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

P.I. – Matthew Thornton, NREL

Presenter – Kriston Brooks, PNNL

Additional Contributors:

-- David Tamburello, SRNL

-- Sam Sprik, NREL

SRNL
SAVANNAH RIVER NATIONAL LABORATORY

NREL
National Renewable Energy Laboratory

Pacific Northwest
NATIONAL LABORATORY

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Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Project ID# ST008

PNNL-SA-125680

Overview

Timeline

- Start: October 1, 2015
- End: September 30, 2018
- 50% Complete (as of 4/1/17)
  - $461,839 Spent (as of 4/1/17)

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: $1,100,000
  - FY16 Funding: $336,000
  - FY17 Funding: $389,000
  - FY18 Funding: $375,000

Partners

NREL NATIONAL RENEWABLE ENERGY LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

HSECoE

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, and enhance 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 modeling tools that will be used by researchers to evaluate the performance their new materials in engineered systems relative to the DOE Technical Targets**.

Barriers Addressed with Models

Barrier	Model Addressing Barrier
A. System Weight and Volume	System Estimator
B. System Cost	Tank Volume/Cost Model
C. Efficiency	Framework Model - On-Board 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

Challenge to Materials Researchers: Evaluating Material Relative to DOE Technical Targets

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

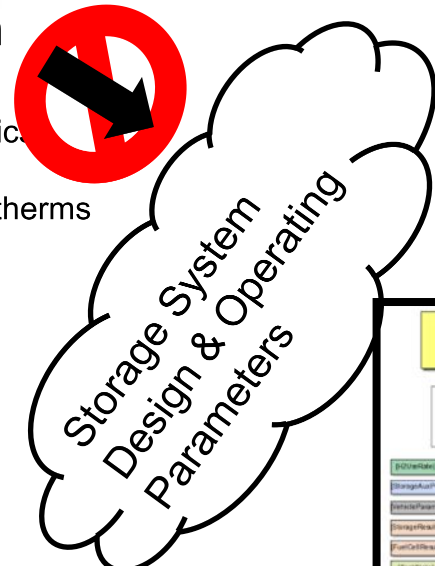
DOE Technical Targets

- Gravimetric & Volumetric Capacity
- Durability & Operability
  - Operating Temperature and Pressure
  - On-Board Efficiency
- Charging/Discharging Rates
  - Startup
  - Refueling

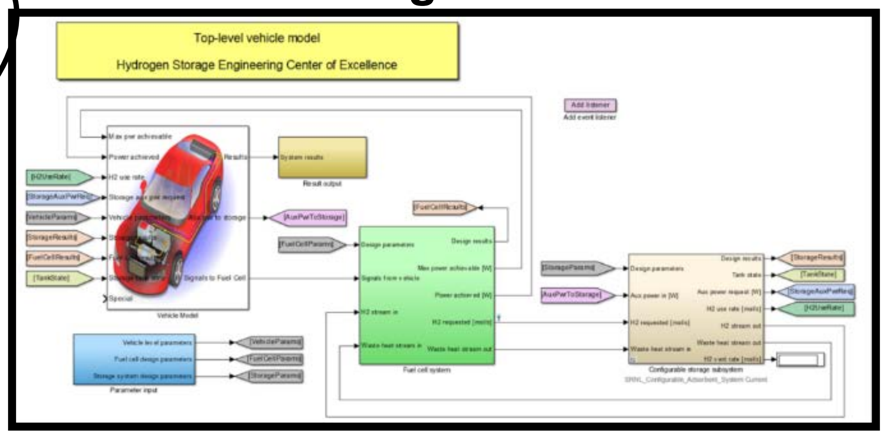
Original Framework Does Not Provide Entire Solution

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms



Modeling Framework



DOE Technical Targets

Gravimetric & Volumetric Capacity
Durability & Operability
- Operating Temperature and Pressure
- On-Board Efficiency

Charging/Discharging Rates
- Startup
- Refueling

HSECoE

Focus: Improve Framework Utility for Materials Researchers

Materials Research

H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

New Isotherm Fitting Tool

DA Parameters

Improved Website

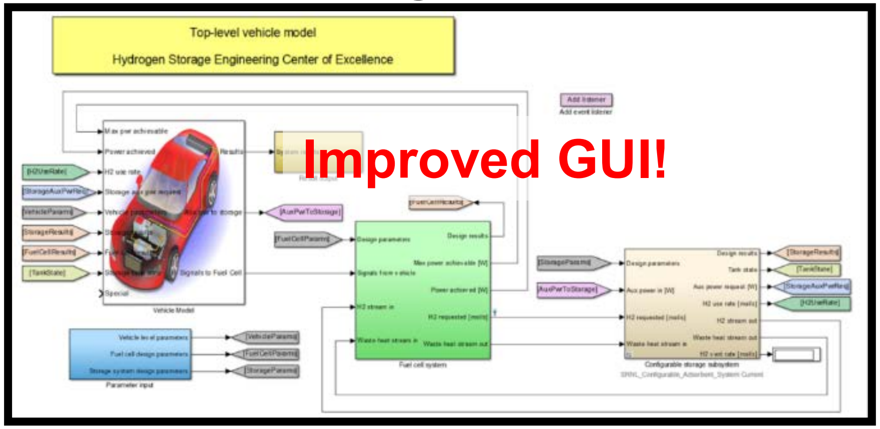
New System Estimator Tool

Component and System Mass & Volume

Stand-Alone Values

Estimated Gravimetric & Volumetric Capacity

Modeling Framework



DOE Technical Targets

Gravimetric & Volumetric Capacity
Durability & Operability
- Operating Temperature and Pressure
- On-Board Efficiency

Charging/Discharging Rates
- Startup
- Refueling

Approach

Modeling Tools Available

MH Acceptability Envelope	**SRNL**	Evaluate Material Properties
Tank Volume/Cost Model	**PNNL**	Estimate tank material, design and cost
Finite Element Models		
Metal Hydride (MH)	**SRNL**	Tank Heat and Mass Transfer Models
Adsorbent (AD)	**SRNL**	
Framework Model with		
Physical Storage	**UTRC/NREL**	Estimate light-duty vehicle performance for each storage system with four drive cycles
Metal Hydride (MH)	**UTRC/SRNL/NREL**	
Chemical Hydride (CH)	**PNNL/NREL**	
Adsorbent (AD)	**SRNL/NREL**	
AD/CH System Estimator	**PNNL/SRNL**	**This Year’s Work**
AD Isotherm Fitting Tool	**SRNL**	**This Year’s Work**

