H_2 Vehicle Simulation Framework

MODEL DESCRIPTION AND USER MANUAL

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MODEL DESCRIPTION

The H_2 Vehicle Simulation Framework is a 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 hydrogen storage systems may be compared on a single vehicle, keeping constant the vehicle-level and fuel cell system assumptions. The goal is to be able to separate the differences in performance that arise from the vehicle and fuel cell and those that arise from the storage system. In the following we describe the model embodied by the H_2 Vehicle Simulation Framework. More details may be found in Pasini et al. (2012) and Thornton et al. (2012). An example of the use of this framework is in Pasini et al. (2013).

The main components of the simulation framework are presented in Figure 1. They are the vehicle-level model, the fuel cell system, and the hydrogen storage systems. The interfaces between modules are designed so that the different storage systems are interchangeable, without need to modify the vehicle and fuel cell assumptions.

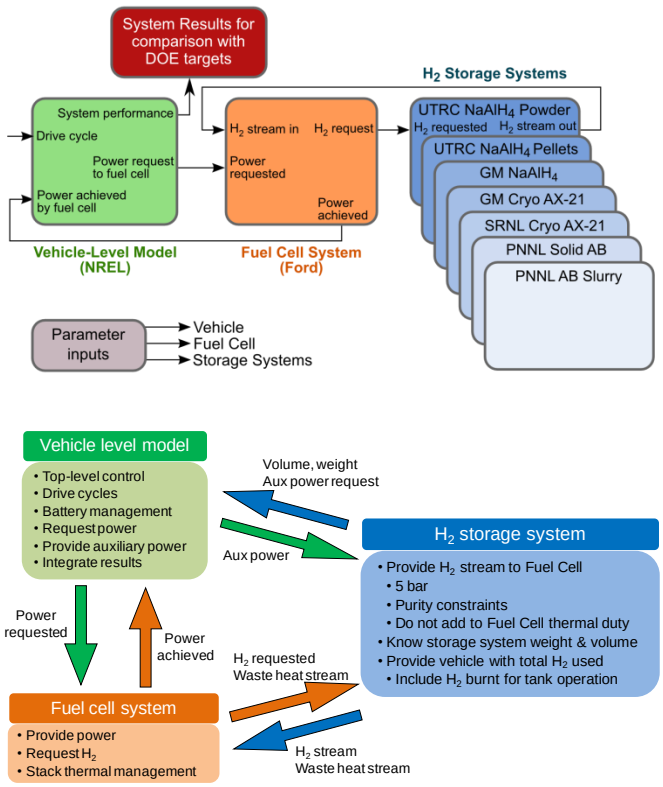

Figure 1. Top: high-level view of components of the vehicle simulation framework. Bottom: responsibilities of the three main modules.

DRIVE CYCLES

The vehicle simulation framework exercises the storage system via Test Cases. Each Test Case corresponds to different driving conditions associated with standard drive cycles, as shown in Figure 2 The simulation starts with the system at ambient temperature and then, for the chosen Test Case,

repeats the corresponding drive cycle indefinitely, until the power demand of the vehicle cannot be met.

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

Figure 2. Drive cycles associated with different test cases.
***Note that the simulation framework does not include Test Case 5, as it does not involve driving.**
****Note that Test Cases 3 & 4 do not simulate increased auxiliary loads due to heating or cooling in the vehicle.**

VEHICLE MODEL

The vehicle model is designed to evaluate high-level attribute improvements. To accomplish this, the inputs, such as the glider and powertrain components, are also defined at a high level. The vehicle glider is defined with a specific frontal area, drag coefficient, mass, center of gravity, front axle weight fraction, and wheel base. The wheels are defined by inertia, a rolling resistance coefficient, coefficient of friction, and radius. The inputs for the motor are power, peak efficiency, mass per unit of power, cost per unit of power, and time to full power. The battery inputs include power, energy, mass per unit of energy, and round trip efficiency. Auxiliary loads are assumed to be a specified constant plus an amount required for the fuel cell and hydrogen storage systems. These inputs match the DOE's technical target units, such as battery kilograms per kilowatt hour, so that the impact of improvements can be evaluated over time as the targets change. The model outputs adjusted fuel economy based on the urban dynamometer driving schedule (UDDS) and the highway fuel economy test (HFET), and applying the shortcut formula to derive the U.S. Environmental Protection Agency's (EPA's) real-world window sticker fuel economy estimate[1]. The model also outputs on-board efficiency and range.

The vehicle model uses the inputs in a power-based modeling approach. This approach starts by calculating all the component limits ahead of each time step to simplify the logic required while calculating the power of each component as the power demand goes from the wheels to the fuel storage system, as seen in Figure 3. The powertrain portion of the model starts by calculating the road loads, including the power to overcome drag, accelerate to a specified cycle speed (portion of a drive cycle), and overcome the rolling resistance and inertia. It then steps through the rest of the powertrain starting with the brakes.

If the vehicle is slowing, the friction brakes are applied if the motor and battery cannot achieve sufficient regenerative braking to meet the drive cycle. The remaining power is then reduced by the transmission, motor, and battery charging efficiency before adding to the battery's state of charge. If the vehicle is accelerating, the road load power is similarly adjusted by transmission and motor efficiencies. The amount of power supplied by the battery and fuel cell to meet the motor demand is determined by the battery's energy management strategy. The battery use strategy is based on the vehicle's kinetic energy. At high speeds, the battery state of charge *target* is lowered. This causes the vehicle to use the battery to accelerate and makes room for regenerative braking for the next slow-down event. At low speeds, the battery state-of-charge target increases, readying it to assist in the next acceleration event. The battery state-of-charge targets are not used if the fuel cell or upstream hydrogen storage system needs assistance from the battery to meet the drive cycle or for auxiliaries. The result is a second-by-second power demand from the fuel cell, which the fuel cell system translates into hydrogen demand from the storage system.

