Hydrogen Storage System Modeling:

Public Access, Maintenance, and Enhancements

Pacific Northwest NATIONAL LABORATORY

Team: Matthew Thornton (PI), Sam Sprik, Kriston Brooks, and David Tamburello

NREL NATIONAL RENEWABLE ENERGY LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

DOE Hydrogen and Fuel Cells Program

2020 Annual Merit Review and Peer Evaluation Meeting

May 20, 2020 **Project ID # ST008**

Hydrogen Storage Engineering CENTER OF EXCELLENCE

Overview

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

NREL – National Renewable Energy Laboratory
SRNL – Savannah River National Laboratory
Pacific Northwest National Laboratory

*Project continuation and direction determined annually by DOE.

Relevance

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.
- **Ultimate Goal**: **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

Approach – Improving Model Utilities for Materials Researchers

Materials Research

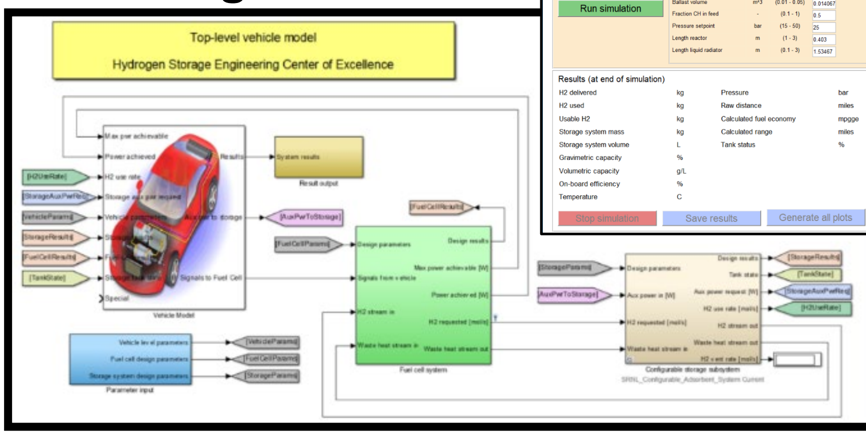
H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

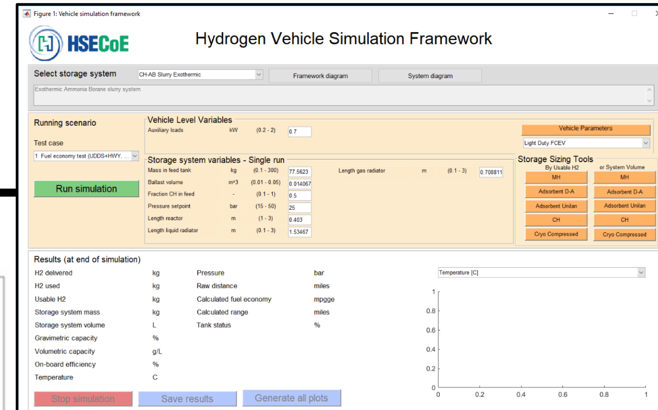
Isotherm Fitting Tool

DA Parameters

Available at
www.hsecoe.org

Modeling Framework





Stand-Alone System Design Tools

Component and System Mass and Volume

Stand-Alone Values

Estimated Gravimetric and Volumetric Capacity

DOE Technical Targets

Gravimetric and Volumetric Capacity
Durability and Operability
- Operating Temperature and Pressure
- Onboard Efficiency

Charging/Discharging Rates
- Start-up
- Refueling

Modeling Tools Available or In Progress

Framework Model with:

• Physical Storage	UTRC/NREL	Estimate performance of light-duty vehicles with four drive cycles for each storage system
• Compressed/Cryo-Compressed H_2	SRNL/NREL	
• Chemical Hydrogen (CH)	PNNL/NREL	
• Adsorbent (AD)	SRNL/NREL	
• Metal Hydride (MH)	PNNL/NREL	

Stand-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	

Additional Tools/Models:

• MH Acceptability Envelope (MHAE)	SRNL
• Tank Volume/Cost Model	PNNL
• AD Isotherm Fitting Tool	SRNL

Finite Element Models:

• Metal Hydride (MH) Finite Element (MHFE)	SRNL	Tank heat and mass transfer models
• Adsorbent (AD) – HexCell and MATI	SRNL	

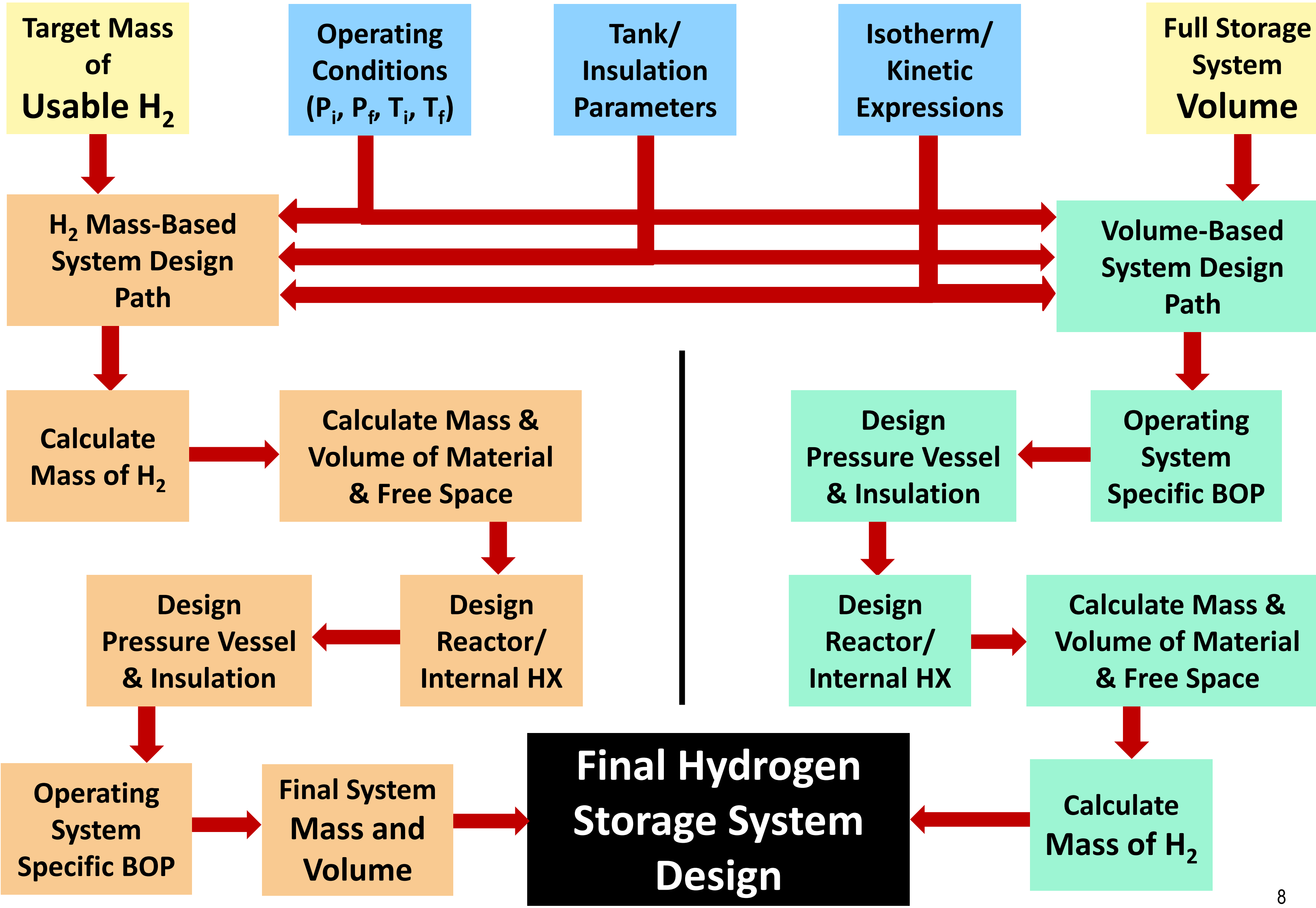
UTRC: United Technologies Research Center

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-H_2-mass-based and full storage-system-volume-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 material-specific 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 Hydride 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

