grav_Cap	g_H2/g_sys
/emp_Op	3		Operating Temperature: 1) Room temperature, 2) Cold Ope	ration, 3) Cryogenic Operation		System-based volumetric capacity	Vol_Cap	g_H2/L_sys
Add Cool	0		Additional Coolant Lines (1) if present			Overall system rank based on mass, volume, and		
444_0001			Additional Cooldrik Enros (1) II prosonik			cost (better systems have higher values)"	Rank	
Emax	5040.27	Jimol _{H2}	UNILAN Parameter Maximum isosteric heat					Input values
Emin	1061.55	Jłmol _{H2} /K	UNILAN Parameter Minimum isosteric heat			Initial/Full tank pressure	Pi	bar
nmax	67.75003	mol _{H2} /kg _A	UNILAN Parameter Maximum H2 loading per mass of ac	Isorbent		Initial/Full tank temperature	Ti	К
Va	0.0014039	m³kg _{A4} ,	UNILAN Parameter Adsorbed volume per mass of adsort	bent		Final/Empty tank pressure	Pf	bar
Vv	0.00725	m³kg _{A4} ,	UNILAN Parameter Void volume per mass of adsorbent			Final/Empty tank temperature	Tf	к
rho_ads	130	kg _{ad} /m³	Bulk Density of the MOF-5			Total H2 Storage System Volume	System_vol	L
k	0.3	WimK	Thermal conductivity of the adsorbent	Output	ts	Type of adsorbent/HX: 1) Powder/HexCell, 2) Compact/MATI	type_Ads	
Ср	780	Ji ka / K	Specific Heat of the adsorbent			Operating Temperature: 1) Cryogenic Operation,		
		-				2) Room Temperature Operation	Temp_Op	
ds_Cost	11.8	\$/kg _{Adr}	Projected cost of the adsorbent per unit mass			Additional coolant (1) present	Add_Cool	
Therm	0		LN2 chiller (1) if present			UNILAN Parameter Maximum isosteric heat	Emax	J/mol_H2
HemUbl	0		Hemispherical (1) or oblate (≠1) endcaps			UNILAN Parameter Minimum isosteric heat	Emin	J/mol_H2/K
Vessel	1		Vessel only (0) or full sizing (≠0)			UNILAN Parameter Maximum H2 loading per mass of adsorbent	nmax	mol_H2/kg_ads
ТТуре	4		Type of pressure vessel:			UNILAN Parameter Adsorbed volume per mass of adsorbent	Va	m^3/kg_ads
			1 = Aluminum Type 1	Inputs		UNILAN Parameter Void volume per mass of adsorbent	Vv	m^3/kg ads
			2 = 316 Stainless Steel Type 1			Bulk Density of the MOF-5	rho ads	kg ads/m^3
			3 = Aluminum + CF Type 3			Thermal conductivity of the adsorbent	k	W/m/K
			4 = SS + CF Type 3			Specific Heat of the adsorbent	Co	J/kg/K
			5 = Plastic + CF Type 4			Projected cost of the adsorbent per unit mass	Ads Cost	\$/kg ads
						Presence of LN2 pre-chiller	Therm	9/ N8_000
•	DA_I	Mass	DA_Volume UNILAN_Mass	UNILAN_Volume	Den	sity CompFact Enthalpy	+	: (

- Separate tabs for Dubinin-Astakhov (D-A) adsorption theory isotherm and UNILAN isotherm
- Models can evaluate mass-of-usable-H₂-constrained and system-volume-constrained design tools
- Can evaluate materials at cryogenic, cold, and room-temperature conditions