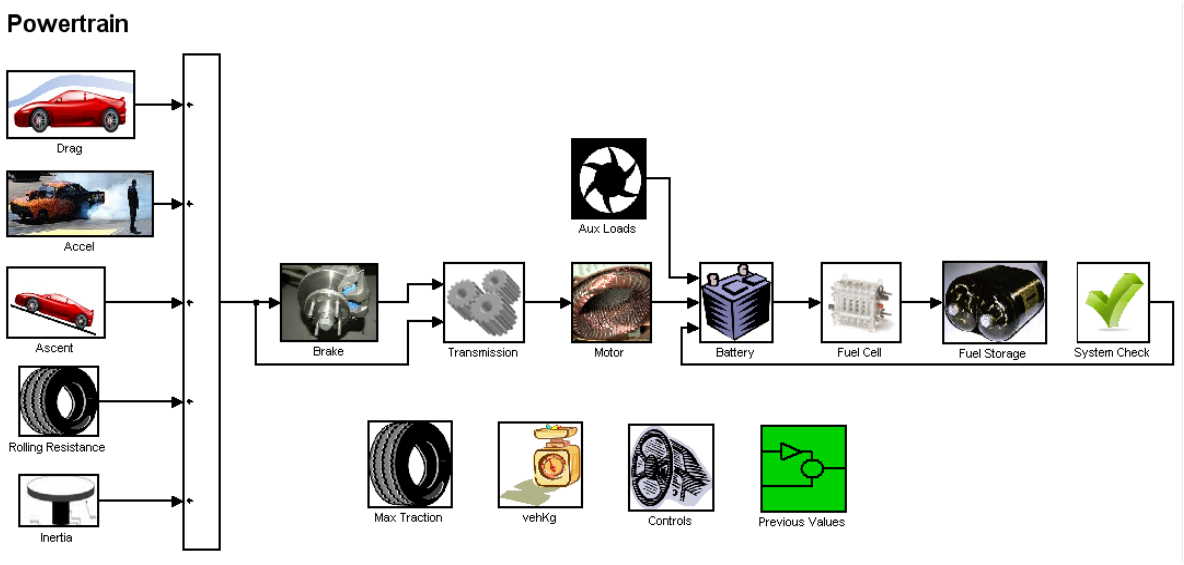

Figure 3. Top-level vehicle model structure.

The hydrogen demand is limited by the storage system and fuel cell models to estimate the amount of hydrogen used, which then goes into the fuel economy estimate. The fuel economy is estimated by running the model using the EPA's city and highway tests (Test Case 1). The hydrogen used is converted to miles per gallon gasoline equivalent (mpgge) on an energy basis. Then, EPA equation (1), which approximates the five-cycle test with the two-cycle test, is used to calculate the reported fuel economy.[1] This corresponds to Test Case 1 in Figure 2.

[1] 40 CFR Part 600 – Fuel Economy of Motor Vehicles, §600.210-08 – Calculation of fuel economy values for labeling.

$$\text{Adjusted\_City\_MPGGE} = \frac{1}{0.003259 + \frac{1.1805}{\text{Model\_City\_MPGGE}}}$$

$$\text{Adjusted\_Highway\_MPGGE} = \frac{1}{0.001376 + \frac{1.3466}{\text{Model\_Highway\_MPGGE}}} \quad (1)$$

$$\text{Adjusted\_Combined\_MPGGE} = \text{Adjusted\_City\_MPGGE} \times 0.55 + \text{Adjusted\_Highway\_MPGGE} \times 0.45$$

Because the adjusted MPGGE and, correspondingly, the range associated with a full tank, are only defined consistently for Test Case 1, those results are not shown in the GUI when running other cases.

The vehicle model will end the simulation in one of the following cases: the energy error beyond the limits of the components indicates that the components cannot meet the drive cycle, the difference between the fuel cell power request from the vehicle and achieved from the fuel cell exceeds a certain error, or the fuel cell power does not meet the minimum required by the vehicle.

FUEL CELL SYSTEM

The fuel cell system model was sized for 80 kW net operating power at 80°C in order to maintain consistency with previous DOE analyses and assumptions. Within the simulation framework, the fuel cell model was developed by Ford Motor Company and based on the cell performance model used by Pukrushpan et al. (2004). As shown in Figure 4, the fuel cell system model parameters were aligned at 80°C to match the DOE's fuel cell system targets for efficiency at rated power (50%) and quarter power (60%). The model has the ability to adjust to the operating temperature based on the test conditions, which will affect the polarization curve and fuel cell system efficiency.