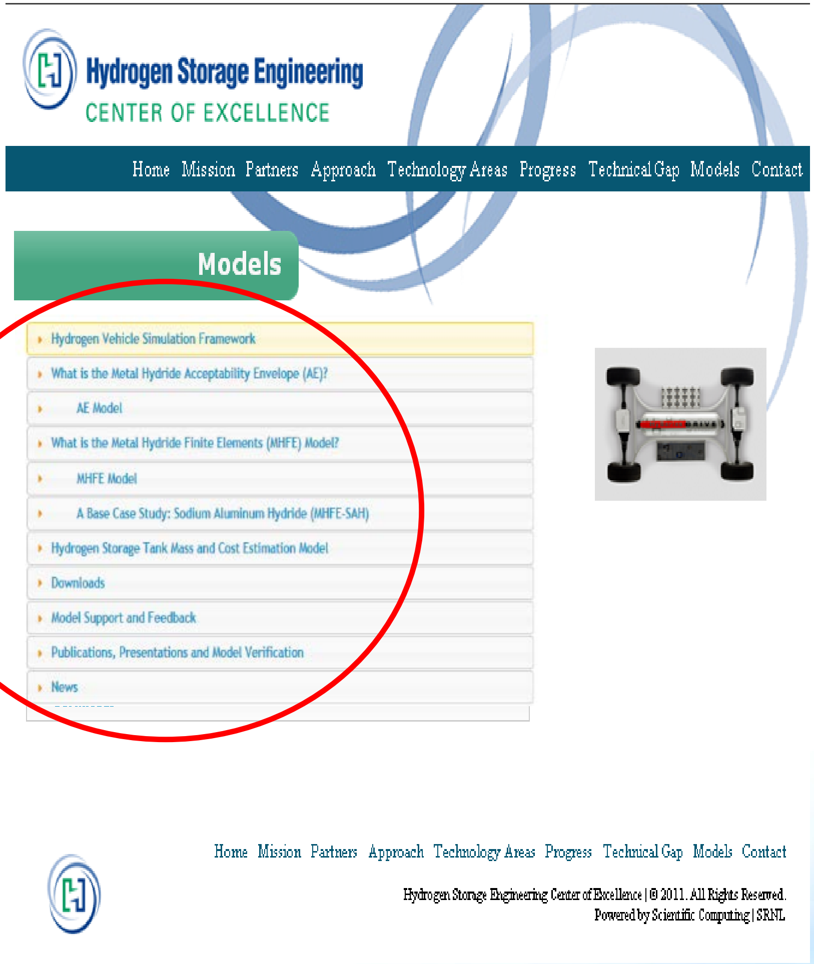
HSECoE

Improved Website Access and Support

HSECoE website:
http://hsecoe.org/

Model Support and Feedback:
HSECoE@nrel.gov

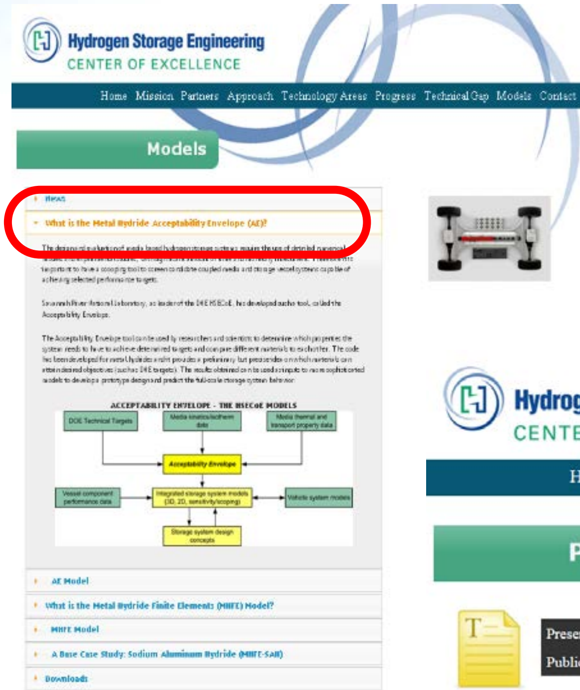
Improved model access/description



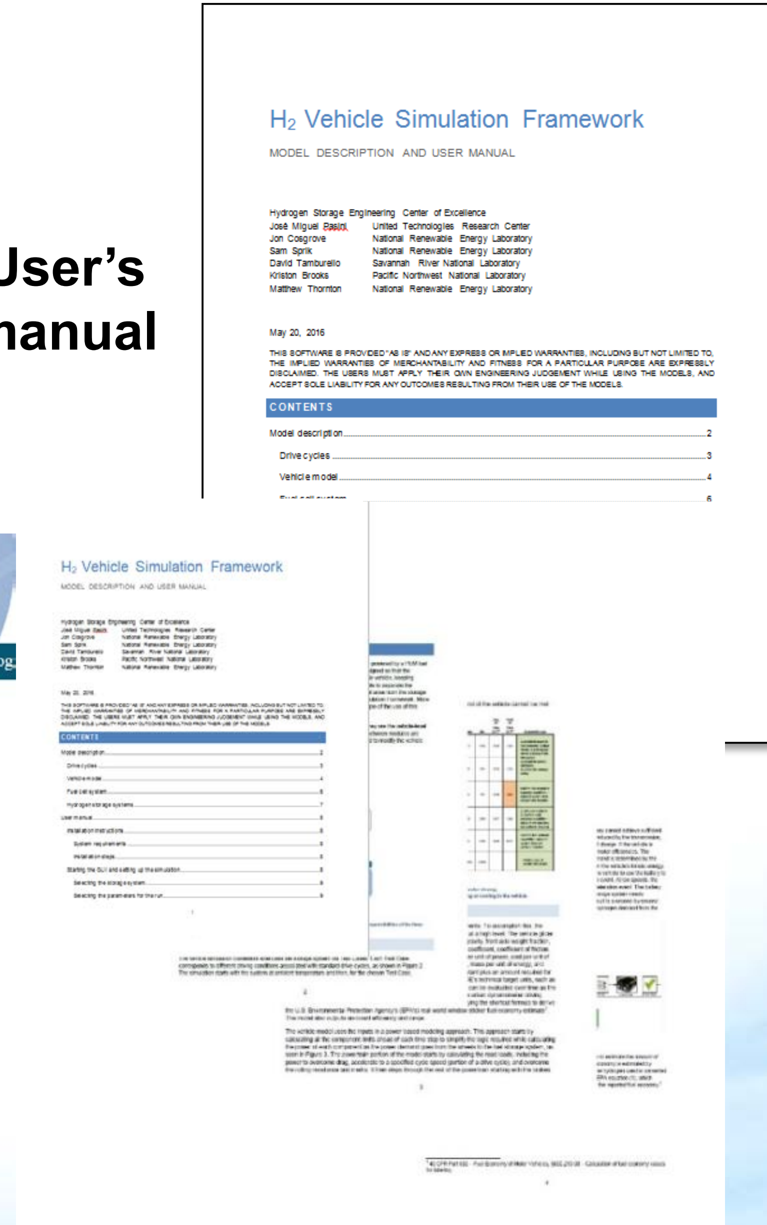
HSECoE

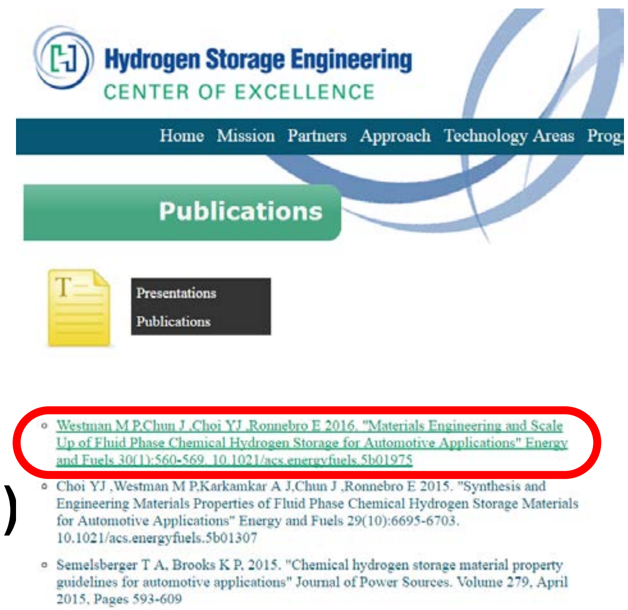
Improved Website Access and Support

Model documentation and downloads



User's manual





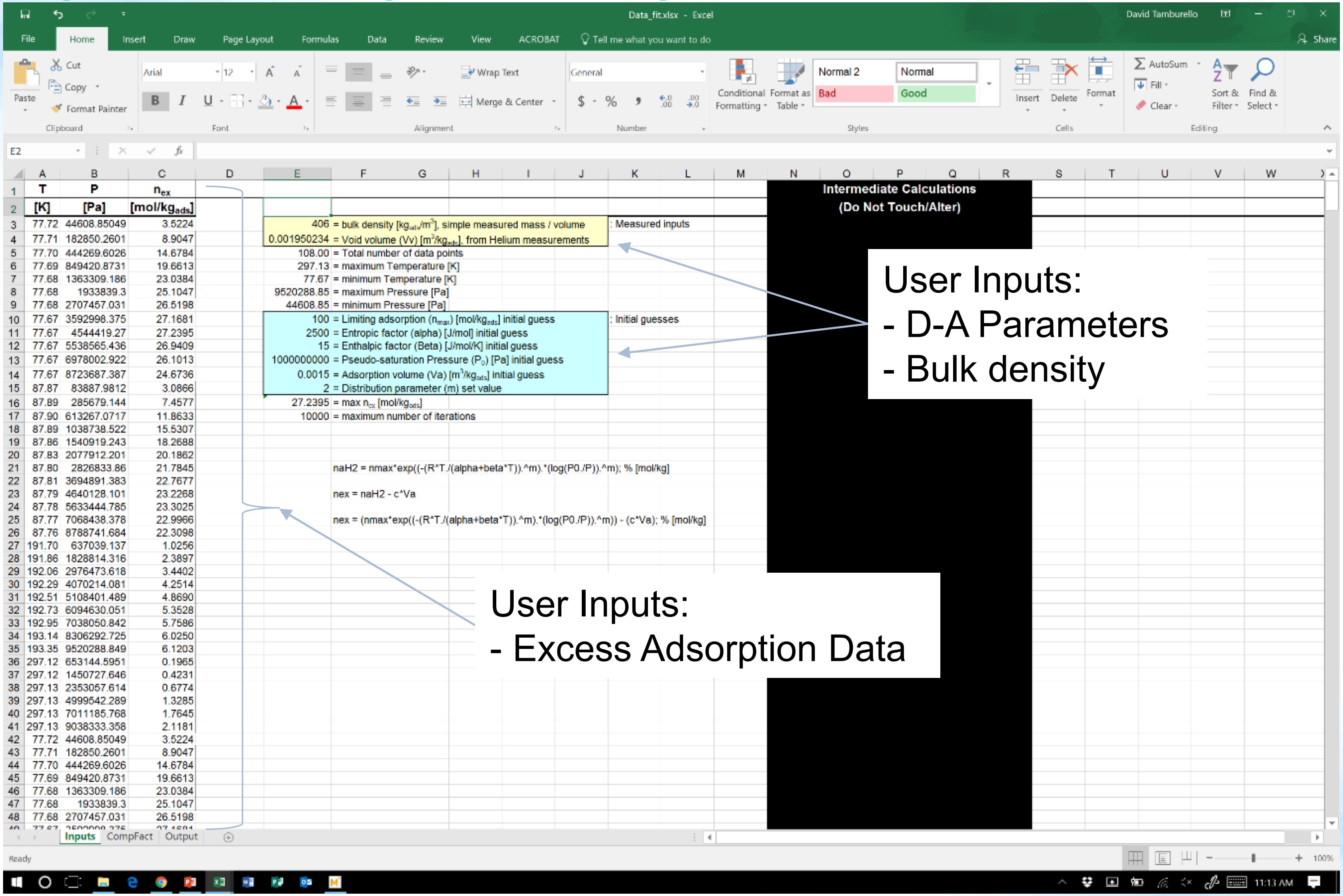
Publications
(now with links)

Automated Isotherm Fitting Simplifies Model Use for Material Developers

- Excess Adsorption Data Fitting Script
  - Written in MathCad™ and I/O in Microsoft Excel
  - Push Button Solution
- Preliminary Model Evaluation:
  - Powder MOF-5
  - Compacted MOF-5 (0.32 g/cc, 0.4 g/cc, and 0.52 g/cc)
  - Activated Carbon

Accomplishments and Progress

Inputs Table Requires Adsorption Parameters in Excel™



	A	B	C
1	T	P	n_{ex}
2	[K]	[Pa]	[mol/kg$_{ads}$]
3	77.72	44608.85049	3.5224
4	77.71	182850.2601	8.9047
5	77.70	444269.6026	14.6784
6	77.69	849420.8731	19.6613
7	77.68	1363309.186	23.0384
8	77.68	1933839.3	25.1047
9	77.68	2707457.031	26.5198
10	77.67	3592998.375	27.1681
11	77.67	4544419.27	27.2395
12	77.67	5538565.436	26.9409
13	77.67	6978002.922	26.1013
14	77.67	8723687.387	24.6736
15	87.87	83887.9812	3.0866
16	87.89	285679.144	7.4577
17	87.90	613267.0717	11.8633
18	87.89	1038738.522	15.5307
19	87.86	1540919.243	18.2688
20	87.83	2077912.201	20.1862
21	87.80	2826833.86	21.7845
22	87.81	3694891.383	22.7677
23	87.79	4640128.101	23.2268
24	87.78	5633444.785	23.3025
25	87.77	7068438.378	22.9966
26	87.76	8788741.684	22.3098
27	191.70	637039.137	1.0256
28	191.86	1828814.316	2.3897
29	192.06	2976473.618	3.4402
30	192.29	4070214.081	4.2514
31	192.51	5108401.489	4.8690
32	192.73	6094630.051	5.3528
33	192.95	7038050.842	5.7586
34	193.14	8306292.725	6.0250
35	193.35	9520288.849	6.1203
36	297.12	653144.5951	0.1965
37	297.12	1450727.646	0.4231
38	297.13	2353057.614	0.6774
39	297.13	4999542.289	1.3285
40	297.13	7011185.768	1.7645
41	297.13	9038333.358	2.1181
42	77.72	44608.85049	3.5224
43	77.71	182850.2601	8.9047
44	77.70	444269.6026	14.6784
45	77.69	849420.8731	19.6613
46	77.68	1363309.186	23.0384
47	77.68	1933839.3	25.1047
48	77.68	2707457.031	26.5198