Excel-Based Chemical Hydrogen Storage Stand-Alone Tool

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

- **Usable-H_2-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**

Input

ExoEndo	1	--	Exothermic/Endotheric Flag (Exo = 1, Endo = 0)
Kinetic_Model	1	--	Kinetic Model Flag (Avrami Kinetics = 1, nth Order Kinetics = 2)
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)
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
E1	29900	J/mol H2	Activation Energy for Rxn 1
n1	3.1	--	Exponent for Avrami or Reaction Order for Rxn 1
DH_rxn_2	0	J/mol H2	Reaction Enthalpy Rxn 2 (negative=exothermic)
Beta2	0	mol H2/mol CH	Molar Ratio H2 maximum for CH material Rxn 2
A2	0	sec-1	Pre-exponential factor for Rxn 2
E2	0	J/mol H2	Activation Energy for Rxn 2
n2	1	--	Exponent for Avrami or Reaction Order for Rxn 2
x_inert	0.5	--	Weight fraction inert with CHS Material to Slurry
Cp_CH	2694	J/kg/K	Heat Capacity CHS Material
Cp_i	1846	J/kg/K	Heat Capacity inert slurrying agent
Cp_p	774	J/kg/K	Heat Capacity CHS Material Product
rho_CH	780	kg/m3	Density CHS Material
rho_i	1000	kg/m3	Density inert slurrying agent
rho_P	1640	kg/m3	Density CHS Material Product
ppm_imp	500	ppm	Concentration of impurity 1
A_imp	0.1	g impurity/g adsorbent	Adsorbent maximum loading impurity 1
MW_imp	17	g/mol	molecular weight impurity 1
ppm_imp2	2000	ppm	Concentration of impurity 2
A_imp2	0.35	g impurity/g adsorbent	Adsorbent maximum loading impurity 2
MW_imp2	80.5	g/mol	molecular weight impurity 2
Usable H2	0	kg	Mass of usable hydrogen required
Total Volume	0.144	m3	Total system volume required
Max Power	25	kW	Maximum Hydrogen Storage H2 Production Required
Ave Power	15	kW	Average Hydrogen Storage H2 Production Required
Pset	25		Ballast Tank Pressure Initial Condition and Setpoint
Q_heater	8000		Reactor heater per length
Tmax	400	°C	Maximum acceptable reactor temperature
vol_flag	1		Flag for either volume or usable H2 constrained design: 1 = volume, 0 = usable H2

Run

Flag for volume- or usable-H_2-constrained design

Output

Name	Value	Units	Description
System Mass and Volume	-----------	-------------	---
TotalMass	131.7338405	kg	Total Estimated System Mass
TotalVolume	144	L	Total Estimated System Volume
Usable H2	5.63829624	kg	Estimated Usable H2 for System
DOE_Mass_Target	0.042800667	kg H2/kg sys	DOE Gravimetric Target 2020
DOE_Vol_Target	0.039154835	kg H2/L sys	DOE Volumetric Target 2020
Design Parameters	-----------	-------------	---
ReactorLength	0.403	m	Reactor Length
Vballast	0.014067745	m3	Ballast Tank Volume
MFeed	78.09274571	kg	Mass Chemical Hydride Required
LiqRadLength	1.534666617	m	Slurry Radiator Length
GasRadLength	0.708811328	m	Hydrogen Gas Radiator Length
RecupLength	0	m	Recuperator Length (if endothermic)
Startup Time	75.96206604	sec	Time to Reach 30% Conversion
Target Temperature	148.9828824	°C	Temperature to Reach 30% Conversion
Maximum Temperature	246.3299437	°C	Maximum Reactor Temperature
End of Parameters	-----------	-------------	---

Excel-Based Metal Hydride Stand-Alone Design Tools

Hydrogen Mass-Based Metal Hydride Storage Design Tool Input Sheet

Name	Value	Units	Description
		Material Properties	
f_H2	0.1	decimal fraction	Hydride Carrying capacity of metal hydride
f_inert	0	decimal fraction	Fraction of inert in metal hydride bed (Enter 0 if f_H2 accour
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 rho_cry = rho_bed)
rho_inert	0	kg/m^3	Density of inert material in hydride bed (Enter 0 if rho_cry = rho_bed)
dH_rxn1	37000	J/mol	Enthalpy per mole H2 rxn 1 (Endothermic +)
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 step rxn)
dS_rxn2	0	J/mol-K	Entropy per mole H2 rxn 2 (set to zero if single step rxn)
beta_rxn1	1	mol/mol	Moles H2 produced per mole feed, Reaction 1 (Enter 0 if no rxn 2)
beta_rxn2	0	mol/mol	Moles H2 produced per mole feed, Reaction 2 (Enter 0 if no rxn 2)
		System Parameters	
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
dT	45	K	acceptable hydride temperature rise during refueling
PH2hi	100	atm	Upper Hydrogen Operating Pressure
PH2lo	5	atm	Lower Hydrogen Operating Pressure
HemObl	1	option	Hemispherical endcap option
Type	2	option	Material Option 1 = 6061-T6 2 = 316 SS 3 = Composite Type III (AL liner) 4 = Composite Type IV (plastic liner)
L/d	4	decimal fraction	Desired **exterior** Ltank over dtank Enter Zero to Calculate
L_tank	0	m	Desired tank **exterior** length Enter 0 to calculate
D_tank	0	m	Desired tank **exterior** diameter Enter 0 to Calculat
dt	300	seconds	Target Refueling time (300 s = DOE 2020 target)
eff_comb	0.8	decimal fraction	Combustion Efficiency if required

Run

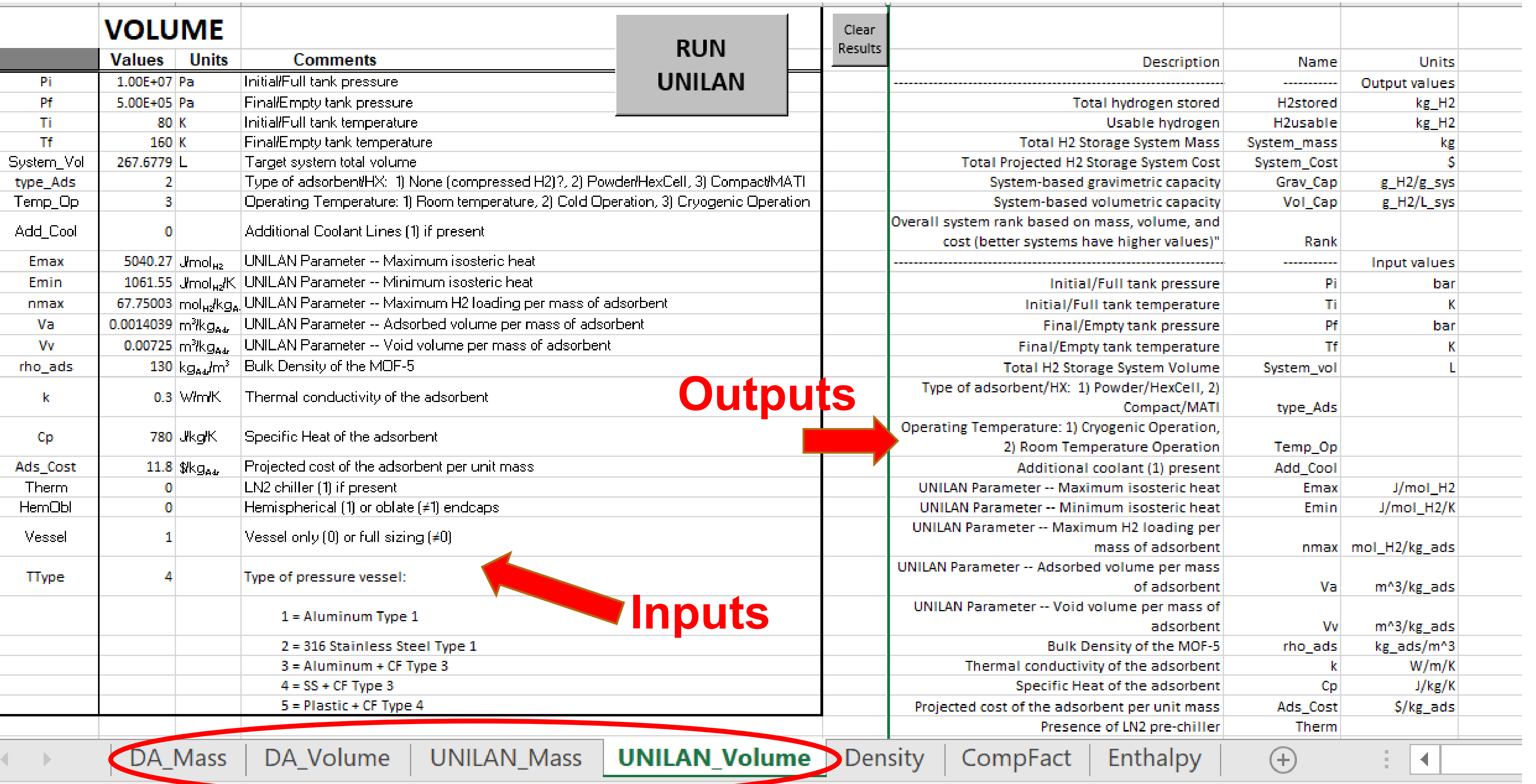
Input

Output

System mass (kg)	225.5653
System volume (m3)	0.112287
Combustor y>0/n=0	1
Mass H2 Burned (kg)	1.321687
Tank Outer Diameter (m)	0.32275
Tank Length (m)	1.249055
Number of coolant Tubes	101
Total Hydride Mass (kg)	69.21687
Tank Mass (kg)	117.0723
Maximum Temperature (°C)	153.45
Percentage of DOE 2025 Gravimetric Target (%)	45.13911
Percentage of DOE 2025 Volumetric Target (%)	124.6804

- **Separate models for mass-of-usable-H_2-constrained and system-volume-constrained design tools**
- **Models based on thermodynamics and heat transfer only; no kinetics or mass transfer included**