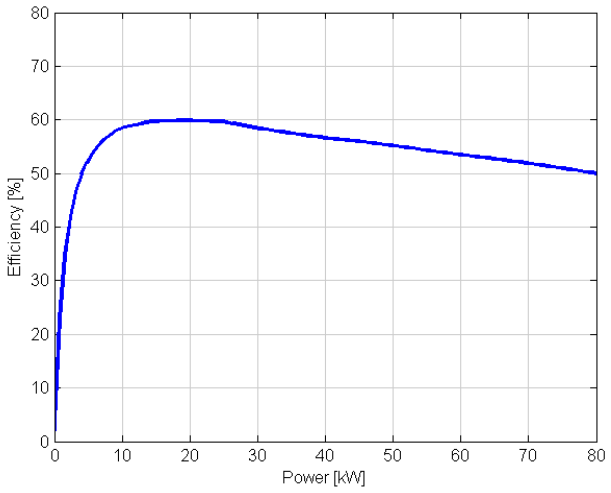

Figure 4. Fuel cell system efficiency used in the model.

Since the simulation framework was focused on the evaluation of material-based storage systems, the fuel cell system model only included the required elements to interface between the vehicle model and the hydrogen storage models. These interface elements include the following: translation of requested vehicle power to current and hydrogen flow request using the polarization curve, compressor parasitic power, and waste heat stream from the fuel cell stack. The interaction between the fuel cell and vehicle

model remain consistent for all of the different material-based storage system model simulations, which is essential to have confidence that the differences are related to the storage system attributes rather than differences in the simulation approach or assumptions.

HYDROGEN STORAGE SYSTEMS

The simulation framework currently contains six storage systems:

- A test system designed for testing the vehicle model and fuel cell separately. This system provides whatever hydrogen demand is placed on it for a finite time.
- A 350 bar compressed gas system. More details are available in Veenstra and Hobein (2011).
- A 700 bar compressed gas system. More details are available in Veenstra and Hobein (2011).
- A metal hydride-based storage system with endothermic hydrogen release at 30 kJ/mol of enthalpy. More details of this system are available in Pasini et al. (2013).
- A chemical hydrogen storage material system selectable for either an exothermic or endothermic hydrogen release enthalphy (Brooks 2014). The exothermic and endothermic systems are represented by an ammonia borane slurry and an alane slurry, respectively. The system design and the material properties can be modified beyond what is shown in the main GUI through the CH Material/Design button. The parameters that can be modified are described in more detail in Appendix A.
- An adsorbent-based hydrogen storage system with heat exchanger and balance of plant components for both powder and compacted forms of the adsorbent. Currently, the only adsorbent available is MOF-5, but additional adsorbents and user inputs for new adsorbents will be available in future versions. Further explanation of the adsorbent system models as well as the parameters that can be modified are described in more detail in Appendix B. The user can explore different designs through the Adsorbent System Design button on the main GUI.

The inclusion of more storage systems is planned for the future. The framework has also been exercised on several other systems based on cryoadsorbent, metal hydride, and chemical hydride materials (Thornton et al., 2012).

Hydrogen Storage System Design Tools

There are two storage system design tools that are accessible from the main GUI. One is for chemical hydride systems and the other for cryo-adsorbents. These tools allow the user to adjust inputs based on different materials and storage parameters which are then used in the system design routine. Results, including volume and mass of the system, are readily viewable from the GUI and can be saved and/or output for running in the vehicle framework. Figures 5 and 6 show the interfaces for these models.

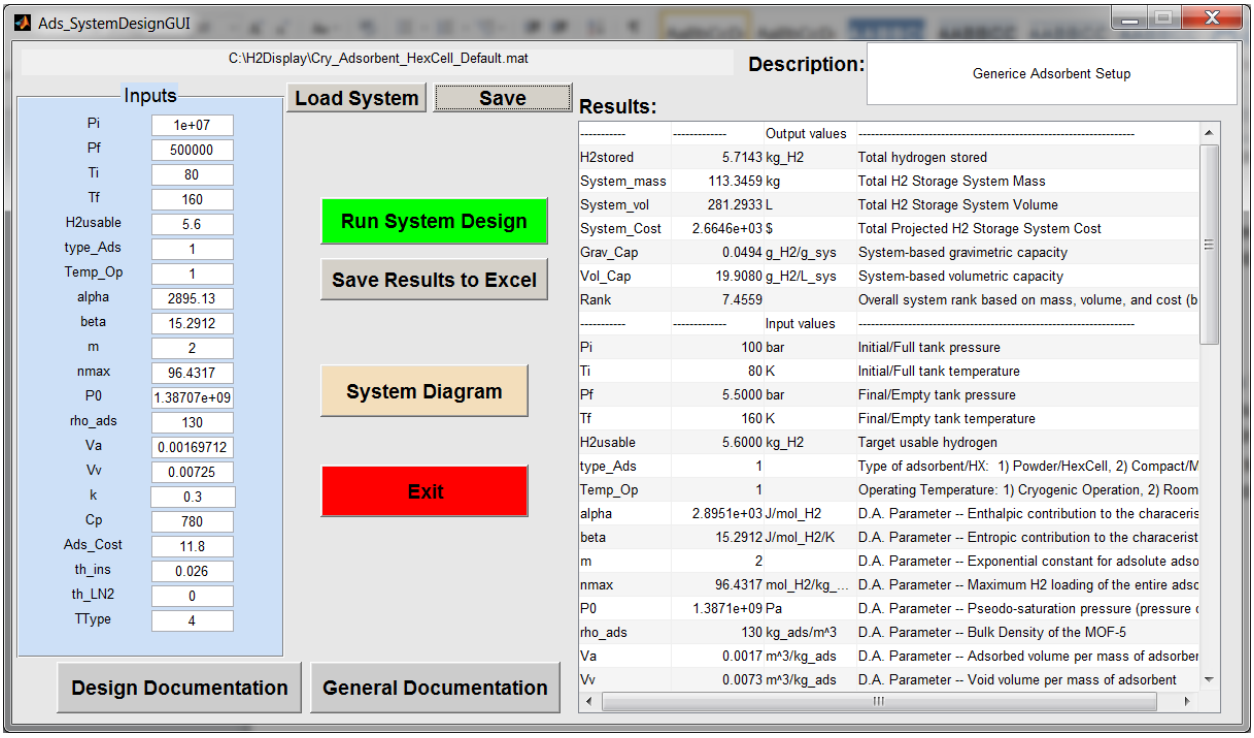

Figure 5. Interface for the Cryo-Adsorbent Storage System Design Tool.