Accomplishments and Progress – Vehicle Framework GUI



Accomplishments and Progress – Adsorbent System

Des	ign Too	o <mark>l in the F</mark>	ramev	vork			Storage Sizing Tools By Usable H2 MH	or System Volume MH
		System Vo	lumo Ir	put			Adsorbent D-A	Adsorbent D-A
		System ve	nume n	iput			Adsorbent Unilan	Adsorbent Unilan
		and Mass	Output				СН	CH
承 Ads_SystemDesig	InGUI	`	<u> </u>				Cryo Compressed	Cryo Compressed
Load S	System	\in	puts\cryo_cds_Defaul	t_HexCell_UNILAN_byv	vol_sys.mat		Save	
Ing	puts	Name:		Cryoadsorbent				
Pi	1e+07	Description:	and a shart sustain by	and a MOE 5. Continu	a during refuel is done either with a p	icrochannel heat eve	hanger (MATI) or with flow th	trough of cold and
Pf	500000	Description. Cry	oausorbent system ba	ased to MOP-5. Cooling	y during reluer is done either with a h	icrochannel neat exc	manger (www.rr) or with now-th	rough of cold gas.
Ti	80		Results	:	Output values			^
Tf	160			H2stored	5.7187 kg_H2	Total hydrogen sto	red	
System_Vol	267.678	Run System	Design	H2usable	5.6043 kg_H2	Usable hydrogen		
type_Ads	2	<u>.</u>		System_mass	151.5204 kg	Total H2 Storage S	System Mass	
Temp_Op	3	Save Results	to Excel	System_Cost	3.3600e+03 \$	Total Projected H2	Storage System Cost	
Add Cool	0	Save Results	IO EXCEI	Grav_Cap	0.0370 g_H2/g_sys	System-based gra	vimetric capacity	
Emay	5040.07			Vol_Cap	20.9367 g_H2/L_sys	System-based volu	imetric capacity	
Emin	5040.27	Create Mo	del File	Rank	6.5186	Overall system ran	k based on mass, volume, a	nd cost (better s
Emm	1061.55				Input values			
nmax	67.75	Sustan Dia		Pi	100 bar	Initial/Full tank pre	ssure	
Va	0.00140392	System Dia	gram	Ti	80 K	Initial/Full tank tem	perature	
Vv	0.00 m3/kgAds. UI	VILAN Parameter Adsorbed	volume per mass of	fadsorbent	5.5000 bar	Final/Empty tank p	pressure	
rho_ads	130			Tf	160 K	Final/Empty tank t	emperature	
k	0.3			System_Vol	267.6779 L	Target H2 Storage	System Volume	
Ср	780	Exit		type_Ads	2	Type of adsorbent/	HX: 1) None? 2) Powder/H	exCell, 3) Comp
Ads Cost	11.8			Temp_Op	3	Operating Tempera	ature: 1) Room Temperature	Operation, 2) Col
 Therm	0			Add_Cool	0	Additional coolant	(1) present	
HamObi	0			Emax	5.0403e+03 J/mol_H2	D.A. Parameter	Enthalpic contribution to the	characeristic free
Nened	0			Emin	1.0616e+03 J/mol_H2/K	D.A. Parameter	Entropic contribution to the o	characeristic free
Vessel	1			nmax	67.7500 mol_H2/kg_ads	D.A. Parameter	Maximum H2 loading of the	entire adsorption
TType	4	— · · —		Va	0.0014 m^3/kg_ads	D.A. Parameter	Adsorbed volume per mass of	of adsorbent
		Design Docu	mentation	Vv	0.0073 m^3/kg_ads	D.A. Parameter	Void volume per mass of ads	sorbent
				rho_ads	130 kg_ads/m^3	D.A. Parameter	Bulk Density of the MOF-5	
		General Docu	mentation	k	0.3000 W/m/K	Thermal conductivi	ty of the adsorbent	
				Ср	780 J/kg/K	Specific Heat of the	e adsorbent	
				Ada Cast	11 0000 ¢// ada	Designated asst of t	ha adaarbaat aar unit maaa	~