Excel-Based Cryo-Adsorbent Stand-Alone Design Tools



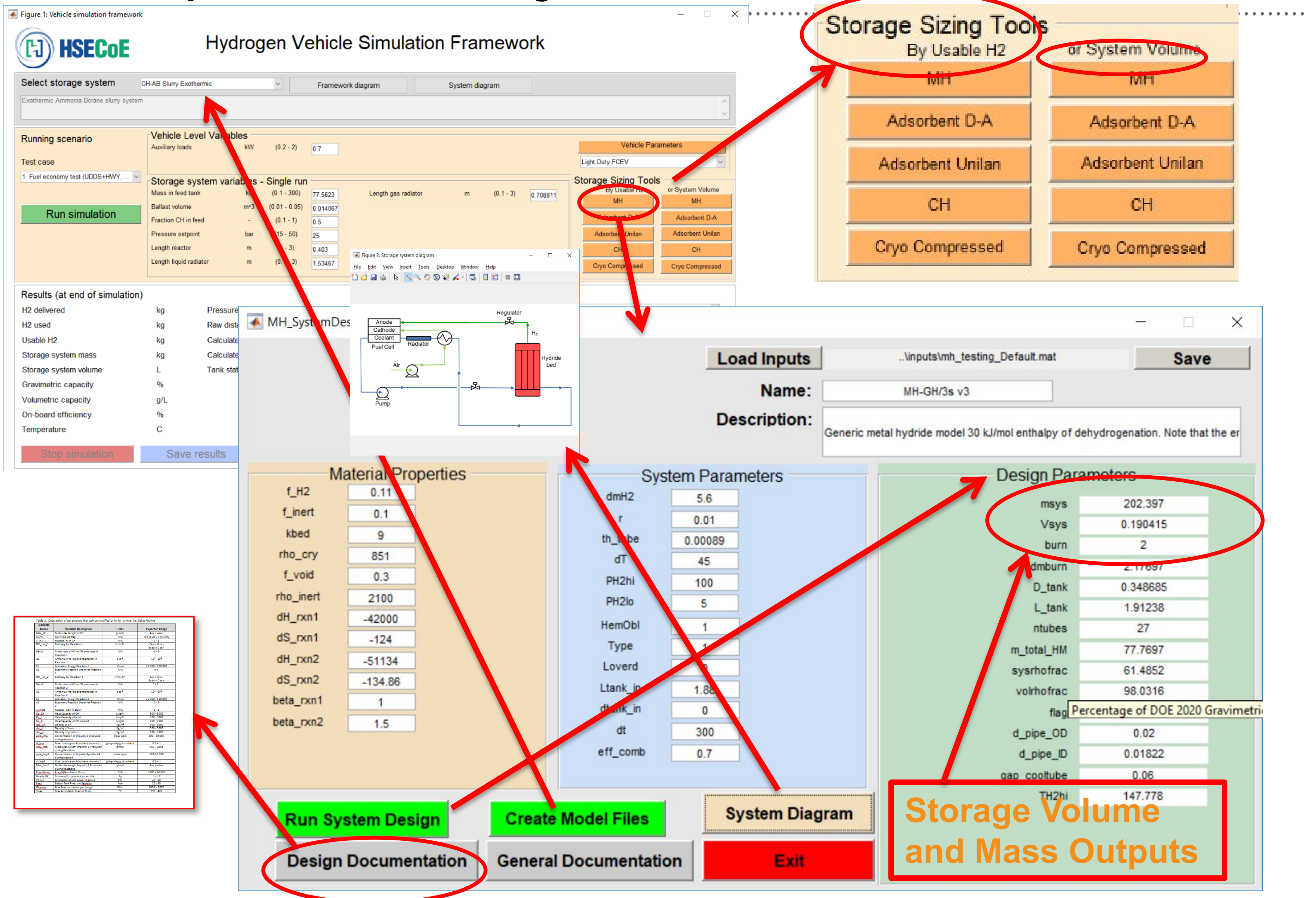
VOLUME

	Values	Units	Comments
Pi	1.00E+07	Pa	Initial/Full tank pressure
Pf	5.00E+05	Pa	Final/Empty tank pressure
Ti	80	K	Initial/Full tank temperature
Tf	160	K	Final/Empty tank temperature
System_Vol	267.6779	L	Target system total volume
type_Ads	2		Type of adsorbent/HX: 1) None (compressed H2)?, 2) Powder/HexCell, 3) Compact/MATI
Temp_Op	3		Operating Temperature: 1) Room temperature, 2) Cold Operation, 3) Cryogenic Operation
Add_Cool	0		Additional Coolant Lines (1) if present
Emax	5040.27	J/mol_{H2}	UNILAN Parameter -- Maximum isosteric heat
Emin	1061.55	$J/mol_{H2}/K$	UNILAN Parameter -- Minimum isosteric heat
nmax	67.75003	mol_{H2}/kg_{A}	UNILAN Parameter -- Maximum H2 loading per mass of adsorbent
Va	0.0014039	m^3/kg_{Ads}	UNILAN Parameter -- Adsorbed volume per mass of adsorbent
Vv	0.00725	m^3/kg_{Ads}	UNILAN Parameter -- Void volume per mass of adsorbent
rho_ads	130	kg_{Ads}/m^3	Bulk Density of the MOF-5
k	0.3	W/m/K	Thermal conductivity of the adsorbent
Cp	780	J/kg/K	Specific Heat of the adsorbent
Ads_Cost	11.8	$\$/kg_{Ads}$	Projected cost of the adsorbent per unit mass
Therm	0		LN2 chiller (1) if present
HemObl	0		Hemispherical (1) or oblate (≠1) endcaps
Vessel	1		Vessel only (0) or full sizing (≠0)
TType	4		Type of pressure vessel:
			1 = Aluminum Type 1
			2 = 316 Stainless Steel Type 1
			3 = Aluminum + CF Type 3
			4 = SS + CF Type 3
			5 = Plastic + CF Type 4

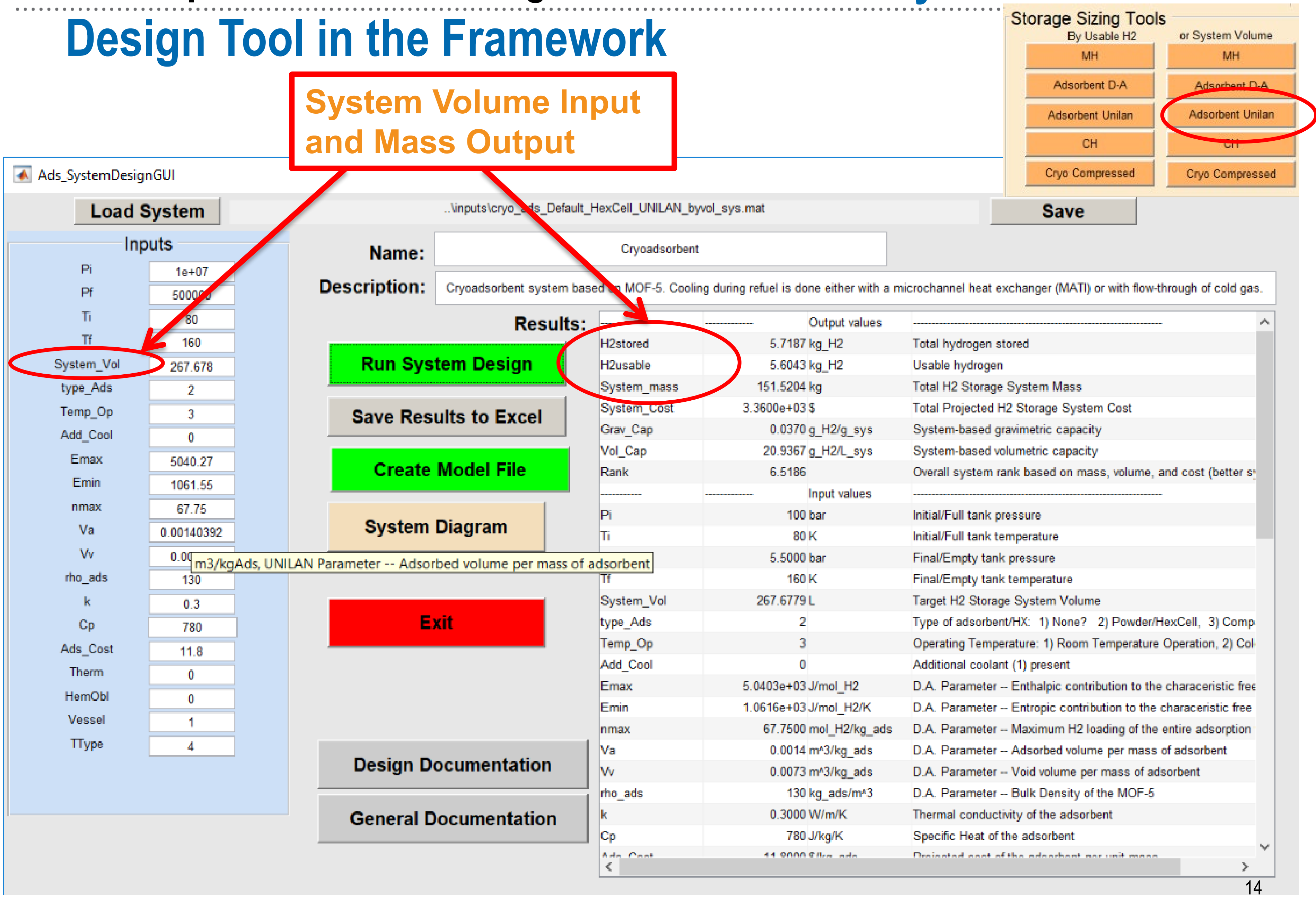
Description	Name	Units
--	-----------	Output values
Total hydrogen stored	H2stored	kg_H2
Usable hydrogen	H2usable	kg_H2
Total H2 Storage System Mass	System_mass	kg
Total Projected H2 Storage System Cost	System_Cost	$
System-based gravimetric capacity	Grav_Cap	g_H2/g_sys
System-based volumetric capacity	Vol_Cap	g_H2/L_sys
Overall system rank based on mass, volume, and cost (better systems have higher values)"	Rank	
--	-----------	Input values
Initial/Full tank pressure	Pi	bar
Initial/Full tank temperature	Ti	K
Final/Empty tank pressure	Pf	bar
Final/Empty tank temperature	Tf	K
Total H2 Storage System Volume	System_vol	L
Type of adsorbent/HX: 1) Powder/HexCell, 2) Compact/MATI	type_Ads	
Operating Temperature: 1) Cryogenic Operation, 2) Room Temperature Operation	Temp_Op	
Additional coolant (1) present	Add_Cool	
UNILAN Parameter -- Maximum isosteric heat	Emax	J/mol_H2
UNILAN Parameter -- Minimum isosteric heat	Emin	J/mol_H2/K
UNILAN Parameter -- Maximum H2 loading per mass of adsorbent	nmax	mol_H2/kg_ads
UNILAN Parameter -- Adsorbed volume per mass of adsorbent	Va	m^3/kg_ads
UNILAN Parameter -- Void volume per mass of adsorbent	Vv	m^3/kg_ads
Bulk Density of the MOF-5	rho_ads	kg_ads/m^3
Thermal conductivity of the adsorbent	k	W/m/K
Specific Heat of the adsorbent	Cp	J/kg/K
Projected cost of the adsorbent per unit mass	Ads_Cost	$/kg_ads
Presence of LN2 pre-chiller	Therm	