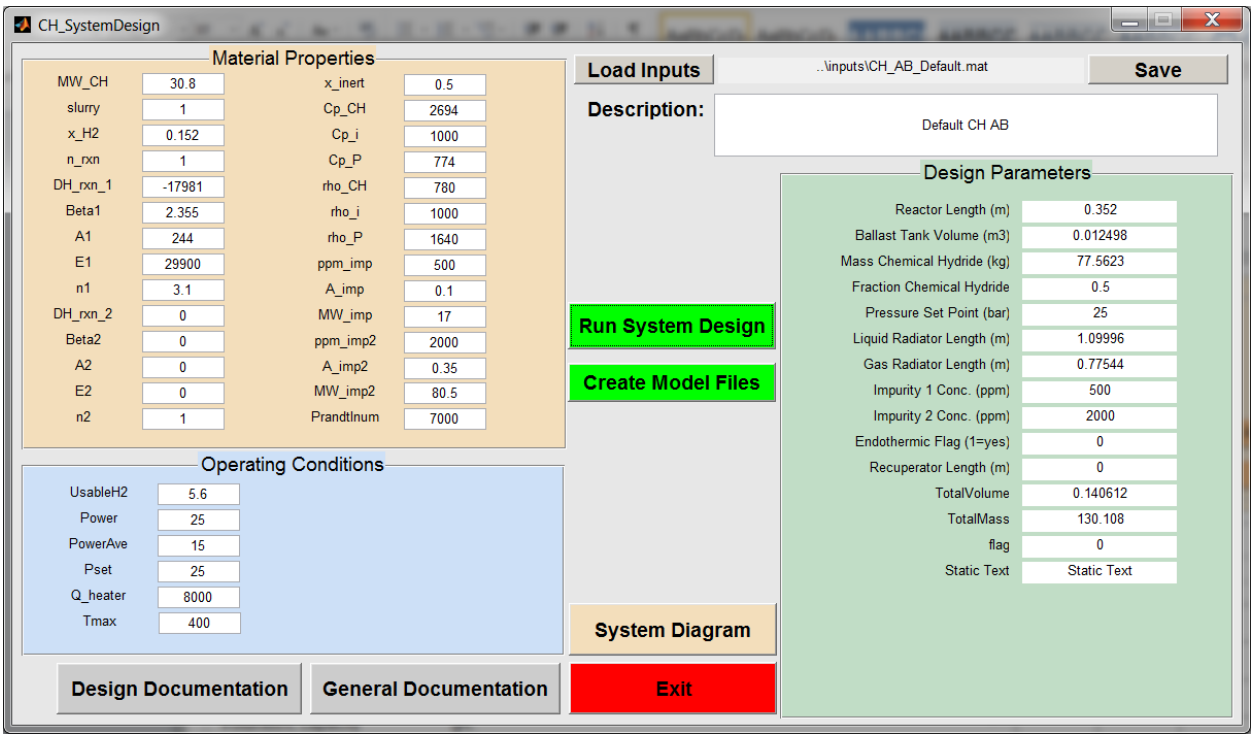

Figure 6. Interface for the CH Storage System Design Tool

USER MANUAL

INSTALLATION INSTRUCTIONS

SYSTEM REQUIREMENTS

In order to run this simulation tool, the user needs to have both MATLAB® (version 2013b has been tested while newer versions should also work) and the corresponding version of Simulink® installed.[2] MATLAB® is the platform that runs the GUI, while Simulink® runs the storage models themselves.

INSTALLATION STEPS

To have the vehicle simulation framework ready to run, please follow the following steps:

1. After downloading the zip file, choose a folder and unzip all the files to this folder. For example, the folder could be “My Documents\vehicle_simulation_framework”. From this point on we will call this folder the simulation framework’s “home” folder.
2. Open MATLAB and set the current folder to the “home” folder mentioned above.
3. Click on the Command Window of MATLAB. If the Command Window is not visible, you can make it visible by typing Ctrl+0 (the “Ctrl” key and the number zero).

STARTING THE GUI AND SETTING UP THE SIMULATION

To start the GUI, open MATLAB and set the current working path to the “home folder.” Then, on the MATLAB command line, execute the command “VehicleSimulatorGUI”. You will be greeted with the screen shown in 7. It has three sections. In the top section, the user selects the storage system to run. In the middle section, the user selects options to run with this specific storage system. The bottom section is where results will appear after the simulation has run to completion.

[2] Both MATLAB and Simulink are trademarks of The Mathworks, Inc.