Accomplishments and Progress – Models Provide Input to Spider Charts



Accomplishments and Progress – Models Provide Input to Spider Charts

NaAlH₄ Estimates

Information provided by Framework Model using available drive cycles



Accomplishments and Progress – Exercise Models



Thermal Conductivity vs. Bed Density on Tank Mass



Approach to Achieving DOE Gravimetric Technical Target

Impact of Metal Hydrides on System Mass



Relationship between Usable H₂ and System Volume

Accomplishments and Progress – Metal Hydride Materials Evaluation

MH Stand-Alone Design Tool Evaluates Promising Materials

Material / Property	Model Input Model Output												
	hydcap	kbed	rhobed	dH	dS.	<u>SysMass</u>	SysVol	Temp	TankMass	HydMass	HydBurn	G-Target	V-Target
<u>ENG,Ti</u> -doped NaAlH₄	0.045	8.96	750	40800	125	612	323	197	400	163	1.77	16.6%	43.2%
TiF ₃ -doped Mg(BH ₄) ₂	0.112	1.43	510	48400	121	566	314	311	415	69.8	2.22	18.0%	44.5%
2LiBH ₄ /MgH ₂	0.097	0.89	550	44200	124	618	348	242	447	78.0	1.97	16.4%	40.1%
∏i-doped LiBH₄	0.104	0.63	470	73200	120	1297	632	622	1038	93.4	4.11	7.8%	22.1%
KH-doped 2LiNH ₂ - MgH ₂	0.040	2.10	640	39500	119	875	479	216	615	182	1.69	11.6%	29.2%
KH-doped Li ₃ N	0.082	0.96	710	67300	126	897	448	493	665	112	3.60	11.3%	31.2%
6nm-Mg(BH ₄) ₂ @C	0.059	7.33	570	45800	109	666	354	374	483	130	2.06	15.3%	39.5%
6nm-LiBH₄@C	0.057	7.06	550	57900	106	904	439	581	694	148	2.86	11.3%	31.9%
6nm-Li₃N@C	0.061	8.32	740	42100	114	507	262	283	337	122	1.84	20.1%	53.4%
KH-6nm-Li₃N@C	0.064	9.61	760	41700	117	466	241	256	304	116	1.82	21.9%	58.1%

Bulk Materials Nano Materials

Learning: Nanoscale materials have higher system gravimetric and volumetric capacity in spite of lower hydrogen storage capacity

- Improved ΔH and ΔS result in significantly reduced operating temperature, reducing tank mass and hydrogen burned
- Improved thermal conductivity improves heat transfer during refueling and reduces the number of coolant tubes required

Framework Model Compares Nanoscaled vs. Bulk Materials



Nano-Li₃N Results from Framework Model



Learning: Nanoscaled Li₃N has fast enough kinetics and low enough temperatures to allow all drive cycles to be met; bulk Li₃N does not

 Bulk Li₃N reaction does not initiate for any of the drive cycles

MH Stand-Alone Design Tool Compares Two Forms of NaAlH₄



- HRL is evaluating NaAlH₄ milled with 0.03TiCl₃ mixed 50:50 wt % with diglyme.
- This mixture has faster kinetics and reaches complete conversion sooner than the control without diglyme.

 2^{nd} : Assuming 20% diglyme and the higher usable H₂ capacity result in nearly the same tank size as Control 1^{st}

An assumed doubling of thermal conductivity reduces system mass and volume by 8.5%

	Control	Best 2 nd	Best 2 nd with					
			higher k					
Useable Hydrogen Capacity	0.04	0.048	0.048					
Inert Fraction	0	0.2	0.2					
Bed Thermal Conductivity	1	1	2					
(W/m/K)								
System mass (kg)	678	680	622					
System volume (m3)	0.315	0.317	0.290					
Mass H2 Burned (kg)	1.63	1.66	1.66					
Tank Outer Diameter (m)	0.475	0.476	0.461					
Tank Length (m)	1.83	1.83	1.77					
Total Hydride Mass (kg)	181	181	181					
Tank Mass (kg)	408	409	372					

Accomplishments and Progress – Metal Hydride Materials Evaluation

Framework Compares Two Forms of NaAlH₄, Maximum T = 160° C



Enhanced material decreases the maximum possible operating temperature with the drive cycles by 5°–10°C

Accomplishments and Progress – Model Website Analytics:

Weekly Activity (April 1, 2019–March 30, 2020)



Activity almost every week; 85% of sessions were by new visitors

Accomplishments and Progress – Model Website Analytics: Web Flow (April 1, 2019–March 30, 2020)