- **Separate tabs for Dubinin-Astakhov (D-A) adsorption theory isotherm and UNILAN isotherm**
- **Models can evaluate mass-of-usable-H_2-constrained and system-volume-constrained design tools**
- **Can evaluate materials at cryogenic, cold, and room-temperature conditions**

Accomplishments and Progress – Vehicle Framework GUI



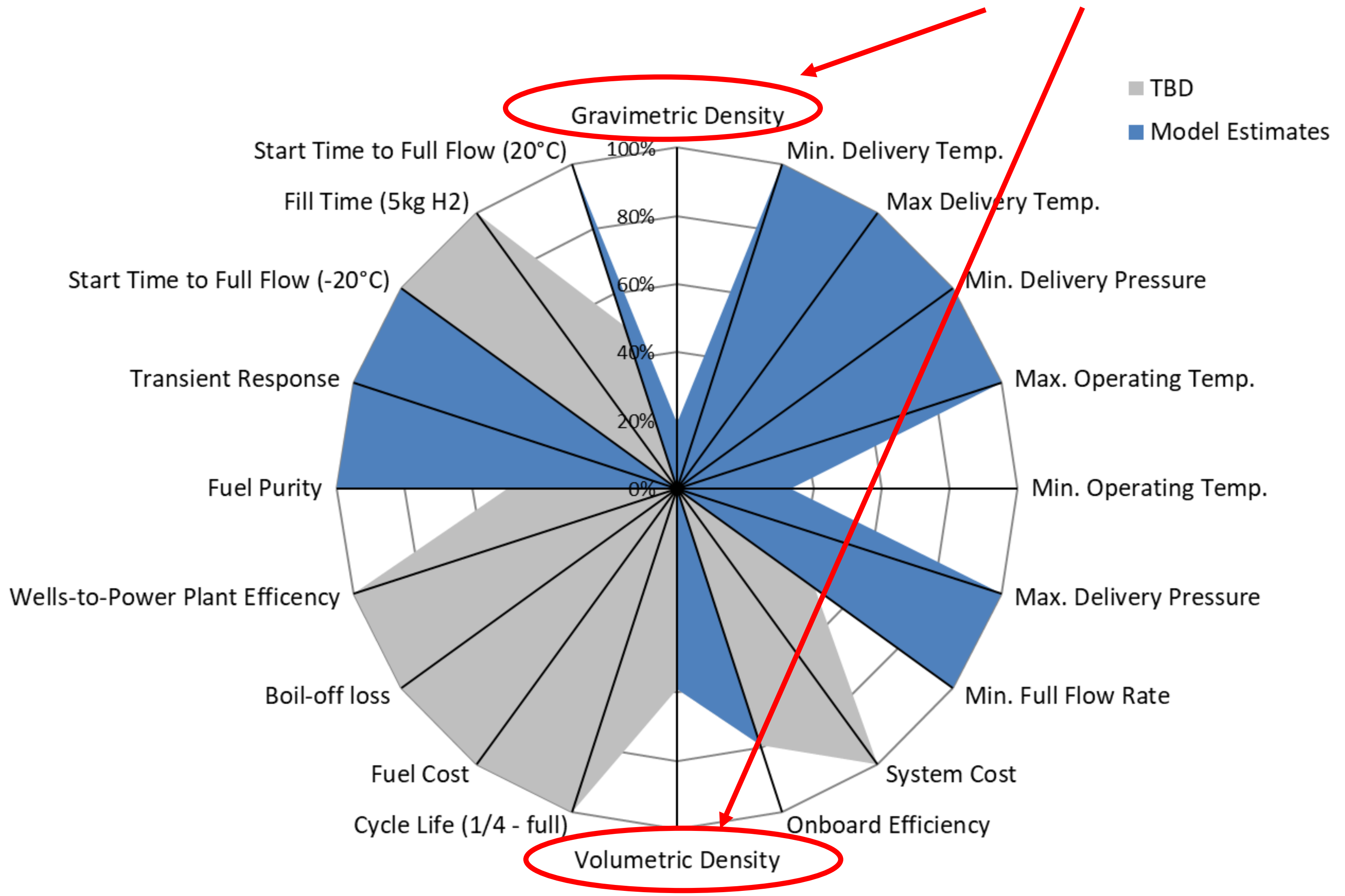
Accomplishments and Progress – Adsorbent System Design Tool in the Framework



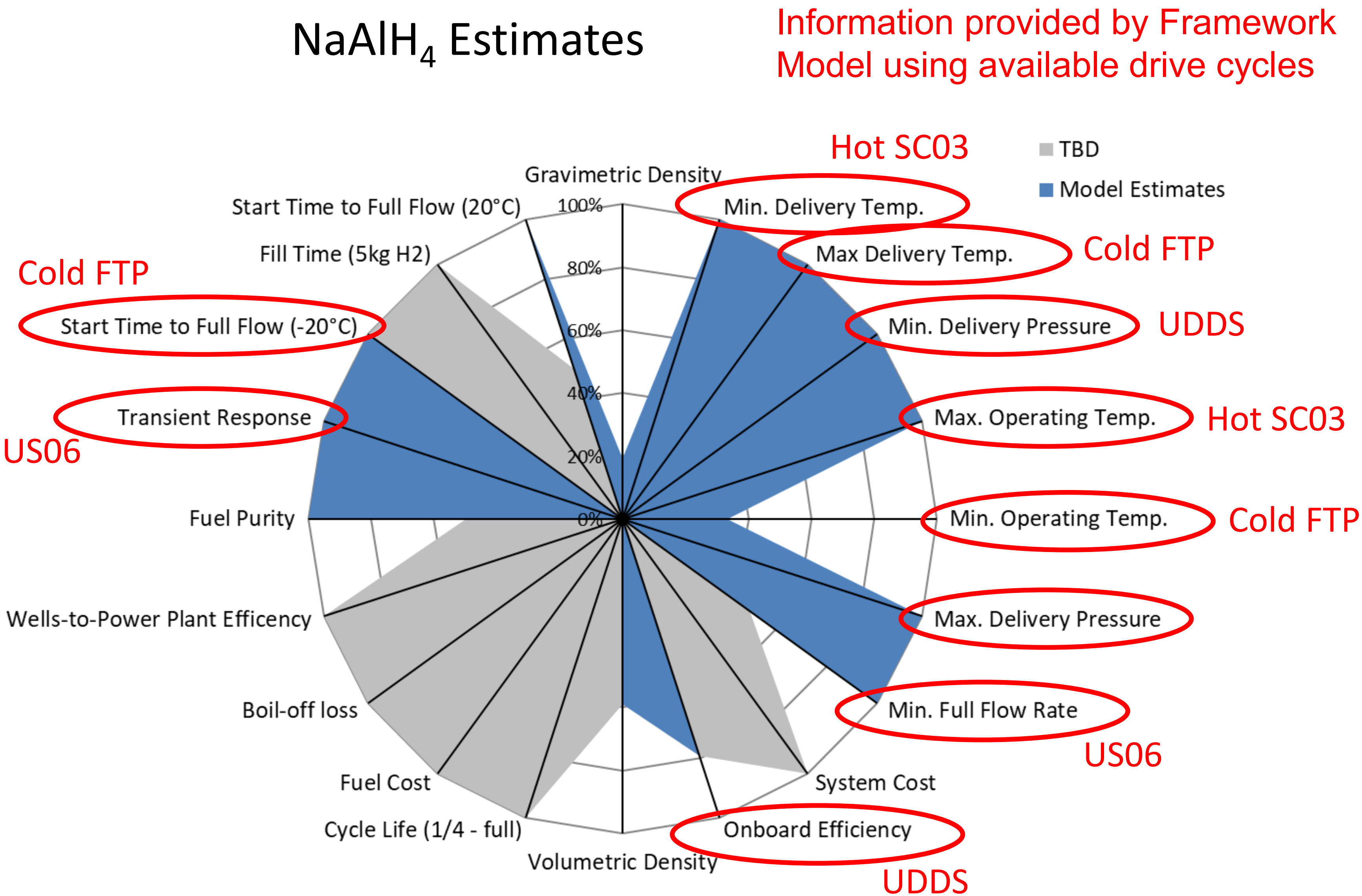
Accomplishments and Progress – Models Provide Input to Spider Charts