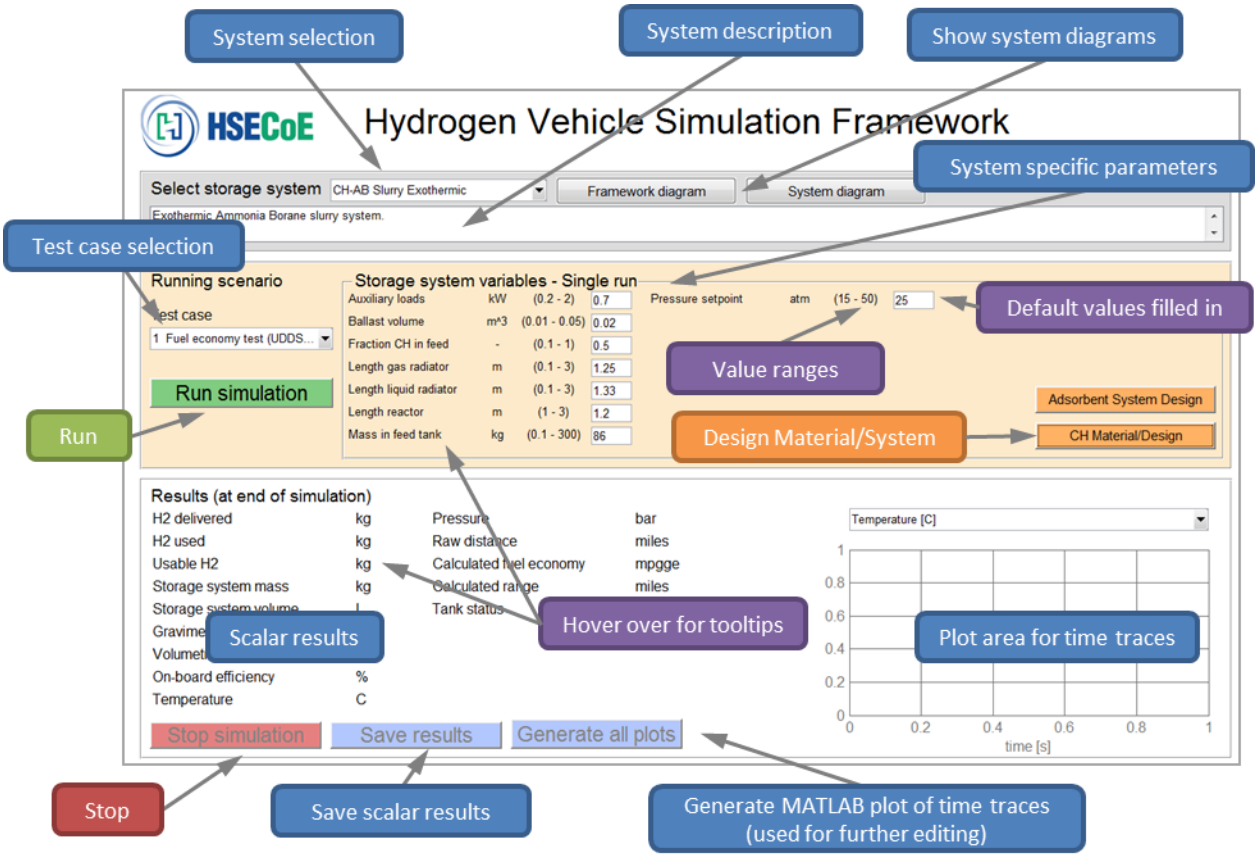

Figure 7. Initial screen of the GUI for the H_2 Vehicle Simulation Framework.

SELECTING THE STORAGE SYSTEM

At the top of the GUI you will see “Select storage system,” followed by a pull-down menu. Using this menu the user can select a different storage system. The larger text area underneath contains a longer description of the currently-selected system.

SELECTING THE PARAMETERS FOR THE RUN

The section “Storage system variables” shows the parameters available for adjustment by the user. Some of these parameters are shared by all storage systems, while others are only meaningful for certain systems. This means that selecting a different storage system may change the appearance of this section.

The entry for each parameter contains a brief description, followed by the units of that parameter (“-“ will appear for dimensionless parameters), the accepted range, and finally the entry itself. When a new system is selected, this field is filled with a default value. Note that hovering over a particular parameter makes a tooltip message appear with a somewhat longer description of the particular parameter.

RUNNING A SIMULATION

Once the running scenario and system variables have been selected, clicking the “Run simulation” button starts the simulation. This triggers a recompilation of some models that may have been modified due to changes in parameters. This is noted by a “Wait ~2 minutes” message on the green button. Once the recompilation is done and the simulation starts running, the current simulated time is also displayed on the green button. The simulation continues until the storage system cannot provide enough hydrogen to the fuel cell for it to satisfy the vehicle’s power demand. At the end of the simulation the scalar results and time traces are added to the “Results” section, as shown in 8.