Value	Description	
406	= bulk density [kg$_{ads}$/m^3], simple measured mass / volume	: Measured inputs
0.001950234	= Void volume (Vv) [m^3/kg$_{ads}$], from Helium measurements	
108.00	= Total number of data points	
297.13	= maximum Temperature [K]	
77.67	= minimum Temperature [K]	
9520288.85	= maximum Pressure [Pa]	
44608.85	= minimum Pressure [Pa]	
100	= Limiting adsorption (n_{max}) [mol/kg$_{ads}$] initial guess	: Initial guesses
2500	= Entropic factor (alpha) [J/mol] initial guess	
15	= Enthalpic factor (Beta) [J/mol/K] initial guess	
1000000000	= Pseudo-saturation Pressure (P_0) [Pa] initial guess	
0.0015	= Adsorption volume (Va) [m^3/kg$_{ads}$] initial guess	
2	= Distribution parameter (m) set value	
27.2395	= max n_{ex} [mol/kg$_{ads}$]	
10000	= maximum number of iterations	

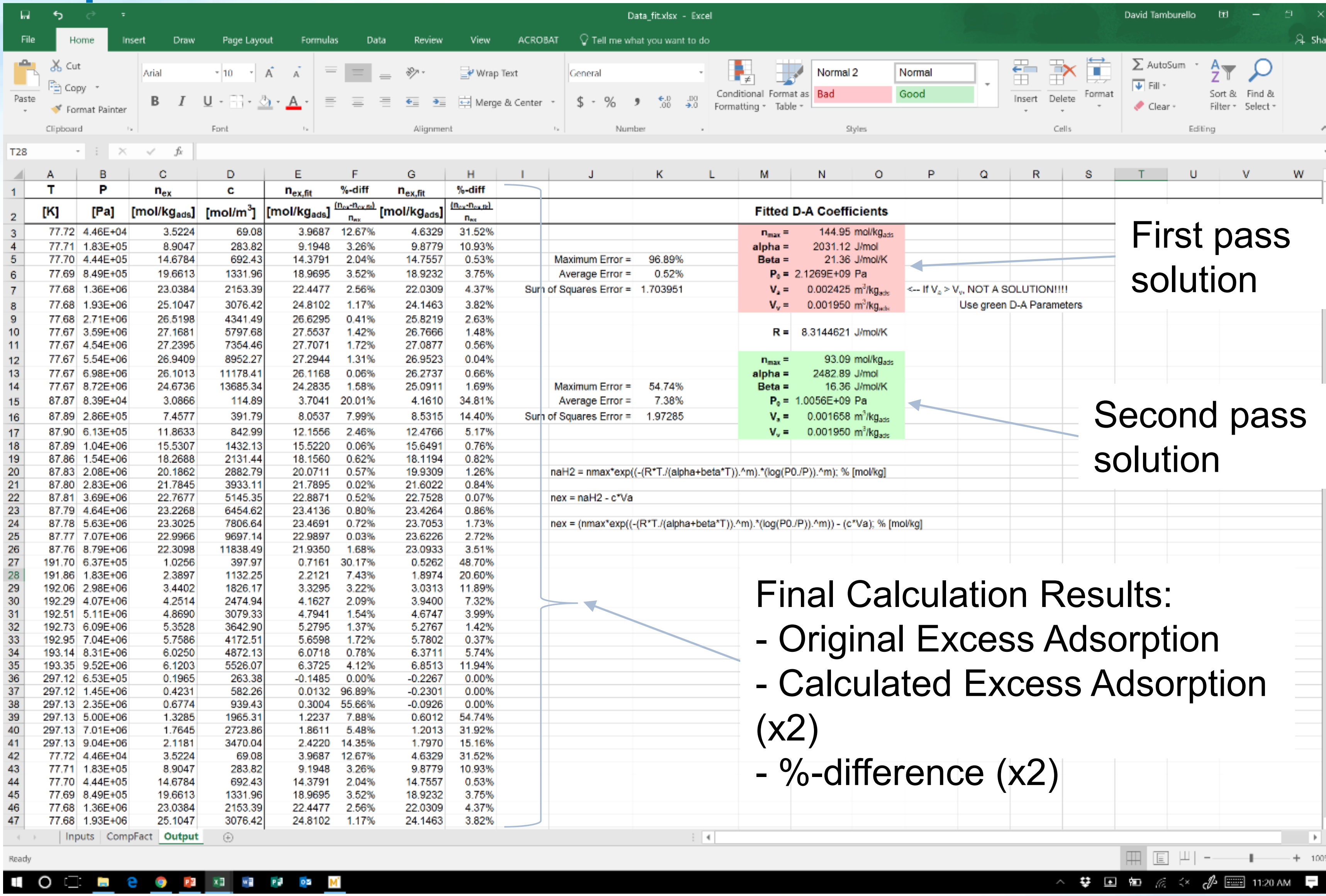
naH2 = nmax*exp((-(R*T./(alpha+beta*T)).^m).*(log(P0./P)).^m); % [mol/kg]

nex = naH2 - c*Va

nex = (nmax*exp((-(R*T./(alpha+beta*T)).^m).*(log(P0./P)).^m)) - (c*Va); % [mol/kg]

Accomplishments and Progress

Output Table Provides DA Parameters and Error



T	P	n_{ex}	c	$n_{ex,fit}$	%-diff	$n_{ex,fit}$	%-diff
[K]	[Pa]	[mol/kg$_{ads}$]	[mol/m^3]	[mol/kg$_{ads}$]	$\frac{(n_{ex}-n_{ex,fit})}{n_{ex}}$	[mol/kg$_{ads}$]	$\frac{(n_{ex}-n_{ex,fit})}{n_{ex}}$
77.72	4.46E+04	3.5224	69.08	3.9687	12.67%	4.6329	31.52%
77.71	1.83E+05	8.9047	283.82	9.1948	3.26%	9.8779	10.93%
77.70	4.44E+05	14.6784	692.43	14.3791	2.04%	14.7557	0.53%
77.69	8.49E+05	19.6613	1331.96	18.9695	3.52%	18.9232	3.75%
77.68	1.36E+06	23.0384	2153.39	22.4477	2.56%	22.0309	4.37%
77.68	1.93E+06	25.1047	3076.42	24.8102	1.17%	24.1463	3.82%
77.68	2.71E+06	26.5198	4341.49	26.6295	0.41%	25.8219	2.63%
77.67	3.59E+06	27.1681	5797.68	27.5537	1.42%	26.7666	1.48%
77.67	4.54E+06	27.2395	7354.46	27.7071	1.72%	27.0877	0.56%
77.67	5.54E+06	26.9409	8952.27	27.2944	1.31%	26.9523	0.04%
77.67	6.98E+06	26.1013	11178.41	26.1168	0.06%	26.2737	0.66%
77.67	8.72E+06	24.6736	13685.34	24.2835	1.58%	25.0911	1.69%
87.87	8.39E+04	3.0866	114.89	3.7041	20.01%	4.1610	34.81%
87.89	2.86E+05	7.4577	391.79	8.0537	7.99%	8.5315	14.40%
87.90	6.13E+05	11.8633	842.99	12.1556	2.46%	12.4766	5.17%
87.89	1.04E+06	15.5307	1432.13	15.5220	0.06%	15.6491	0.76%
87.86	1.54E+06	18.2688	2131.44	18.1560	0.62%	18.1194	0.82%
87.83	2.08E+06	20.1862	2882.79	20.0711	0.57%	19.9309	1.26%
87.80	2.83E+06	21.7845	3933.11	21.7895	0.02%	21.6022	0.84%
87.81	3.69E+06	22.7677	5145.35	22.8871	0.52%	22.7528	0.07%
87.79	4.64E+06	23.2268	6454.62	23.4136	0.80%	23.4264	0.86%
87.78	5.63E+06	23.3025	7806.64	23.4691	0.72%	23.7053	1.73%
87.77	7.07E+06	22.9966	9697.14	22.9897	0.03%	23.6226	2.72%
87.76	8.79E+06	22.3098	11838.49	21.9350	1.68%	23.0933	3.51%
191.70	6.37E+05	1.0256	397.97	0.7161	30.17%	0.5262	48.70%
191.86	1.83E+06	2.3897	1132.25	2.2121	7.43%	1.8974	20.60%
192.06	2.98E+06	3.4402	1826.17	3.3295	3.22%	3.0313	11.89%
192.29	4.07E+06	4.2514	2474.94	4.1627	2.09%	3.9400	7.32%
192.51	5.11E+06	4.8690	3079.33	4.7941	1.54%	4.6747	3.99%
192.73	6.09E+06	5.3528	3642.90	5.2795	1.37%	5.2767	1.42%
192.95	7.04E+06	5.7586	4172.51	5.6598	1.72%	5.7802	0.37%
193.14	8.31E+06	6.0250	4872.13	6.0718	0.78%	6.3711	5.74%
193.35	9.52E+06	6.1203	5526.07	6.3725	4.12%	6.8513	11.94%
297.12	6.53E+05	0.1965	263.38	-0.1485	0.00%	-0.2267	0.00%
297.12	1.45E+06	0.4231	582.26	0.0132	96.89%	-0.2301	0.00%
297.13	2.35E+06	0.6774	939.43	0.3004	55.66%	-0.0926	0.00%
297.13	5.00E+06	1.3285	1965.31	1.2237	7.88%	0.6012	54.74%
297.13	7.01E+06	1.7645	2723.86	1.8611	5.48%	1.2013	31.92%
297.13	9.04E+06	2.1181	3470.04	2.4220	14.35%	1.7970	15.16%
77.72	4.46E+04	3.5224	69.08	3.9687	12.67%	4.6329	31.52%
77.71	1.83E+05	8.9047	283.82	9.1948	3.26%	9.8779	10.93%
77.70	4.44E+05	14.6784	692.43	14.3791	2.04%	14.7557	0.53%
77.69	8.49E+05	19.6613	1331.96	18.9695	3.52%	18.9232	3.75%
77.68	1.36E+06	23.0384	2153.39	22.4477	2.56%	22.0309	4.37%
77.68	1.93E+06	25.1047	3076.42	24.8102	1.17%	24.1463	3.82%