$NaAlH_4$ Estimates

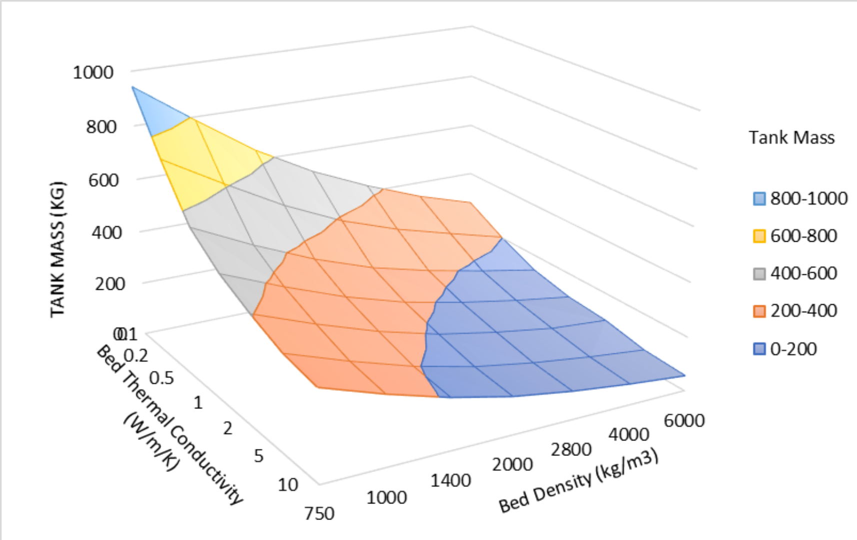
Information provided by design tool



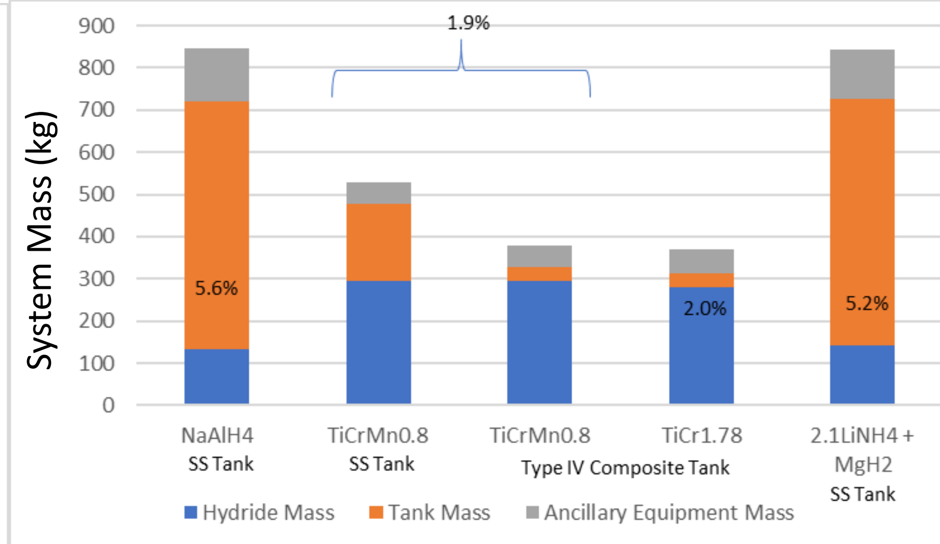
Accomplishments and Progress – Models Provide Input to Spider Charts



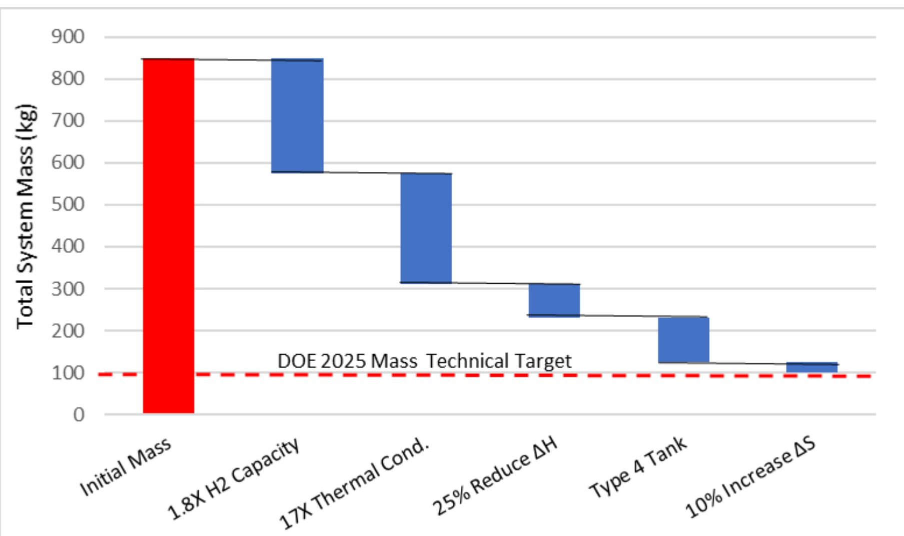
Accomplishments and Progress – Exercise Models



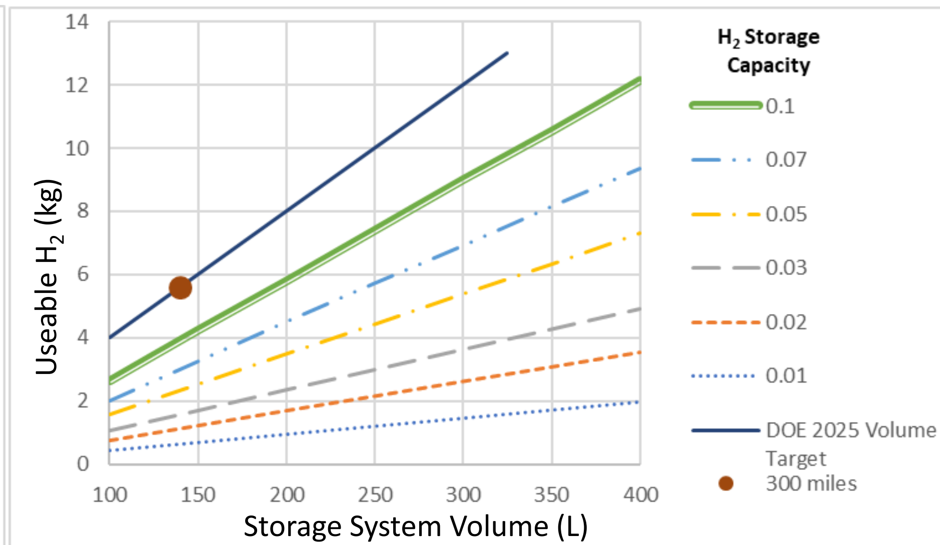
Thermal Conductivity vs. Bed Density on Tank Mass



Impact of Metal Hydrides on System Mass



Approach to Achieving DOE Gravimetric Technical Target



Relationship between Usable H_2 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	SysMass	SysVol	Temp	TankMass	HydMass	HydBurn	G-Target	V-Target
ENG Ti-doped $NaAlH_4$	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%
Ti-doped $LiBH_4$	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_3N	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-$LiBH_4$@C	0.057	7.06	550	57900	106	904	439	581	694	148	2.86	11.3%	31.9%
6nm-Li_3N@C	0.061	8.32	740	42100	114	507	262	283	337	122	1.84	20.1%	53.4%
KH-6nm-Li_3N@C	0.064	9.61	760	41700	117	466	241	256	304	116	1.82	21.9%	58.1%