 1st interaction is mostly on Models page followed by Technology Areas; 2nd interaction is mostly on Models page

Accomplishments and Progress – Model Website Analytics:

Locations (April 1, 2019–March 30, 2020)



Activity by city shows global interest in countries and regions including China, Australia, Japan, EU, and others

Accomplishments and Progress – Model Downloads

(through March 30, 2020)

MODEL	Total	Totals AMR2019	Additional through 2020Q2
H ₂ Storage Tank Mass and Cost Model	268	241	27
MHAE Model	75	66	9
MHFE Model	121	107	14
Vehicle Simulator Framework Model	192	165	27
CH System Design Stand-Alone	44	31	13
Adsorbent System Design Stand-Alone	56	30	26
MH System Design by Usable H ₂	5	-	5
MH System Design by System Volume	4	-	4

Most downloads are for *Tank Mass and Cost Model* and *Vehicle Simulator Model*

Collaboration and Coordination

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Organization	Relationship	Туре	Responsibility
NREL	Team Member	National Lab	Update website and framework
SRNL	Team Member	National Lab	Adsorbent and compressed gas modeling
PNNL	Team Member	National Lab	Chemical hydrogen and metal hydride modeling
Ford	Consultant	Industry	Beta testing, fuel cell model, adsorption data
University of Michigan	Material Developer	Academia	Adsorption data
University of California Berkeley	Material Developer	Academia	Adsorption data
HyMARC Seedling— Liox	Material Developer	National Lab/ Collaboration	Metal hydride data
HyMARC— Sandia	Material Research	National Lab/ Collaboration	Metal hydride data

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Proposed Future Work – FY20 Milestones and Next Steps

D	eliverable	Due
FY20- Q1	Provide update related to HyMARC collaboration and application of models and post new Framework Model version, including Excel version for all Stand-Alone Models.	Complete
FY20- Q2	Provide update on web portal activity—website hits and time on site, website use locations, and model downloads.	Complete
FY20- Q3	SMART Milestone: Update framework storage, fuel cell, and vehicle models to accommodate medium-duty (vocational, class 4–6) and heavy-duty (line-haul, class 8) vehicle platforms in addition to the existing midsize passenger car option. This will also include the modification of the Framework Model test cases to include up to three additional cases based on representative medium- and heavy-duty drive cycles (e.g., heavy-duty UDDS, HHDDT, HTUF-4, NY Comp. or CBD).	6/30/2020
FY20- Q4	Submit at least two of the following three journal articles: (1) New framework paper— demonstrate models by exercising them using available HyMARC material data, (2) paper related to the sensitivity analysis and develop hierarchy of parameters to adjust to assist material developers, and (3) paper on the tank mass and volume estimator (i.e., Tankinator).	9/30/2020

Any proposed future work is subject to change based on funding levels

Technology Transfer Activities – Updated HSECoE Model Website

HSECoE website: http://hsecoe.org/



Pacific Northwest



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Modeling Efforts

As part of the H-SE's modeling effort, it was found useful to develop simplified models that can packly estimate potimal loading and discharge kinetics, effective hydrogen capacilies, system dimensions, and heat removal requirements of vanous materials based hydrogen storage system designs. Parameters obtained from these models were then used as inputs into the detailed models to obtain an accurate assessment of system performance that includes more complete integration of the physical processes. In addition, to meet the obecrives of the Center, there was a need to guickly and efficiently evaluate various materials based storage systems and to compare their performance against DDE light duty vehicle targets. 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. As such a modeling "framework" that was used for system evaluation and comparison by the Center was developed. The framework was used to implement the integrated vehicle, the power plant, and the storage system models. This framework tool was used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent set of assumptions.

It was felt, by DDE, that these models and the modeling harnework could provide benefit to research efforts outside of the HSECoE and therefore should be made available to university and laboratory researchers working in this area. Below are select models, including the center modeling framework, that are available for download and use by the broad research community. Model descriptions, a user's manual and presentations detailing the models validation are also available for download below. These models are open for use by material developers and storage system designers, but caution should be used when applying these models to materials and operating conditions that have not been validated. Please send any questions or comments to the technical assistance e-mail provided.