Fitted D-A Coefficients

n_{max} =	144.95	mol/kg$_{ads}$
alpha =	2031.12	J/mol
Beta =	21.36	J/mol/K
P_0 =	2.1269E+09	Pa
V_a =	0.002425	m^3/kg$_{ads}$
V_v =	0.001950	m^3/kg$_{ads}$

Maximum Error = 96.89%
Average Error = 0.52%
Sum of Squares Error = 1.703951

<-- If $V_a > V_v$, NOT A SOLUTION!!!!
Use green D-A Parameters

R = 8.3144621 J/mol/K

n_{max} =	93.09	mol/kg$_{ads}$
alpha =	2482.89	J/mol
Beta =	16.36	J/mol/K
P_0 =	1.0056E+09	Pa
V_a =	0.001658	m^3/kg$_{ads}$
V_v =	0.001950	m^3/kg$_{ads}$

Maximum Error = 54.74%
Average Error = 7.38%
Sum of Squares Error = 1.97285

```
naH2 = nmax*exp((-(R*T./(alpha+beta*T)).^m).*(log(P0./P)).^m); % [mol/kg]

nex = naH2 - c*Va

nex = (nmax*exp((-(R*T./(alpha+beta*T)).^m).*(log(P0./P)).^m)) - (c*Va); % [mol/kg]
```

First pass solution

Second pass solution

Final Calculation Results:
- Original Excess Adsorption
- Calculated Excess Adsorption (x2)
- %-difference (x2)

Output Table Provides DA Parameters and Error

Data_fit.xlsx - Excel

Row	T [K]	P [Pa]	n_{ex} [mol/kg$_{ads}$]	c [mol/m^3]	$n_{ex,fit}$ [mol/kg$_{ads}$]	%-diff $\frac{\lvert n_{ex}-n_{ex,fit}\rvert}{n_{ex}}$	$n_{ex,fit}$ [mol/kg$_{ads}$]	%-diff $\frac{\lvert n_{ex}-n_{ex,fit}\rvert}{n_{ex}}$
3	77.72	4.46E+04	3.5224	69.08	3.9687	12.67%	4.6329	31.52%
4	77.71	1.83E+05	8.9047	283.82	9.1948	3.26%	9.8779	10.93%
5	77.70	4.44E+05	14.6784	692.43	14.3791	2.04%	14.7557	0.53%
6	77.69	8.49E+05	19.6613	1331.96	18.9695	3.52%	18.9232	3.75%
7	77.68	1.36E+06	23.0384	2153.39	22.4477	2.56%	22.0309	4.37%
8	77.68	1.93E+06	25.1047	3076.42	24.8102	1.17%	24.1463	3.82%
9	77.68	2.71E+06	26.5198	4341.49	26.6295	0.41%	25.8219	2.63%
10	77.67	3.59E+06	27.1681	5797.68	27.5537	1.42%	26.7666	1.48%
11	77.67	4.54E+06	27.2395	7354.46	27.7071	1.72%	27.0877	0.56%
12	77.67	5.54E+06	26.9409	8952.27	27.2944	1.31%	26.9523	0.04%
13	77.67	6.98E+06	26.1013	11178.41	26.1168	0.06%	26.2737	0.66%
14	77.67	8.72E+06	24.6736	13685.34	24.2835	1.58%	25.0911	1.69%
15	87.87	8.39E+04	3.0866	114.89	3.7041	20.01%	4.1610	34.81%
16	87.89	2.86E+05	7.4577	391.79	8.0537	7.99%	8.5315	14.40%
17	87.90	6.13E+05	11.8633	842.99	12.1556	2.46%	12.4766	5.17%
18	87.89	1.04E+06	15.5307	1432.13	15.5220	0.06%	15.6491	0.76%
19	87.86	1.54E+06	18.2688	2131.44	18.1560	0.62%	18.1194	0.82%
20	87.83	2.08E+06	20.1862	2882.79	20.0711	0.57%	19.9309	1.26%
21	87.80	2.83E+06	21.7845	3933.11	21.7895	0.02%	21.6022	0.84%
22	87.81	3.69E+06	22.7677	5145.35	22.8871	0.52%	22.7528	0.07%
23	87.79	4.64E+06	23.2268	6454.62	23.4136	0.80%	23.4264	0.86%
24	87.78	5.63E+06	23.3025	7806.64	23.4691	0.72%	23.7053	1.73%
25	87.77	7.07E+06	22.9966	9697.14	22.9897	0.03%	23.6226	2.72%
26	87.76	8.79E+06	22.3098	11838.49	21.9350	1.68%	23.0933	3.51%
27	191.70	6.37E+05	1.0256	397.97	0.7161	30.17%	0.5262	48.70%
28	191.86	1.83E+06	2.3897	1132.25	2.2121	7.43%	1.8974	20.60%
29	192.06	2.98E+06	3.4402	1826.17	3.3295	3.22%	3.0313	11.89%
30	192.29	4.07E+06	4.2514	2474.94	4.1627	2.09%	3.9400	7.32%
31	192.51	5.11E+06	4.8690	3079.33	4.7941	1.54%	4.6747	3.99%
32	192.73	6.09E+06	5.3528	3642.90	5.2795	1.37%	5.2767	1.42%
33	192.95	7.04E+06	5.7586	4172.51	5.6598	1.72%	5.7802	0.37%
34	193.14	8.31E+06	6.0250	4872.13	6.0718	0.78%	6.3711	5.74%
35	193.35	9.52E+06	6.1203	5526.07	6.3725	4.12%	6.8513	11.94%
36	297.12	6.53E+05	0.1965	263.38	-0.1485	0.00%	-0.2267	0.00%
37	297.12	1.45E+06	0.4231	582.26	0.0132	96.89%	-0.2301	0.00%
38	297.13	2.35E+06	0.6774	939.43	0.3004	55.66%	-0.0926	0.00%
39	297.13	5.00E+06	1.3285	1965.31	1.2237	7.88%	0.6012	54.74%
40	297.13	7.01E+06	1.7645	2723.86	1.8611	5.48%	1.2013	31.92%
41	297.13	9.04E+06	2.1181	3470.04	2.4220	14.35%	1.7970	15.16%
42	77.72	4.46E+04	3.5224	69.08	3.9687	12.67%	4.6329	31.52%
43	77.71	1.83E+05	8.9047	283.82	9.1948	3.26%	9.8779	10.93%
44	77.70	4.44E+05	14.6784	692.43	14.3791	2.04%	14.7557	0.53%
45	77.69	8.49E+05	19.6613	1331.96	18.9695	3.52%	18.9232	3.75%
46	77.68	1.36E+06	23.0384	2153.39	22.4477	2.56%	22.0309	4.37%
47	77.68	1.93E+06	25.1047	3076.42	24.8102	1.17%	24.1463	3.82%

Errors Calculated for First pass solution

Maximum Error =	96.89%
Average Error =	0.52%
Sum of Squares Error =	1.703951

Errors Calculated for Second pass solution

Maximum Error =	54.74%
Average Error =	7.38%
Sum of Squares Error =	1.97285

naH2 = nmax*exp((-(R*T./(alpha+be

nex = naH2 - c*Va

nex = (nmax*exp((-(R*T./(alpha+bet

Fitted D-A Coefficients

n_{max} =	144.95	mol/kg$_{ads}$
alpha =	2031.12	J/mol
Beta =	21.36	J/mol/K
P_0 =	2.1269E+09	Pa
V_a =	0.002425	m^3/kg$_{ads}$
V_v =	0.001950	m^3/kg$_{ads}$