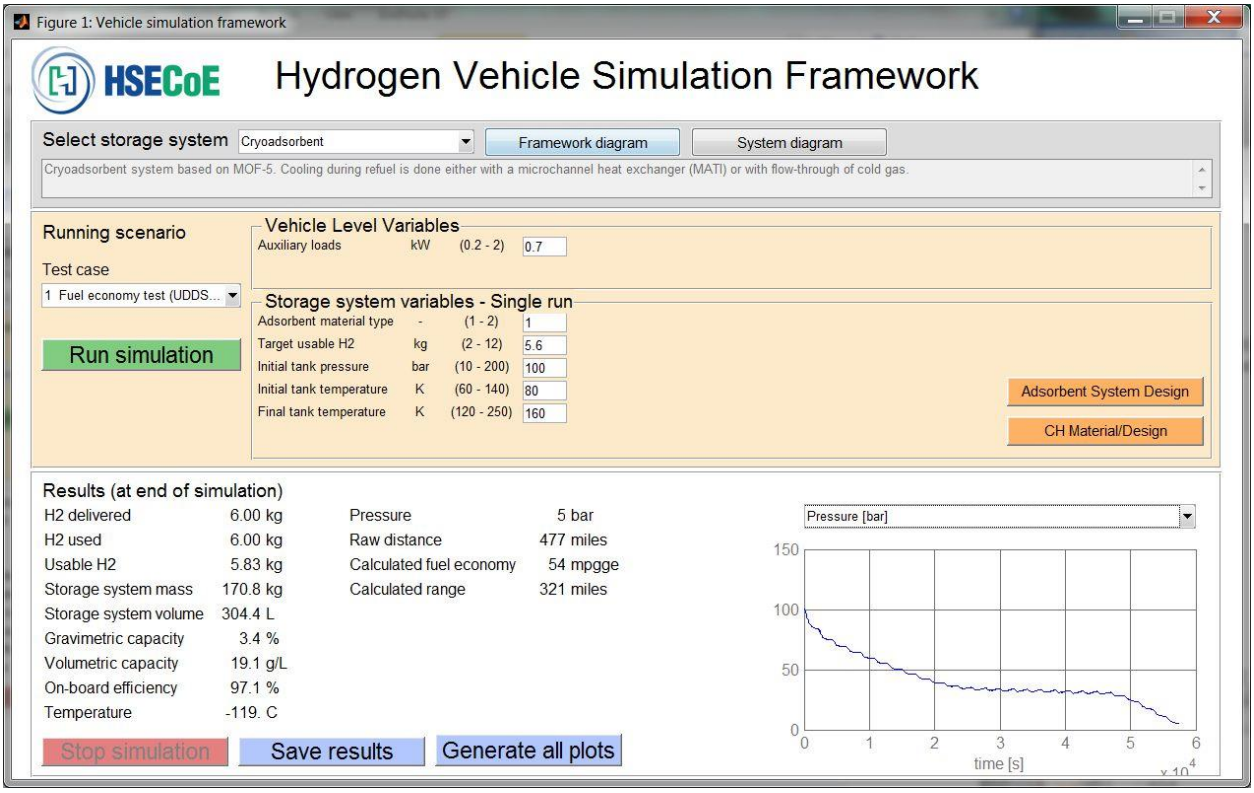

Figure 8. GUI after completing a simulation.

PLOTTING AND SAVING THE RESULTS

Once the simulation has finished, the “Save results” button may be used to save the results for future use. The resulting text file is tab-separated, so it can be directly opened with Excel for additional processing. It includes the scalar results as well as the time traces.

The “Generate all plots” button generates a MATLAB figure from each time trace, so as to make it available for saving as a MATLAB “fig” file, as well as for modification.

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APPENDIX A: CHANGING THE SETUP FILE FOR THE CHEMICAL HYDROGEN STORAGE MATERIAL MODELS

There is a small set of parameters that can be readily adjusted as part of the main Vehicle Framework GUI. If changes are required in the design of the system beyond this GUI or the model is run with a different material, the parameters can be changed through the “CH Material/Desgin” button in the main GUI. The details of the system components such as the reactor, radiators, phase separator and other balance of plant components are provided. Additionally, the kinetic, transport and thermodynamic parameters of a new material can be implemented into the design by adjusting the parameters in the material properties section. This data can be accessed for both ammonia borane and alane in the storage system design GUI by loading “ch_ab_slurry_Default.mat” and “ch_alane_slurry_Default.mat,” respectively from the “inputs” folder. The name of each of the parameters in these files along with their current value, units, and a short description are provided in Table A-1. When using the “run system design” button, several design parameters are displayed but many are behind the GUI and stored under the “Sized” field in the “*.mat” file. **Care should be taken when these variables are adjusted manually as it may result in the model crashing or stopping prematurely**. For example, the tuning parameters for the PI controllers used to control feed and recycle flow and the heat addition to the reactor have not been optimized for all possible cases.

In addition to the input file, there are additional parameters that provide the properties of the slurrying agent, hydrogen, and air that are used in the model.

Table A-1: Input Parameters to the CHS System Design Tool

	Values	Units	Comments
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
Useable H2	5.6	kg	Mass of usable hydrogen required
Power	40	kW	Maximum Hydrogen Storage H2 Production Required
PowerAve	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

Table A-2: Description of the Parameters for the Chemical Hydrogen Storage Materials

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
MW_CH(1)	30.8	30	g/mol	molecular weight of CH	
rhoCH	780	1486	kg/m3	solid density of CH without slurrying agent	
cpCH	2694	1000	J/kg/K	heat capacity of CH without slurrying agent	
rhoCHProd	1640	2700	kg/m3	solid density of CH product without slurrying agent	