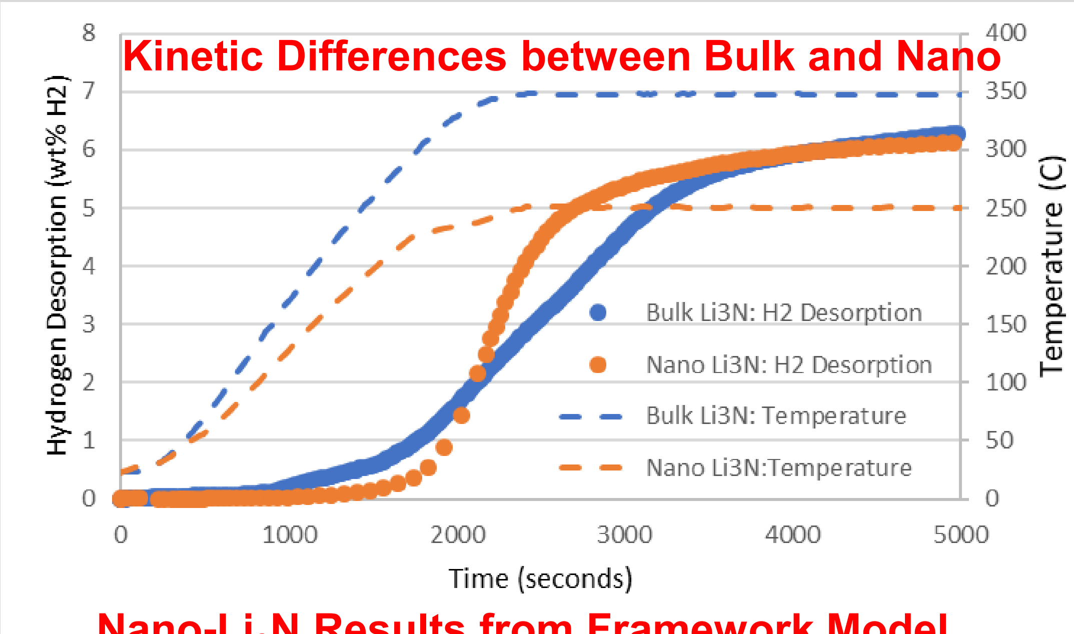
Bulk Materials   Nano Materials

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*

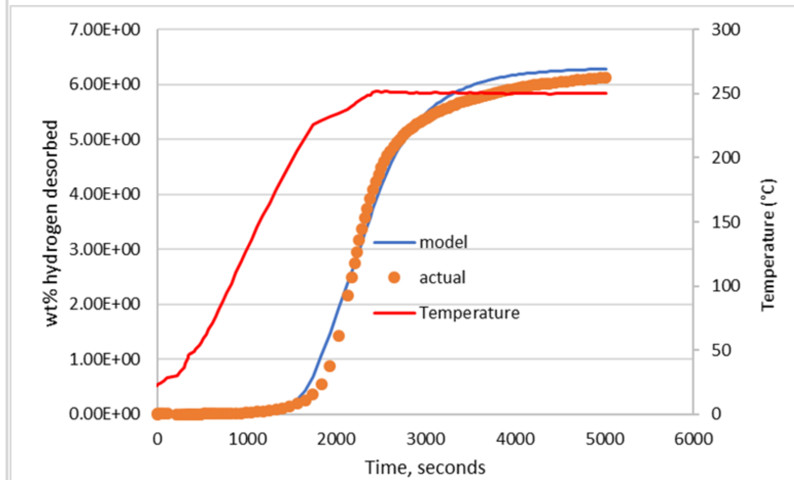
Accomplishments and Progress – Metal Hydride Materials Evaluation

Framework Model Compares Nanoscaled vs. Bulk Materials

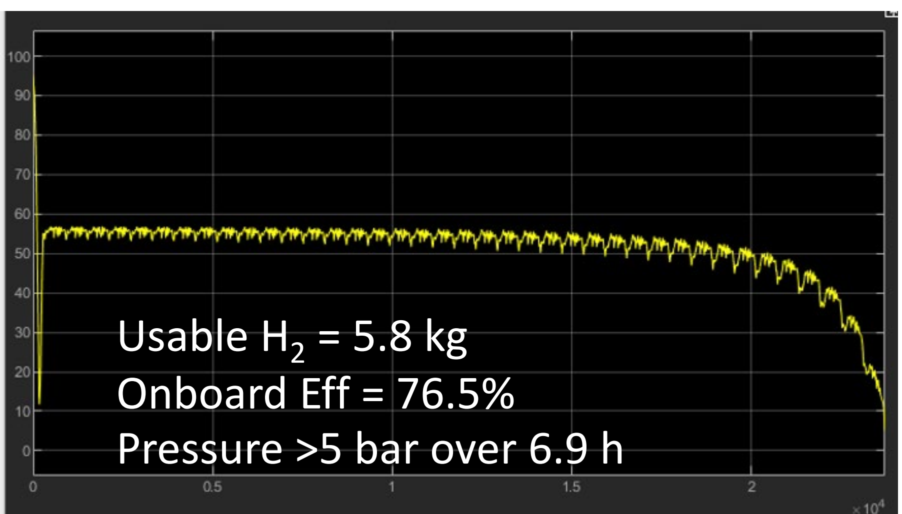


Fit Data with First Order Reaction

$$r = -\left(161{,}154e^{-\frac{79677}{RT}}\right) C_{Li3N}$$



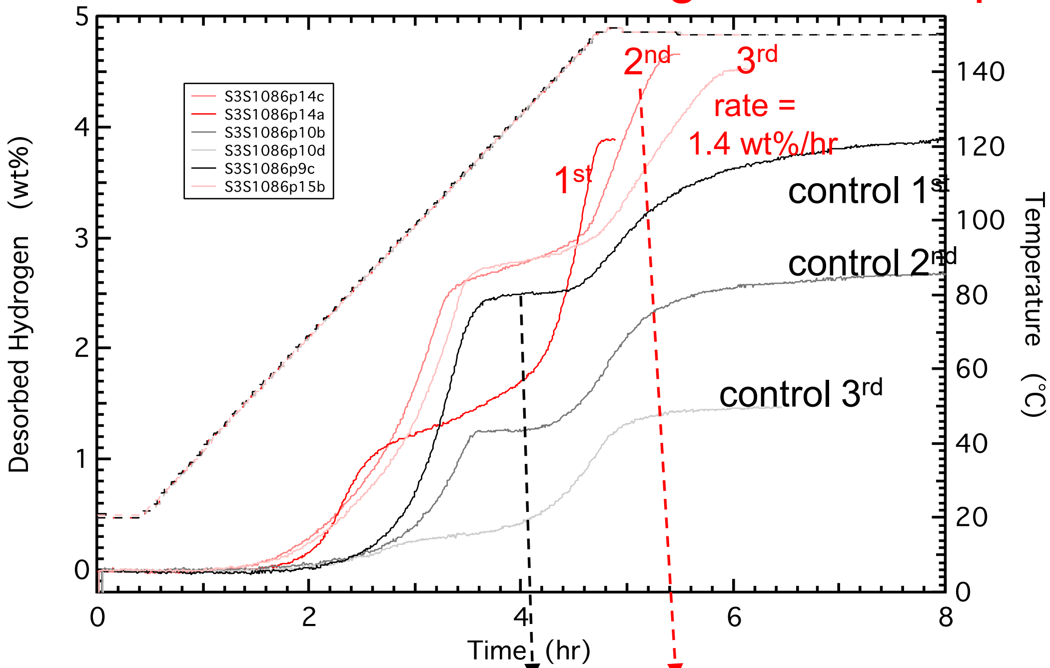
Nano-Li_3N Results from Framework Model



Learning: Nanoscaled Li_3N has fast enough kinetics and low enough temperatures to allow all drive cycles to be met; bulk Li_3N does not

- *Bulk Li_3N reaction does not initiate for any of the drive cycles*

MH Stand-Alone Design Tool Compares Two Forms of $NaAlH_4$



- HRL is evaluating $NaAlH_4$ milled with $0.03TiCl_3$ mixed 50:50 wt % with diglyme.
- This mixture has faster kinetics and reaches complete conversion sooner than the control without diglyme.

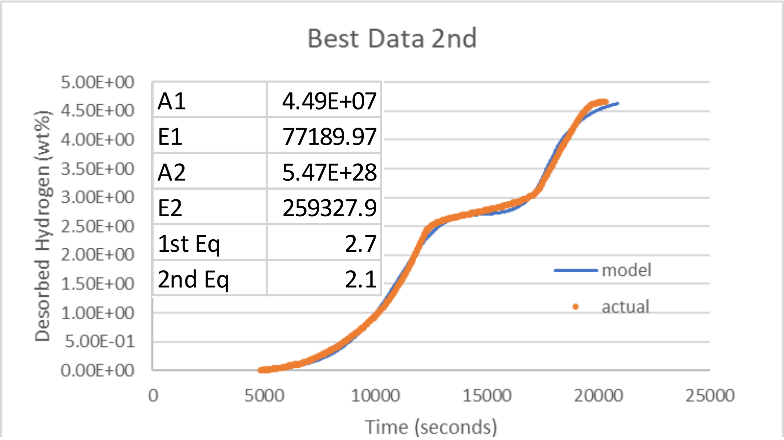
	Control	Best 2nd	Best 2nd with higher k
Useable Hydrogen Capacity	0.04	0.048	0.048
Inert Fraction	0	0.2	0.2
Bed Thermal Conductivity (W/m/K)	1	1	2
System mass (kg)	678	680	622
System volume (m3)	0.315	0.317	0.290
Mass H2 Burned (kg)	1.63	1.66	1.66
Tank Outer Diameter (m)	0.475	0.476	0.461
Tank Length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