<-- If V_a > V_v, NOT A SOLUTION!!!! Use green D-A Parameters

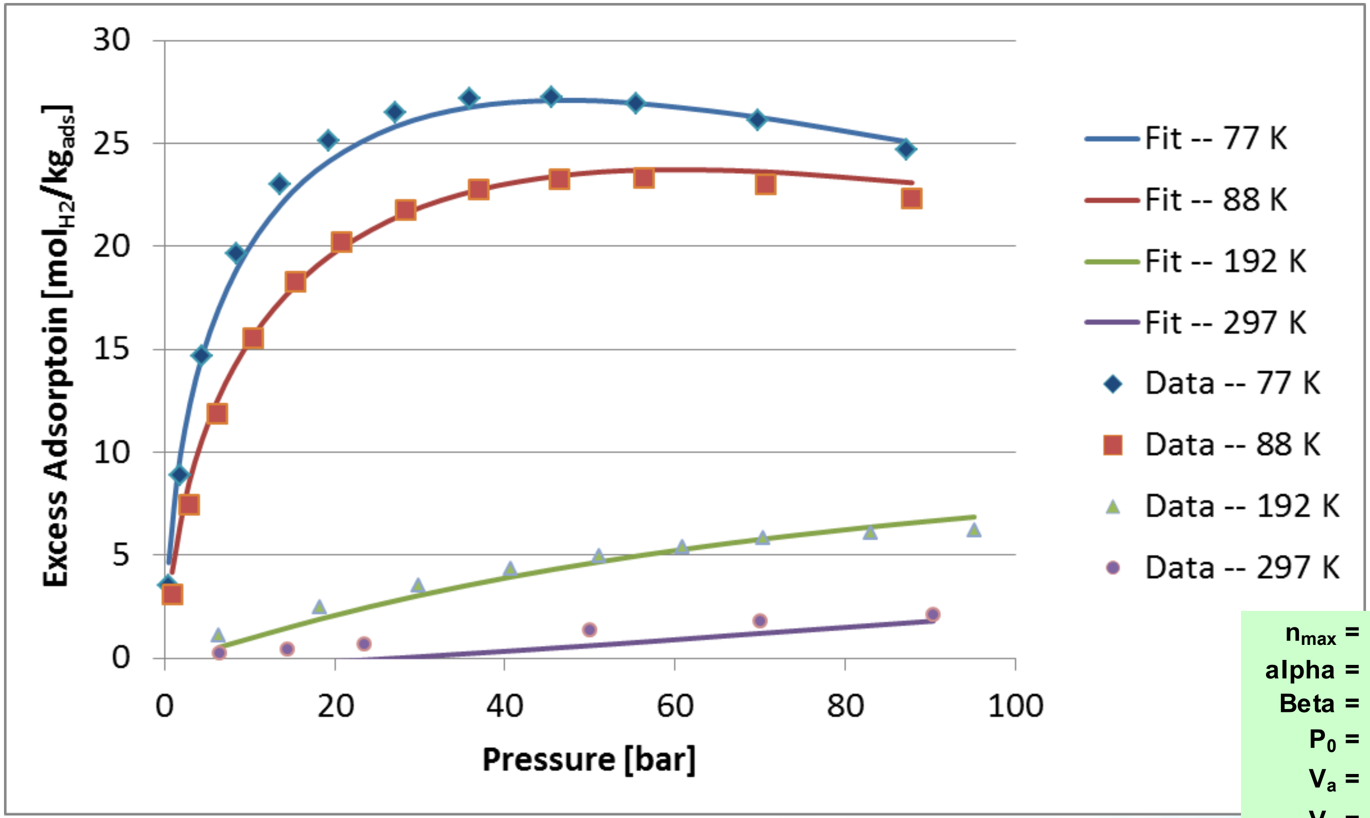
R = 8.3144621 J/mol/K

n_{max} =	93.09	mol/kg$_{ads}$
alpha =	2482.89	J/mol
Beta =	16.36	J/mol/K
P_0 =	1.0056E+09	Pa
V_a =	0.001658	m^3/kg$_{ads}$
V_v =	0.001950	m^3/kg$_{ads}$

Inputs | CompFact | Output

Isotherm Fitting Results

- All fitting results performed had a sum of squares error less than 5.0
- All but one had a sum of squares error of less than 2.0
- **Sample Result:** 0.4 g/cc Compacted MOF-5



n_{max} =	93.09 mol/kg_{ads}
alpha =	2482.89 J/mol
Beta =	16.36 J/mol/K
P_0 =	1.0056E+09 Pa
V_a =	0.001658 m^3/kg_{ads}
V_v =	0.001950 m^3/kg_{ads}

Sizing Routine Estimates All Input Parameters Needed for Framework

- **Benefit**
  - **Availability (No Simulink license required)**
  - **Uses inputs measured by materials researchers to calculate Framework parameters**
  - **Estimates system mass and volume for preliminary comparison to the DOE Technical Targets**
  - **Can be run separate or can be run as a GUI within the framework**

Executable Sizing Routine – Chemical Hydrogen Input File

input_AB.xlsx - Excel

	Values	Units	Comments
ExoEndo	1	--	Exothermic/Endothermic 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
Useable H2	5.6	kg	Mass of usable hydrogen required
Power	40	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

Reaction Parameters
Weight Fraction H_2

Heat Capacity & Density

Impurities

Operating Conditions

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Executable Sizing Routine – Chemical Hydrogen Output

Name	Value	Units	Description
		System Mass and Volume	
TotalMass	218.8343	kg	Total Estimated System Mass
TotalVolume	236.6091	L	Total Estimated System Volume
DOE_Mass_Target	0.02559	kg H2/kg sys	DOE Gravimetric Target 2020
DOE_Vol_Target	0.023668	kg H2/L sys	DOE Volumetric Target 2020
		Framework Input Parameters	
ReactorLength	1.574	m	Reactor Length
Vballast	0.092683	m3	Ballast Tank Volume
MFeed	128.1465	kg	Mass Chemical Hydride Required
x_CH	0.5	kg/kg	Fraction chemical Hydride in Slurry or Liquid
LiqRadLength	3.671969	m	Slurry Radiator Length
GasRadLength	0.961873	m	Hydrogen Gas Radiator Length
ppm_imp	0	ppm	Impurity 1 Conc.
ppm_imp	0	ppm	Impurity 2 Conc.
Recup	1	--	Recuperator Flag (1 = endothermic)
RecupLength	1.78423	m	Recuperator Length (if endothermic)
		Intermediate Values	
Startup Time	187.6743	sec	Time to Reach 30% Conversion
		Framework Values: Reactor Parameters	
reactparam.A1	1.2E+10	1/sec	Arrhenius Parameter Reaction 1
reactparam.E1	102200	J/mol	Activation Energy Reaction 1
reactparam.n1,	2	--	Exponential Factor Reaction 1
reactparam.beta1	1.5	mol H2/mol CH	Ratio H2 to CH Produced Reaction 1
reactparam.DH1	-7600	J/mol	Reaction 1 Enthalpy
reactparam.A2	0	1/sec	Arrhenius Parameter Reaction 2
reactparam.E2	1000	J/mol,	Activation Energy Reaction 2
reactparam.n2	1	--	Exponential Factor Reaction 2
reactparam.beta2	0	mol H2/mol CH	Ratio H2 to CH Produced Reaction 2
reactparam.DH2	0	J/mol	Reaction 2 Enthalpy
reactparam.rxntyp	1	--	Type of Reaction(1=Avrami, 2=nth Order
reactparam.D	0.0444	m	Reactor Diameter
reactparam.thick	0.0017	m	Reactor Wall Thickness
reactparam.rhoslui	1244.147	kg/m3	Density Slurry
reactparam.MW	30	g/mol	Chemical Hydride Molecular Weight
reactparam.Cpsluri	1423	J/kg/K	Heat Capacity Slurry
reactparam.rhome	8000	kg/m3	Density Steel
reactparam.Cpmet	470	J/kg/K	Heat Capacity Steel
reactparam.CpH2	14400	J/kg/K	Heat Capacity H2
		Framework Values: Liquid Radiator Parameters	

System Mass & Volume

Key Design Parameters used in Framework

Intermediate Values

Other Framework Values For each Unit Operation

Output: Provides all parameters needed for full Chemical Hydrogen storage system.

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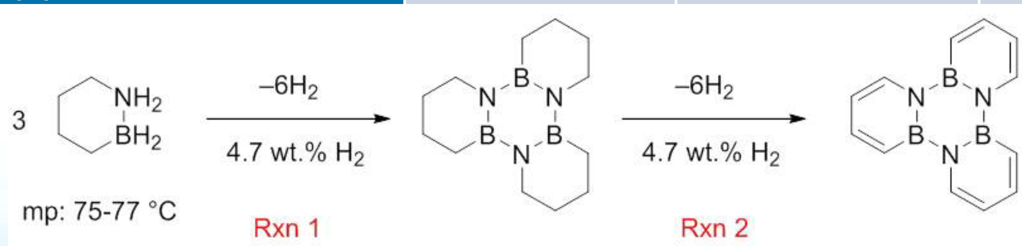
Executable Sizing Routine – Representative Results for CHS

Calculated System Parameter	Ammonia Borane	Alane	CBN*
Total System Mass (kg)	133	188	117
Total System Volume (L)	146	161	135
System Gravimetric Capacity (kg H_2/kg system)	0.042	0.029	0.048
System Volumetric Capacity (kg H_2/L system)	0.038	0.035	0.041
Reactor Length (m)	0.64	1.28	2.3
Ballast Tank Volume (L)	14	22	32
Mass Chemical Hydride (kg)	77	128	70
Fraction Chemical Hydride	0.5	0.5	1
Liquid Radiator Length (m) (3 tubes)	2.4	1.6	0.9
Gas Radiator Length (m) (1 tube)	1.2	1.0	1.4
Recuperator Length (m) (3 tubes)	0	3.22	0.8
Startup Temperature (°C)	178	202	279
Ballast Time (s)	75	117	176

*CBN:



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Executable Sizing Routine – Adsorbent Input File

A	B: Values	C: Units	D: Comments
Pi	1.00E+07	Pa	Initial/Full tank pressure
Pf	5.00E+05	Pa	Initial/Full tank temperature
Ti	80	K	Final/Empty tank pressure
Tf	160	K	Final/Empty tank temperature
H2usable	5.6	kg_{H2}	Target usable hydrogen
type_Ads	1		Type of adsorbent/HX: 1) Powder/HexCell, 2) Compact/MATI
alpha	2895.12802	J/mol_{H2}	D.A. Parameter -- Enthalpic contribution to the characeristic free energy of adsorption
beta	15.29117	$J/mol_{H2}/K$	D.A. Parameter -- Entropic contribution to the characeristic free energy of adsorption
m	2		D.A. Parameter -- Exponential constant for adsolute adsorption
nmax	96.43165	mol_{H2}/kg_{Ads}	D.A. Parameter -- Maximum H2 loading of the entire adsorption volume
P0	1.39E+09	Pa	D.A. Parameter -- Pseodo-saturation pressure (pressure of the gas phase)
rho_ads	130	kg_{Ads}/m^3	D.A. Parameter -- Bulk Density of the MOF-5
Va	0.00169712	m^3/kg_{Ads}	D.A. Parameter -- Adsorbed volume per mass of adsorbent
Vv	0.00725	m^3/kg_{Ads}	D.A. Parameter -- Void volume per mass of adsorbent
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
th_ins	0.026	m	Pressure vessel insulation thickness
th_LN2	0	m	Pressure vessel LN2 chiller channel thickness (minimum value of 1/4" if pressent)
TType	4		Type of pressure vessel:
			0 = Aluminum Type 1
			1 = 316 Stainless Steel Type 1
			2 = Aluminum + CF Type 3
			3 = SS + CF Type 3
			4 = Plastic + CF Type 4

Operating Conditions (rows Pi – Tf)

Adsorbent condition and Dubinin-Astakhov (D.A.) Parameters (rows type_Ads – Vv)

Thermal properties (rows k – Cp)

Pressure vessel design considerations (rows th_ins – TType)

Operating Condition Limits: 5.0 bar < P < 700 bar
40 K < T < 400 K

Calculations should be limited to the adsorbent excess adsorption data range

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Accomplishments and Progress