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
cpCHProd	774	950	J/kg/K	heat capacity of CH product without slurrying agent	
rhoCHPmin	300	34	kg/m3	minimum density of foam product exiting reactor	assumes some H2 stays in slurry as a foam
MaxCHtoMaxH2	0.152	0.1	kg H2/kg CH	maximum mass fraction H2 in CH	
preExpRxn1_SAB	281	1.20E+10	s-1	Arrhenius pre-exponential factor "first equivalent"	"first equivalent" represents the reaction that can be described by the first Avrami equation and is not limited to exactly one equivalent of H2
actNrgRxn1_SAB	2.99E+04	1.02E+05	J/mol	activation energy "first equivalent"	
preExpRxn2_SAB	4.18E+15	0	s-1	Arrhenius pre-exponential factor "second equivalent"	"first equivalent" represents the reaction that can be described by the second Avrami equation and is not limited to exactly one equivalent of H2
actNrgRxn2_SAB	1.49E+05	0	J/mol	activation energy "second equivalent"	
n1_SAB	3.1	2		Avrami exponent "first equivalent"	
n2_SAB	1.2	1		Avrami exponent "second equivalent"	
beta1_SAB	1.43	1.5		hydrogen generated in "first equivalent"	amount of equivalents of H2 produced from first Avrami equation
beta2_SAB	0.925	0		hydrogen generated in "second equivalent"	amount of equivalents of H2 produced from second Avrami equation
beta1factor_SAB	1.20E-04	1		multiplier to calculate Beta1 at reduced temperatures	

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
beta2factor_SAB	4.20E-07	1		multiplier to calculate Beta2 at reduced temperatures	
betan1_SAB	2	1		exponent to calculate Beta1 at reduced temperatures	
betan2_SAB	3	1		exponent to calculate Beta2 at reduced temperatures	
deltaHRxn1_SAB	19895	-7600	J/mol H2	reaction enthalpy "first equivalent"	negative for endothermic, positive for exothermic
deltaHRxn2_SAB	1500	0	J/mol H2	reaction enthalpy "second equivalent"	
OuterDiaRtr	4.44E-02	4.44E-02	m	outer diameter of reactor metal shell	
InnerDiaShaft	4.76E-03	4.76E-03	m	diameter of stir shaft	area displaced by central stirrer is removed from flow area
OuterDiaCha	4.11E-02	4.11E-02	m	inner diameter of reactor	
Dslurry	1.50E-02	1.50E-02	m	estimated interface diameter between gas and slurry	model assumes gas flows through the center of the reactor near the stirrer and slurry flows along the outside
k1_limit	1.36	2.03E+02	s-1	maximum reaction rate constant "first equivalent"	
k2_limit	0.766	0	s-1	maximum reaction rate constant "second equivalent"	
c_shaft	3.38E-04	3.38E-04	m/rpm	axial displacement of auger (if present)	auger not in current design
shaftrpm	0	0	rpm	shaft rotational speed	slurry flow due to auger is added to pressure drop flow

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
viscosity	0.5	0.5	kg/m/s	slurry viscosity	
Prandtlnum	7000	7000		slurry Prantl number	
thick_tube	8.89E-04	8.89E-04	m	reactor wall thickness	
k_insulation	0.06	0.06	W/m/K	thermal conductivity of reactor insulation	
hinf	10	10	W/m2/K	convection coefficient on outside of reactor insulation	
t_insulation	0.0254	0.0254		thickness of reactor insulation	
Q_heater	8000	8000	W	power to reactor heater	
mass_ps	0.8	0.8	kg	mass of phase separator in contact with slurry	only heating bottom 1/4 of phase separator
lenPS	0.302	0.302	m	length of phase separator	
diaPS	0.089	0.089	m	diameter of phase separator	
n_tubes_liq	1	1		number of parallel tubes in slurry radiator	
intdia_hx_liq	0.007747	0.007747	m	inner diameter of slurry radiator	radiator is finned tube design
extdia_hx_liq	0.009525	0.009525	m	outer diameter of slurry radiator	
thick_fin	0.00046	0.00046	m	fin thickness in slurry radiator	
dia_fin	0.0254	0.0254	m	diameter of the fin in slurry radiator	
pitch_fin	0.00254	0.00254	m	pitch of fins in slurry radiator	
pitchturb	0.0762	0.0762		pitch of turbulator inside of slurry radiator tube	

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
n_tubes_gas	1	1		number of parallel tubes in gas radiator	
extdia_hx_gas	0.00635	0.00635	m	outer diameter of gas radiator	
intdia_hx_gas	0.0052	0.0052	m	inner diameter of gas radiator	fin pitch and thickness same as slurry radiator
dia_fin_gas	0.0159	0.0159	m	diameter of the fin in gas radiator	pitch of turbulator same as slurry radiator
intdia	0	0.0127	m	outer diameter of inner tube	recuperator is a counterflow tube-in-tube configuration
extdia	0	0.0196	m	outer diameter of outer tube	
t_int	0	5.59E-04	m	wall thickness of inner tube	
t_ext	0	8.89E-04	m	wall thickness of outer tube	
MParam(1)	51.924	51.924	kg/L	mass coefficient for feed tank	used for system mass calculation
VParam(1)	1.75	1.75	kg	intercept for feed tank mass	used for system mass calculation
MParam(3)	0.316	0.316	kg/m length	specific mass gas radiator	used for system mass calculation
VParam(3)	2.00E-04	2.00E-04	m3/m length	specific volume gas radiator	used for system volume calculation
MParam(4)	0.544	0.544	kg/m length	specific mass slurry radiator	used for system mass calculation
VParam(4)	8.66E-04	8.66E-04	m3/m length	specific volume slurry radiator	used for system volume calculation
MParam(5)	173.9	173.9	kg/m3/atm	specific mass ballast tank	used for system mass calculation