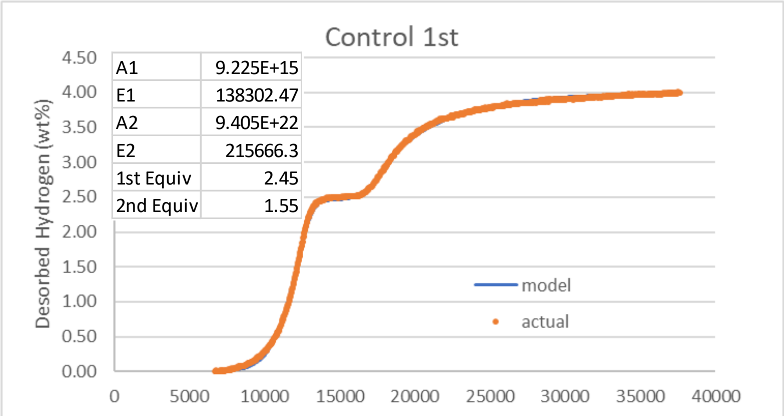
2nd: Assuming 20% diglyme and the higher usable H_2 capacity result in nearly the same tank size as Control 1st

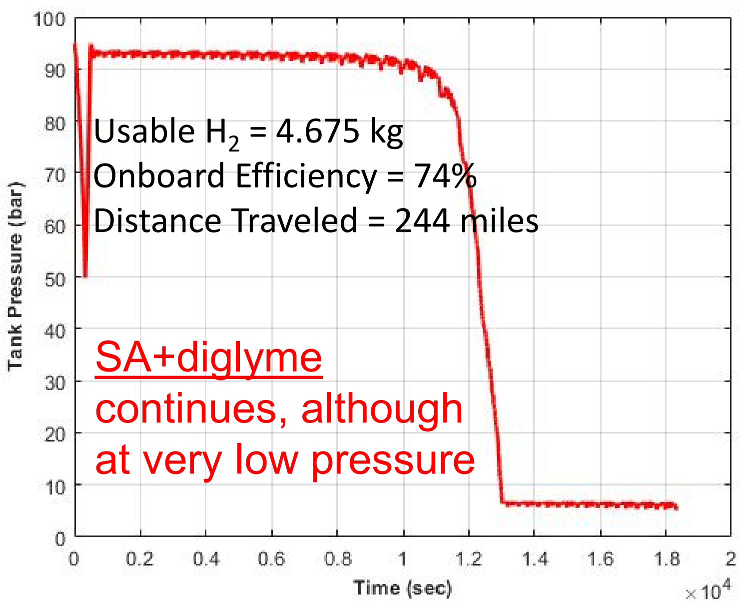
An assumed doubling of thermal conductivity reduces system mass and volume by 8.5%

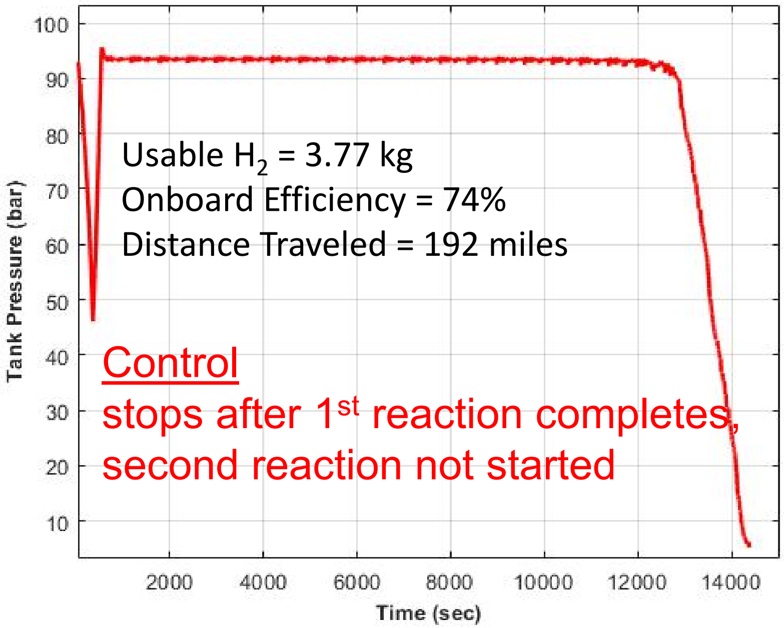
Accomplishments and Progress – Metal Hydride Materials Evaluation