Executable Sizing Routine – Adsorbent Output File

Output.xlsx - Excel

A1 | Name

	A	B	C	D
1	Name	Value	Units	Description
2	----------	------------	Output values	--
3	H2stored	5.714285714	kg_H2	Total hydrogen stored
4	System_mass	113.3458877	kg	Total H2 Storage System Mass
5	System_vol	281.2933333	L	Total H2 Storage System Volume
6	System_Cost	2664.635557	$	Total Projected H2 Storage System Cost
7	Grav_Cap	0.049406292	g_H2/g_sys	System-based gravimetric capacity
8	Vol_Cap	19.9080438	g_H2/L_sys	System-based volumetric capacity
9	Rank	7.455876711		Overall system rank based on mass, volume, and cost (better systems have higher values"
10	----------	------------	Input values	--
11	Pi	100	bar	Initial/Full tank pressure
12	Ti	80	K	Initial/Full tank temperature
13	Pf	5.5	bar	Final/Empty tank pressure
14	Tf	160	K	Final/Empty tank temperature
15	H2usable	5.6	kg_H2	Target usable hydrogen
16	type_Ads	1		Type of adsorbent/HX: 1) Powder/HexCell, 2) Compact/MATI
17	alpha	2895.12802	J/mol_H2	D.A. Parameter -- Enthalpic contribution to the characeristic free energy of adsorption
18	beta	15.29117	J/mol_H2/K	D.A. Parameter -- Entropic contribution to the characeristic free energy of adsorption
19	m	2		D.A. Parameter -- Exponential constant for adsolute adsorption
20	nmax	96.43165	mol_H2/kg_ads	D.A. Parameter -- Maximum H2 loading of the entire adsorption volume
21	P0	1387070830	Pa	D.A. Parameter -- Pseodo-saturation pressure (pressure of the gas phase)
22	rho_ads	130	kg_ads/m^3	D.A. Parameter -- Bulk Density of the MOF-5
23	Va	0.00169712	m^3/kg_ads	D.A. Parameter -- Adsorbed volume per mass of adsorbent
24	Vv	0.00725	m^3/kg_ads	D.A. Parameter -- Void volume per mass of adsorbent
25	k	0.3	W/m/K	Thermal conductivity of the adsorbent
26	Cp	780	J/kg/K	Specific Heat of the adsorbent
27	Ads_Cost	11.8	$/kg_ads	Projected cost of the adsorbent per unit mass
28	th_ins	0.026	m	Pressure vessel insulation thickness
29	th_LN2	0	m	Pressure vessel LN2 chiller channel thickness (minimum value of 1/4" if pressent)
30	TType	4		Type of pressure vessel: 0 = Type 1 Al, 1 = Type 1 SS, 2 = Type 3 Al+CF, 3 = Type 3 SS+CF, 4 = Type 4 Plastic+CF
31	----------	------------	Intermediate Calculations	--
32	ntotal	0.259938979	kg_H2/kg_ads	Mass of H2 stored per mass of adsorbent
33	mass_inHX	10.12628399	kg	Mass of the internal Heat Exchanger
34	vol_inHX	3.750475553	L	Volume of the internal Heat Exchanger
35	Cost_inHX	67.59294565	$	Projected cost of the internal Heat Exchanger
36	mass_ads	21.98318138	kg_ads	Mass of the adsorbent material
37	vol_ads	174.035335	L	Volume of the adsorbent material
38	Cost_ads	11.8	$	Projected cost of the adsorbent material
39	m_H2	5.714285714	kg_H2	Total mass of hydrogen stored
40	m_H2_ads	5.714285714	kg_H2	Mass of hydrogen associated with the adsorbent
41	m_H2_gas	0	kg_H2	Mass of hydrogen in the free space (outside of the adsorbent)
42	vol_gas	0	L	Volume of gas in the free space (outside of the adsorbent)
43	Cost_H2	15.42857143	$	Projected cost of the hydrogen
44	mass_tank	58.79413661	kg	Total mass of the tank (pressure vessel, insulation, etc.)
45	vol_tank	264.7503333	L	Outer volume of the tank
46	Cost_tank	1330.759166	$	Projected cost of the tank
47	N_tank	1		Total number of tanks (pre-set to 1 tank)
48	L_tank	1800.328516	mm	Outer length of the tank
49	D_tank	446.2418486	mm	Outer diameter of the tank
50	L-to-D	4.03442331		Length-to-Diameter ratio of the outside of the tank
51	L_cyl	1477.74755	mm	Length of the cylinder section of the tank
52	L_int	1725.069316	mm	Internal length of the tank
53	D_int	370.9826486	mm	Internal diameter of the tank
54	R1	185.4913243	mm	Radius of the tank interior
55	R2	189.4913243	mm	Outer radius of the tank pressure vessel (type 1) or the pressure vessel liner (type 3 or 4)
56	R3	197.7209243	mm	Outer radius of the tank pressure vessel (carbon fiber of type 3 or 4)
57	R4	197.7209243	mm	Outer radius of the LN2 chilling channels (if pressent)
58	R5	221.1209243	mm	Outer radius of the tank insulation
59	R6	223.1209243	mm	Outer radius of the outer shell of the tank (outer shell thickness pre-set to 2mm)
60	m_BOP	16.728	kg	Mass of the balance of plant of the H2 storage system
61	vol_BOP	16.543	L	Volume of the balance of plant of the H2 storage system

Sheet1 | Sheet2 | Sheet3

System level outputs

Repeat of the calculation inputs

Intermediate calculation results:

- -- Pressure vessel description
- -- Internal heat exchanger
- -- hydrogen storage breakdown

Output: Details needed for a full adsorbent H_2 storage system.

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Executable Sizing Routine – Representative Results for ADS

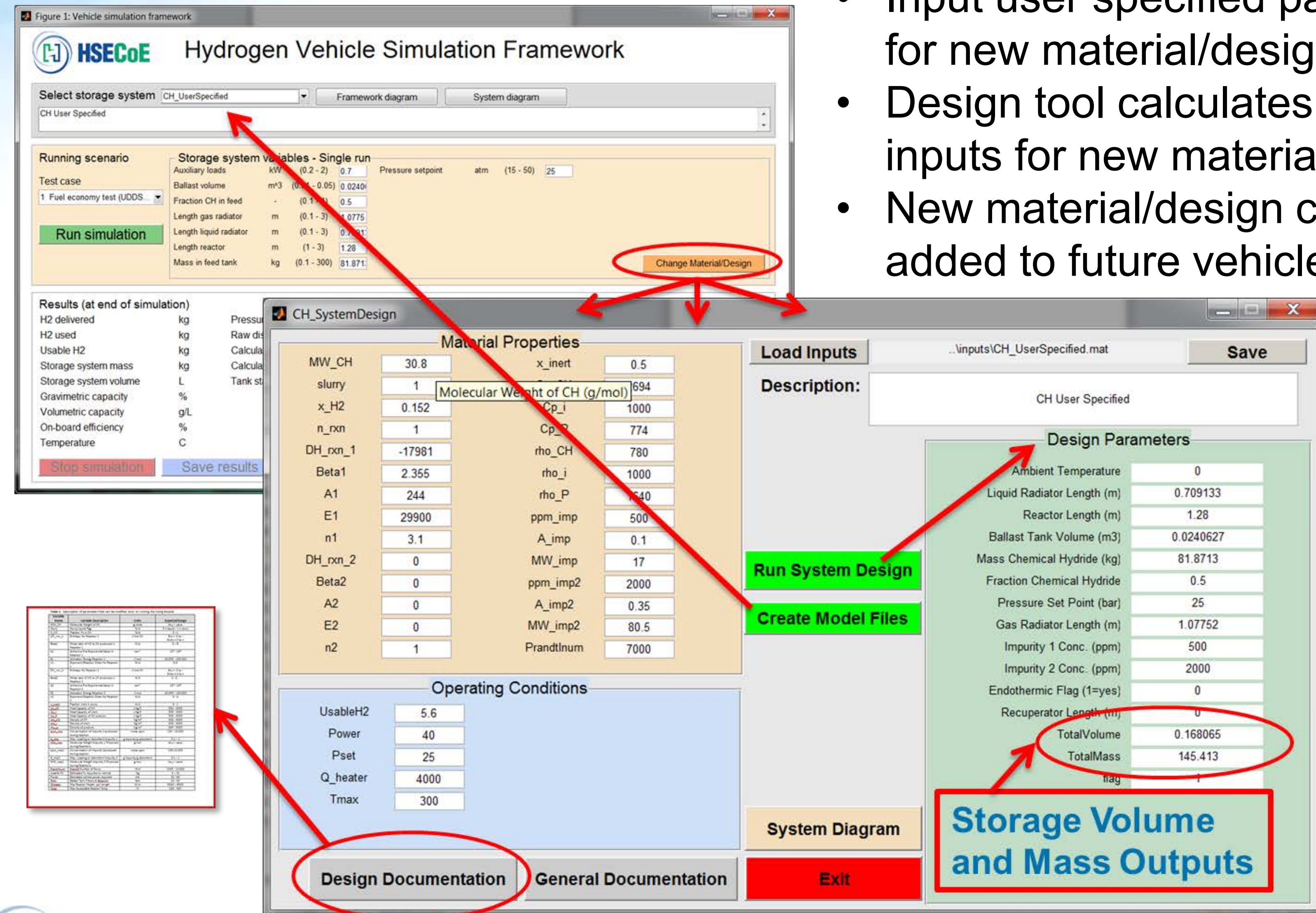
	Gravimetric Capacity [g_{H2}/g_{sys}]	Volumetric Capacity [g_{H2}/L_{sys}]	Source
MOF-5 Powder [130 kg/m^3]	0.0338 g_{H2}/g_{sys}	18.6 g_{H2}/L_{sys}	HSECoE
MOF-5 Compact [406 kg/m^3]	0.0314 g_{H2}/g_{sys}	21.3 g_{H2}/L_{sys}	HSECoE
DUT-23 (Co) Powder* [200 kg/m^3]	0.0348 g_{H2}/g_{sys}	20.7 g_{H2}/L_{sys}	Ford / University of Michigan
IRMOF-20 Powder* [200 kg/m^3]	0.0341 g_{H2}/g_{sys}	20.3 g_{H2}/L_{sys}	Ford / University of Michigan
MOF-5 Powder [200 kg/m^3]	0.0332 g_{H2}/g_{sys}	19.6 g_{H2}/L_{sys}	HSECoE