Cick here to view our current publications and presentations

Models

Hydrogen Vehicle Simulation Framework

The H2 Vehicle Simulation Framework is a MATLAB/Simulink tool for simulating a light duty vehicle powered by a PEM fuel cell, which in turn is fueled by a hydrogen storage system. The framework is designed so that the performance of different storage systems may be compared on a single vehicle, maintaining the vehicle and fuel cell system assumptions.

The Framework is composed of a vehicle module, a fuel cell module, and a hydrogen storage module. The figure below shows these components and the main responsibilities and interfaces.

The vehicle module computes demand for a given drive cycle. Power demand is based on acceleration, aerodynamic orag, rolling resistance and component efficiencies. The drive cycles are repeated until some failure condition is encountered. This could be that the hydrogen has been depleted, the flow rate is insufficient, or some components are undersized for the vehicle's demand

The fact cell block's responsibility is to translate power demand from the vehicle into hydrogen demant to the storage system. It also manages thermal balance and makes waste heat stream available for harvesting by the storage system. Note that this is not a fuel cell sizing tool. The performance curve is chosen to match DOE targets for efficiency (50% at rated power, 60% at 20% of rated power).

The hydrogen storage system responds to hydrogen flow demands from the fuel cell system it may also request auxiliary electrical powr from the vehicle if needed, such as for heating and powering balance of plant components.

Summary

Relevance	 Provide materials-based hydrogen storage researchers with models and materials requirements to assess their material's performance in an automotive application.
Approach	 Improve stand-alone model and framework utility by bridging the gap between the information generated by the materials researcher and the DOE Technical Targets.
Technical Accomplishments and Progress	 Stand-alone tools have been developed in Microsoft Excel as a replacement for MATLAB and placed on the modeling website. These models allow easier use by the hydrogen storage community. Stand-alone tools and framework have been used to evaluate materials for HyMARC and help better understand the benefits (or not) of new materials.
Collaborations	 Project team includes NREL, SRNL, and PNNL. Consultants from industry participate in team meetings and provide input. Material developers from HyMARC and academia provide new material properties.
Proposed Future Research	 Expand the use of models by demonstrating their utility with other storage materials and vehicle class options.

Remaining Challenges and Barriers

- Increase the use of the models by material developers
 - Expand the researcher base that uses the models
 - Simplify the model use for nonmodelers
- Increase the use of the models by systems engineers
 - Potential expansion of the model capabilities to other vehicle classes and system platforms
- Demonstrate the models' utility to other researchers
 - Applying the models to their applications
- Find available data to validate the models
- Reverse engineering—using the models to better inform materials developers of what properties are most important

Publications and Presentations

Brooks, K., D. Tamburello, S. Sprik, M. Thornton. 2018. "Design Tool for Estimating Chemical Hydrogen Storage System Characteristics for Light-Duty Fuel Cell Vehicles." *International Journal of Hydrogen Energy* 43, no. 18 (May): 8846–8858.

Brooks, K., D. Tamburello, S. Sprik, M. Thornton. 2020. "Design Tool for Estimating Metal Hydride Storage System Characteristics for Light-Duty Fuel Cell Vehicles." *International Journal of Hydrogen Energy*, forthcoming (submitted January 2020).

Tamburello, D. 2018. "Cryo-Adsorbent Hydrogen Storage Systems for Fuel Cell Vehicles" (presented at the 70th Southeastern Regional Meeting of the American Chemical Society, Augusta, GA, November 2, 2018).

Tamburello, D., B. Hardy, M. Sulic, M. Kesterson, C. Corgnale, D. Anton. 2018. "Compact Cryo-Adsorbent Hydrogen Storage Systems for Fuel Cell Vehicles" (POWER2018-7474, Proceedings of the ASME Power and Energy Conference, Buena Vista, FL, June 24, 2018).

Responses to Previous Year Reviewers' Comments

• This project was not reviewed last year

NREL/PR-5400-76602

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 the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Fuel Cell Technologies Office. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.