Framework Compares Two Forms of $NaAlH_4$, Maximum T = 160°C



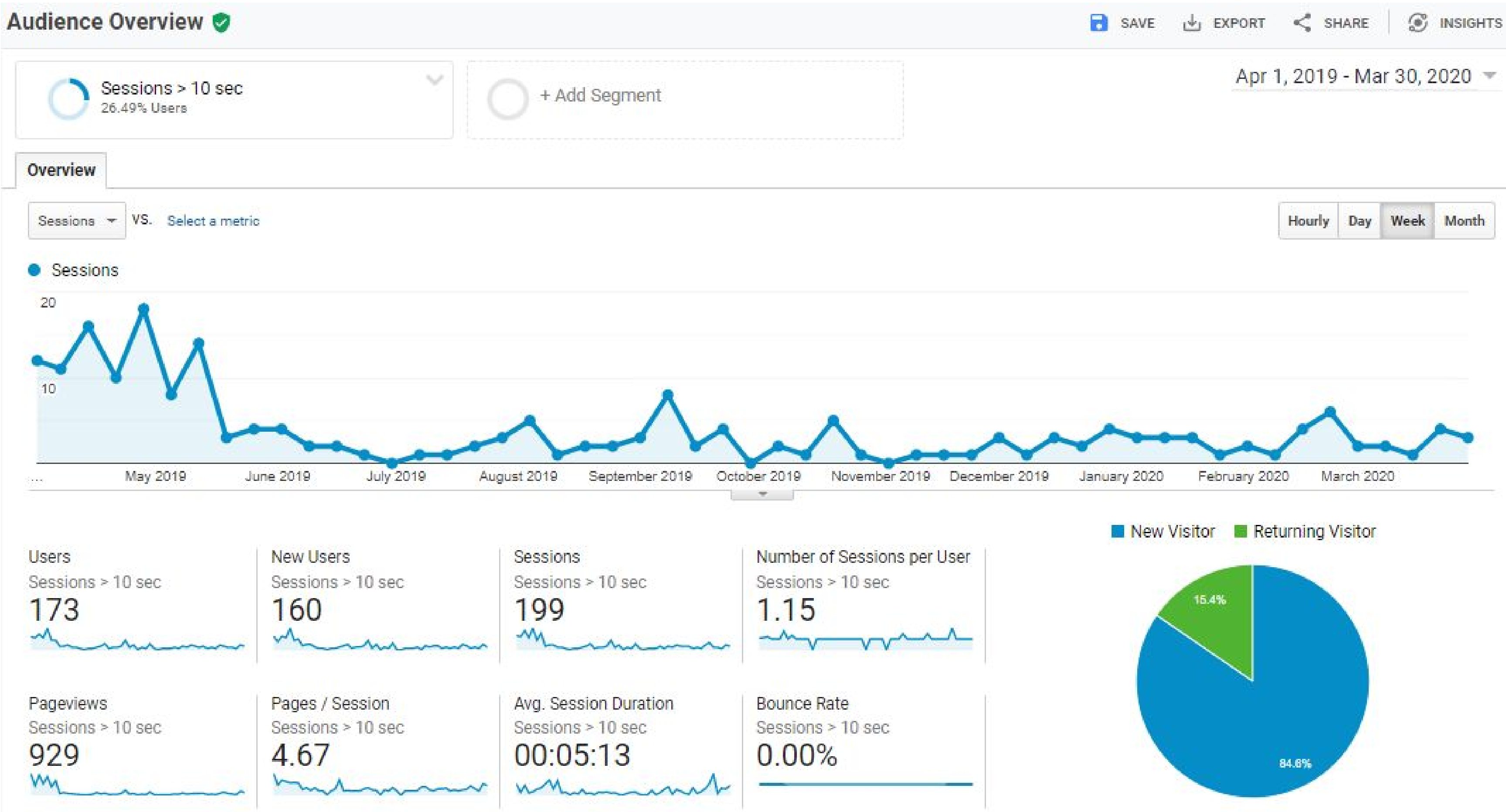






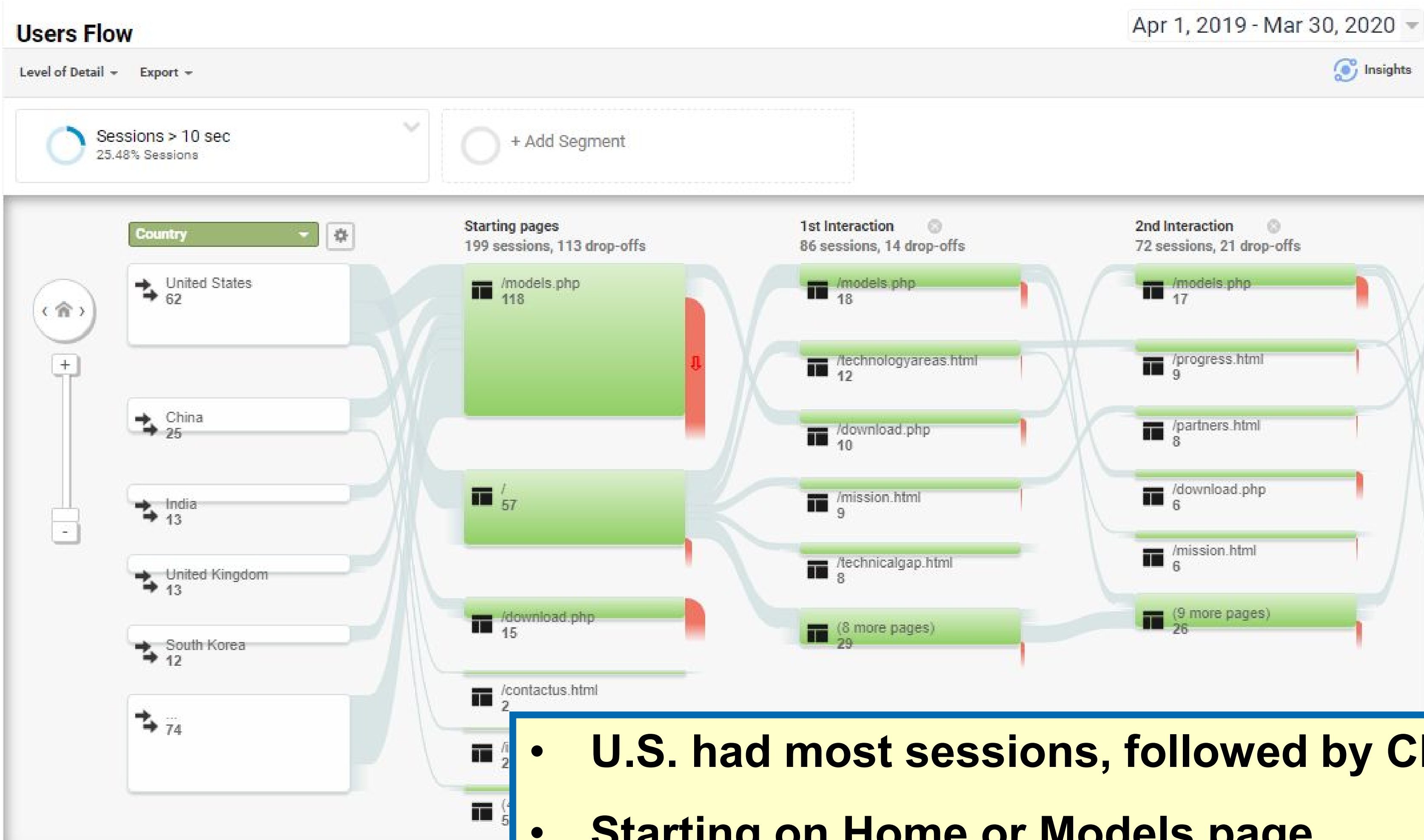
Enhanced material decreases the maximum possible operating temperature with the drive cycles by 5°–10°C

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



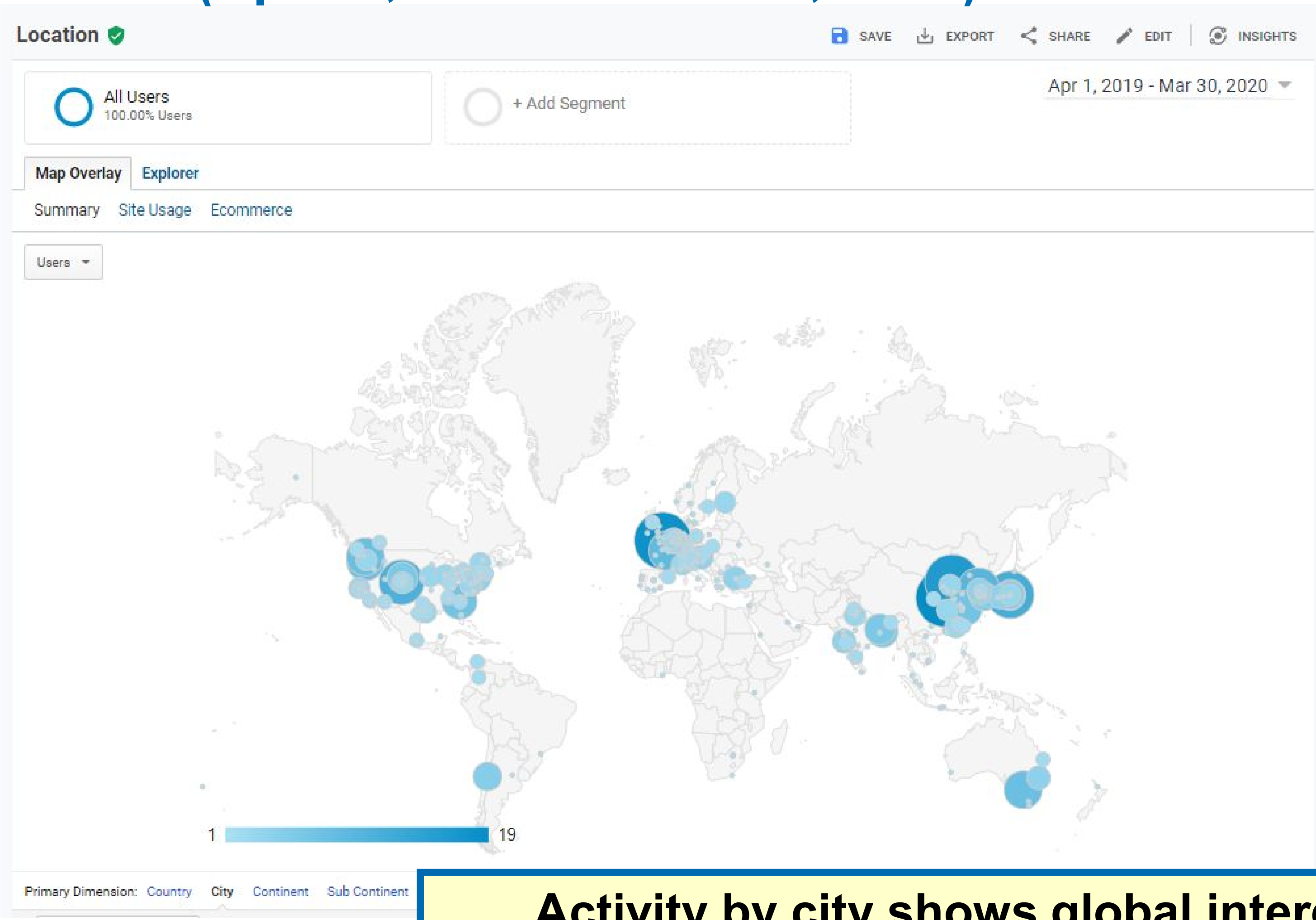
Activity almost every week; 85% of sessions were by new visitors

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



- **U.S. had most sessions, followed by China**
- **Starting on Home or Models page**
- **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

Organization	Relationship	Type	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

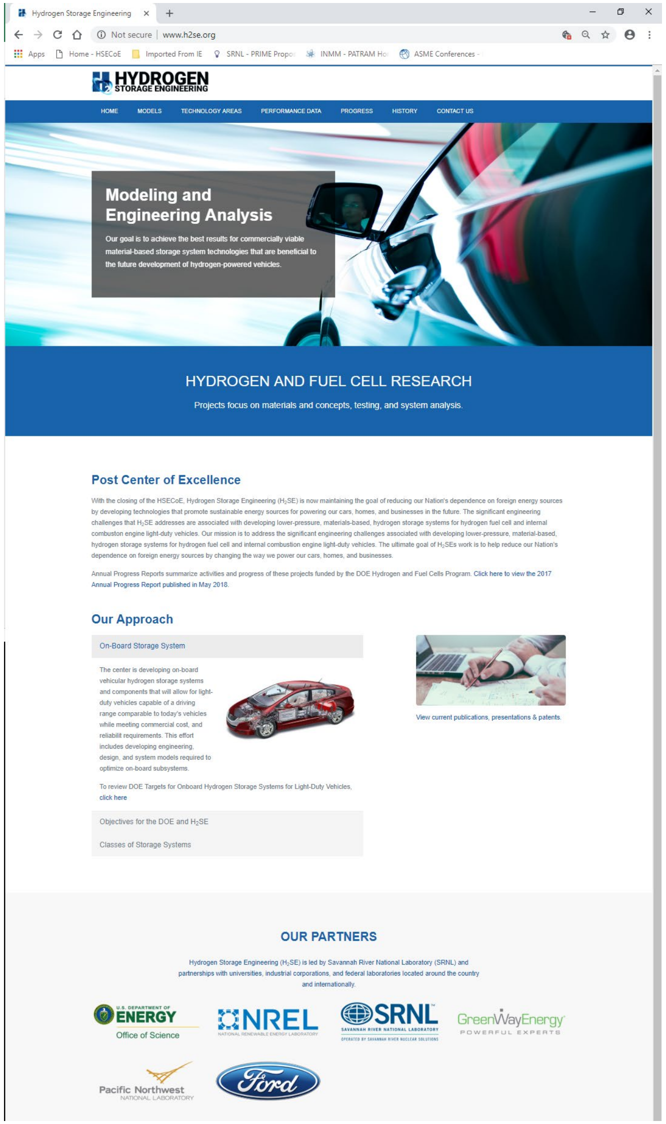
Proposed Future Work – FY20 Milestones and Next Steps

Deliverable		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/



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*