***Special thanks to Ford and the University of Michigan for sharing their data**

System Design Assumptions:

- Operating Conditions: 80 K, 100 bar to 160 K, 5 bar
- 5.6 kg of usable hydrogen (~5.714 kg of actual hydrogen storage)
- Type 1 aluminum pressure vessel
- LN_2 pressure vessel chiller channel thickness of 9.525 mm
- Uniform insulation thickness of 23 mm, with a 2 mm outer aluminum shell

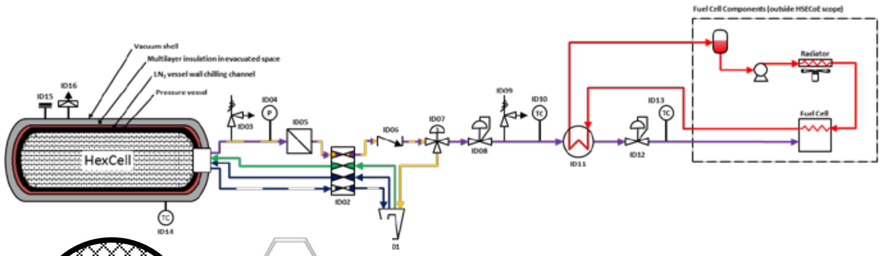
GUI Improvements: Storage System Design Tool Incorporated into Framework

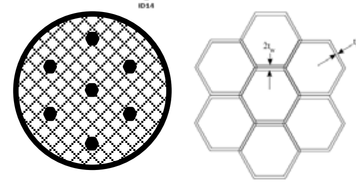


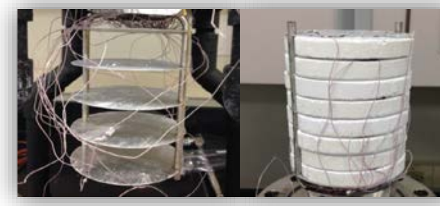
- Input user specified parameters for new material/design
- Design tool calculates framework inputs for new material/design
- New material/design can then added to future vehicle simulation

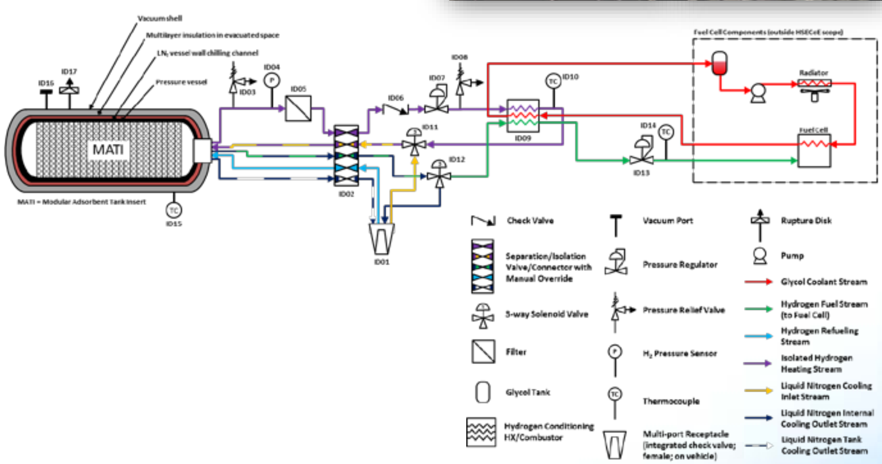
AD Model Improvements: Expand Model Capability

- Adsorbent model updates:
  - Improved hydrogen properties calculations for **faster time steps / improved solution convergence**.
  - **Validated the adsorbent model** estimates using powder MOF-5 and 0.32 g/cc, 0.4 g/cc, and 0.52 g/cc compacted MOF-5 excess adsorption.
- System model updates:
  - Updated tank design controls to **include Type 1, Type 3, and Type 4 pressure vessels**.
  - **Included insulation thickness control** to the design space to account for cryogenic to room temperature operation.









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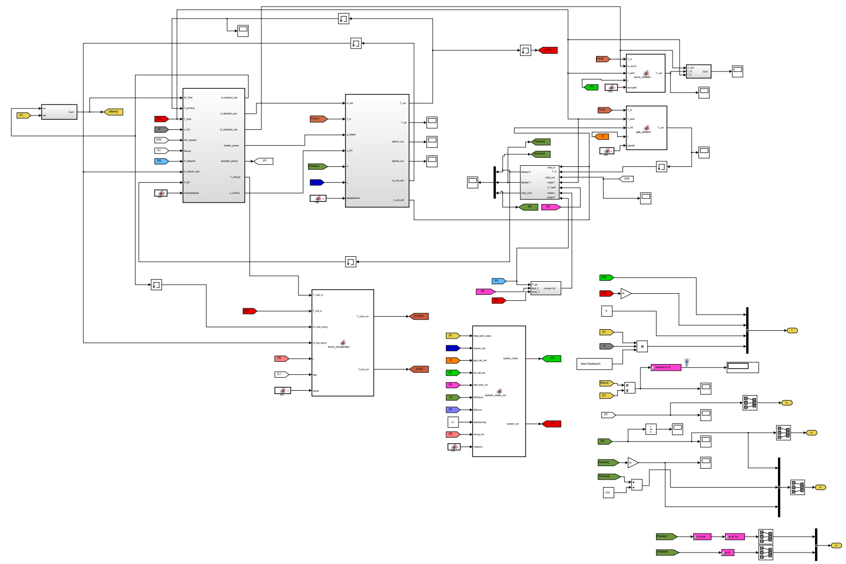
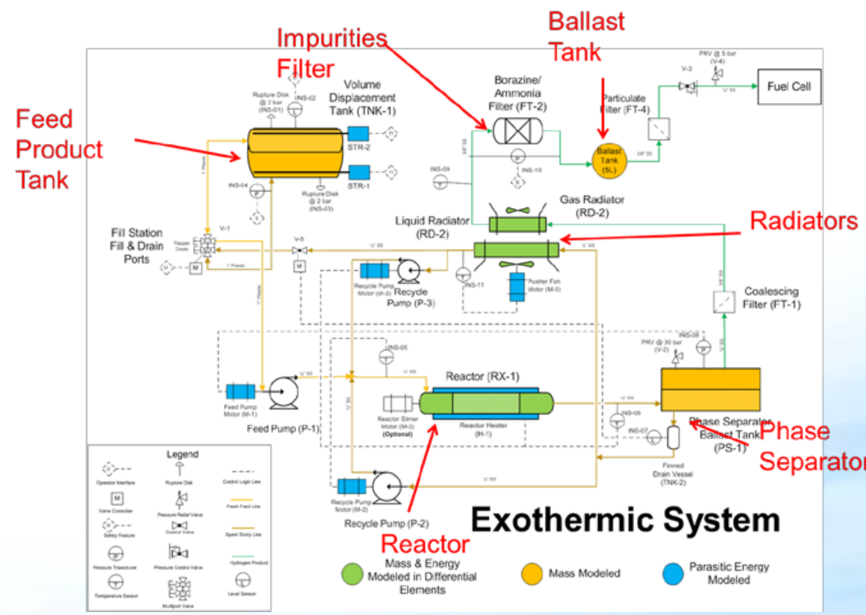
CH Model Updates/Improvements (Kriston)

- Remove unneeded complexity to **decrease model computation time**
  - Radiator, Recuperator, Ballast Tank
- **Added n^{th} order reaction kinetics** with two series reactions as an alternative to two parallel Avrami reactions
  - A → B → C

$$\left.\frac{\partial \alpha_1}{\partial t}\right|_{kinetics} = k_1\left[C_0\left(1-\alpha_1\right)\right]^{n_1} \qquad \left.\frac{\partial \alpha_2}{\partial t}\right|_{kinetics} = k_2\left[C_0\left(\alpha_1-\alpha_2\right)\right]^{n_2}$$

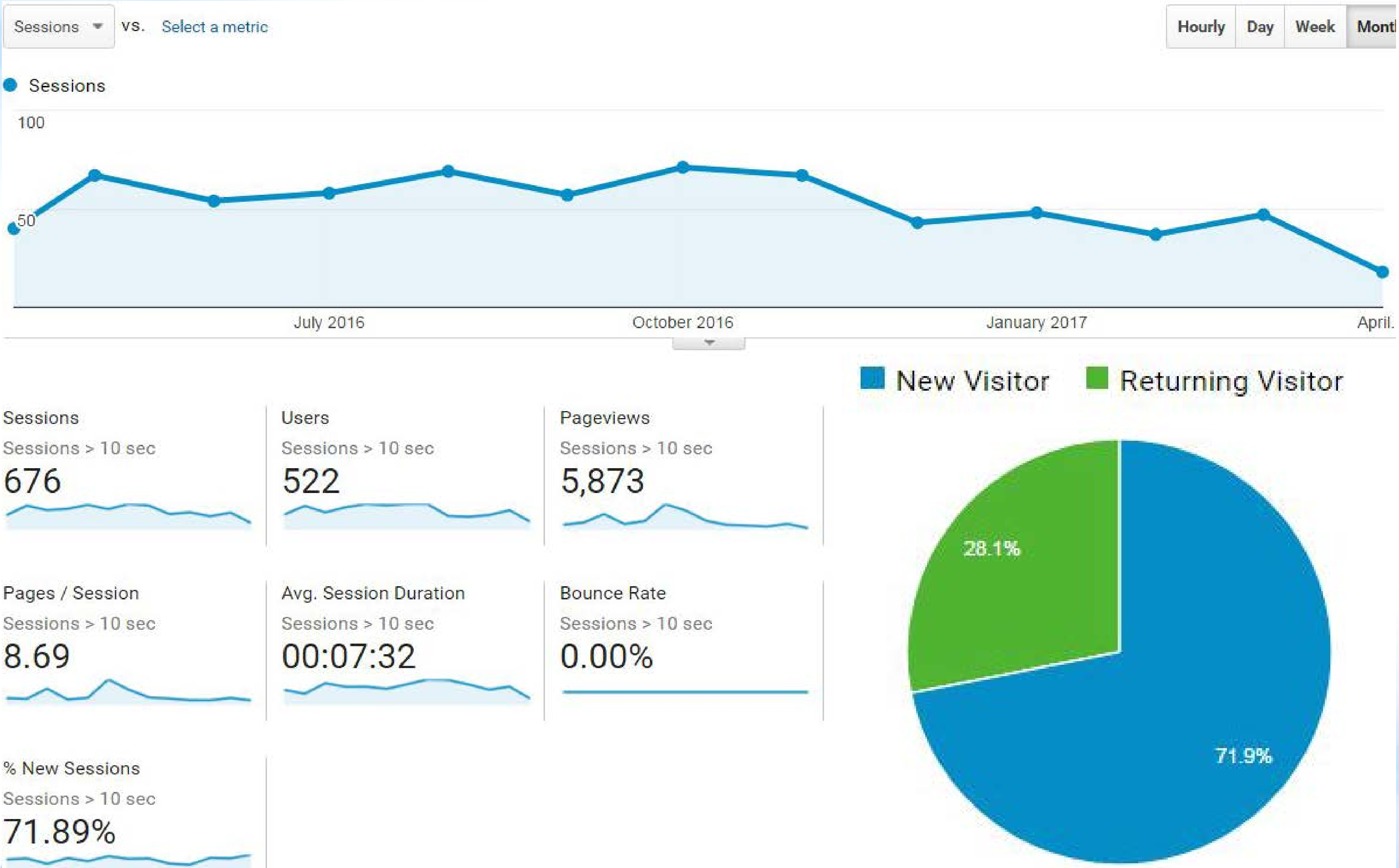
- **Eliminate need for separate C++ Compiler**
  - Use MatLAB functions rather than S-Functions
  - New version of MatLAB require importing separate C++ compiler





Accomplishments and Progress

Model Website Analytics (through April 2017)



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Model Website Analytics Web Flow

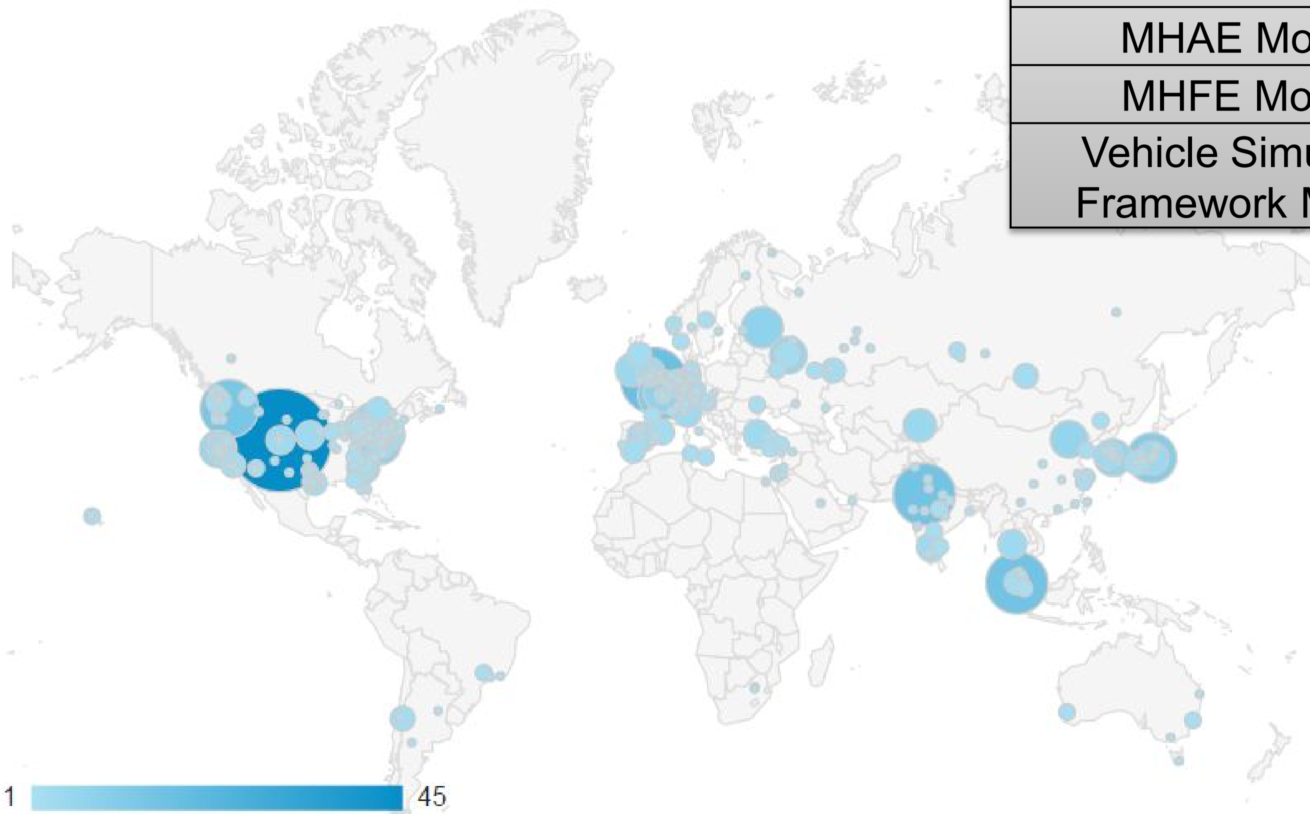
25% of users go directly to modeling webpage

Largest fraction of subsequent interactions are to the modeling webpage

Website users are going to the model webpage

Model Website Analytics

MODEL	DOWNLOADS (Since AMR16)
H_2 Storage Tank Mass and Cost Model	150 (49)
MHAE Model	46 (17)
MHFE Model	74 (33)
Vehicle Simulator Framework Model	107 (39)



39 new downloads of the Vehicle Simulator Framework Model since April, 2016.

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AMR Comments

2016 AMR Comment	2017 Response/Approach
Models written in MatLAB/Simulink may not be utilized by material researchers	Have developed executable sizing routines that do not require MatLAB/Simulink
Outside materials developers would find it useful to have access to the source codes.	Source code is available on the website and can be modified (user beware)
Make accommodations for RT Adsorbents	Model currently can accommodate RT adsorbents but BOP not yet accounted for properly.
Documentation of the instructions for the models should be provided--including specific software requirements and critical assumptions	User manual provides specific software requirements and critical assumptions. Journal articles provide documentation of approach.
The project should obtain feedback from "outside" users that are not HSECoE members and then make adjustments based on their input—users workshop	Evaluating materials from others, including non-HSECoE members: -- Mike Veenstra, Ford Motor Co. -- Don Siegel, University of Michigan -- Jeff Long*, UC Berkeley

*New collaboration – the team is altering the codes to accommodate Jeff's room temperature adsorbent material.

Collaborations

Organization	Relationship	Type	Responsibility
NREL	Team Member	Federal Lab	Update Website and Framework
SRNL	Team Member	Federal Lab	Adsorbent and Compressed Gas Modeling
PNNL	Team Member	Federal Lab	Chemical Hydrogen and Metal Hydride Modeling
Ford	Consultant	Industry	Beta Testing, Fuel Cell Model, Adsorption Data
RCB Hydrides LLC	Consultant	Industry	Beta Testing, H_2 Storage Expertise
University of Michigan	Material Developer	Academia	Adsorption Data
University of California Berkeley	Material Developer	Academia	Adsorption Data

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Remaining Challenges and Barriers

- Increase the use of the models by material developers
    - *Expand the capability of the models to include other kinetic and thermodynamic expressions*
    - *Simplify the model use for non-modelers*
- Increase the use of the models by systems engineers
    - *Potential expansion of the model capabilities to other vehicle classes*
- Demonstrate the model's utility to other researchers
    - *Applying the models to their applications*
- Find available data to validate the model

Model Path Forward – Next Steps

- Convert isotherm fitting routine into MatLAB and stand-alone executable file
- Update Adsorbent model to address room temperature BOP
- Develop stand-alone system executable for MH and Compressed Gas Storage
- Develop volume-based design to target specific vehicle volume limitations/designs and/or, potentially, additional vehicle classes
- Update Adsorbent model with Unilan (or the 2-state Langmuir) models in addition to the D-A model.
- Expand model to other vehicle classes (beyond light duty)
- Work with Material Based H_2 Storage Developers to Apply model to their materials
- Maintain and enhance exiting framework models and track web activity and downloads.

Proposed Future Work

Past and Proposed Future Deliverables

	Deliverable	Date
3	Develop storage system sizing pre-processor (CH storage system).	**Complete**
4	**SMART milestone –** Develop a stand-alone isotherm data fitting routine to convert raw excess adsorption H_2 data into its D-A parameters.	**Complete**
5	GUI Update for user input capability and documentation.	**Complete**
6	**SMART milestone -** Stand-alone System Estimator: Executable version of the sizing functions for Adsorbent and CH models to create first-order storage system estimates based on material properties.	**Complete**
7	Update web models: Executable System Estimators, Isotherm Fitting Tool, GUI/framework.	**6/2017**
8	Develop MH and compressed gas storage system estimators	**9/2017**
9	Provide update on web portal activity—web site hits and time on site, web site use locations and model down loads.	**12/2017**
10	Update Adsorbent and CH models with volume-based design to target specific vehicle classes	**3/2018**
11	Alternative Storage System Formulations: Update the hydrogen storage equations for additional theoretical formulations. (i.e. Unilan or 2-state Langmuir)	**6/2018**
12	Update models with expanded vehicle class options and newly available data from other DOE programs	**9/2018**

Technology Transfer Activities

- Tracking model downloads
- Requesting feedback from users
- Utilizing Beta Testers from industry to evaluate the utility of the models and suggest improvements

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 framework utility by bridging the gap between the information generated by the materials researcher and the parameters required for the framework model.
Technical Accomplishments and Progress	• Developed system estimator for CH and Adsorbents. • System estimator used with framework GUI and as stand-alone executable. • Developed a stand-alone isotherm data fitting routine for D-A parameters. • Improved website and model accessibility.
Collaborations	• Project team includes NREL, SRNL, and PNNL. • Consultants from industry participate in team meetings and provide input.
Proposed Future Research	• Expand the use of models by demonstrating their utility with other storage materials, theoretical formulations, and vehicle class options.

Questions?

HSECoE Models on the WEB Team:

Matthew Thornton

David Tamburello

Kriston Brooks

Sam Sprik

With support from Bob Bowman and Mike Veenstra

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