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
VParam(5)	1	1	m3/m3 volume	specific volume ballast tank	used for system volume calculation
MParam(6)	0.004	0.004	kg/ppm	mass NH3 scrubber	used for system mass calculation
VParam(6)	6.80E-06	6.80E-06	m3/ppm	volume NH3 scrubber	used for system volume calculation
MParam(7)	0.0042	0.0042	kg/ppm	mass borazine scrubber	used for system mass calculation
VParam(7)	0.000003	0.000003	m3/ppm	volume borazine scrubber	used for system volume calculation
MParam(8)	32.1	27.8	kg	mass BOP	used for system mass calculation
VParam(8)	0.0268	0.0193	m3	volume BOP	used for system volume calculation
TargetTemp	150	280	°C	setpoint reactor temperature	exothermic: target reactor inlet tempature endothermic: target reactor outlet temperature
StartupTemp	200	220	°C	temperature when flow to reactor begins	prior to startup temperature, reactor is warming
Recycle_Ratio	2.5	0	kg/kg	maximum recycle ratio	recycle:feed mass ratio
mdot_feed_max	0.0167	0.0167	kg/min	limit on total mass flow of feed	
mdotrecycle_max	0.04175	0.0167	kg/min	limit on total mass flow of recycle	
Tproduct_max	250	280	°C	setpoint for maximum reactor temperature	
kp	0.0001336	1.34E-04	kg/s/atm	proportional gain for feed flow controller	compares ballast tank pressure to setpoint
ki	1.34E-06	1.34E-06	kg/s2/atm	integral time constant for feed flow controller	

Parameter	Exothermic Model Value	Endothermic Model Value	Units	Description	Notes
kd	0	0	kg/s2/atm	derivative time constant for feed flow controller	
kp_heat	0	26.7	W/°C	proportional gain for reactor heater	compares reactor temperature to setpoint
ki_heat	0	2.67	W/s/°C	integral time constant for reactor heater	used for endothermic systems only
kd_heat	0	0	W/s/°C	derivative time constant for reactor heater	used for endothermic systems only
kpt	5.00E-05	0	kg/s/°C	proportional gain for cold feed recycle	compares reactor temperature to setpoint
kit	3.00E-07	0	kg/s2/°C	integral time constant for cold feed recycle	used for exothermic systems only

Table A-2: Description of the Constants for the Chemical Hydrogen Storage Models

Parameter	Value	Units	Description	Notes
k_liq	1	W/m/K	Thermal conductivity of slurrying agent	Assumed to be AR-20 silicone oil and increased to account for slurry mixture
rhoInert	1070	kg/m^3	Density of slurrying agent	Assumed to be AR-20 silicone oil
cpInert	1846	J/kg/K	Heat capacity of slurrying agent	Assumed to be AR-20 silicone oil
rhometal	8000	kg/m^3	reactor metal density	Assumed to be stainless steel
cpmetal	480	J/kg/K	reactor metal heat capacity	Assumed to be stainless steel, 300K
k_metal	177	W/m/K	heat exchanger fin heat capacity	fin assumed to be aluminum
cpH2	14500	J/kg/K	H_2 heat capacity	based on film temp of 450K

Parameter	Value	Units	Description	Notes
MW_H2	2	g/mol	H_2 molecular weight	
Pr_H2	0.690		H_2 Prandtl Number	based on film temp of 450K
mu_H2	117.2e-7	kg/m/s	viscosity of H_2 gas (dynamic)	based on film temp of 450K
k_H2	0.247	W/m/K	H_2 thermal conductivity	based on film temp of 450K
cpair	1009	J/kg/K	air heat capacity	based on film temp of 350K
Pr_air	0.7		air Prandtl Number	based on film temp of 350K
k_air	0.03	W/m/K	air thermal conductivity	based on film temp of 350K
v_air	4.5	m/s	air velocity across the radiators	based on 10 mph speed
mu_air	2.08e-7	kg/m/s	air viscosity (dynamic)	based on film temp of 350K
rho_air	0.995	kg/m^3	air density	based on film temp of 350K

APPENDIX B: SYSTEM EXPLANATION AND OPTIONS AVAILABLE FOR THE ADSORBENT HYDROGEN STORAGE SYSTEM MODELS

The adsorbent hydrogen storage system models were originally written as a scoping tool to evaluate individual options and combinations of adsorbent materials, internal and external heat exchangers, pressure vessel designs, and balance of plant components. In all cases, the goal was to store 5.6 kg of usable hydrogen and calculate the resulting system response capabilities, overall system efficiency, gravimetric capacity, and volumetric capacity. The two system designs with the best balance of capabilities and versatility are provided, with their schematics shown in Figure 7.

Adsorbent system #1 is a powder-based system that utilizes a honeycomb heat exchanger with resistance heating (called HexCell) and a simplified balance of plant (BOP), as shown in Figure 7a. The powder adsorbent currently available for this system is MOF-5, with a density of 0.18 g/cc. A glycol-water heat exchanger connected to the fuel cell radiator is used to warm the hydrogen above the minimum acceptable fuel cell temperature (-40 ^{o}C). Adsorbent system #2 is a compacted adsorbent system that utilizes an isolated-fluid super-fin heat exchanger (called MATI) with a recirculating BOP, as shown in Figure 7b. The compacted adsorbent is MOF-5, which has been compacted to 0.52 g/cc. The recirculating BOP uses a hydrogen combustor coupled with the external heat exchanger connected to the fuel cell radiator to heat hydrogen before sending it back through the pressure vessel via the MATI to release more hydrogen. The hydrogen passing through the MATI is then re-heated by re-passing it through the external heat exchanger to warm the hydrogen above the minimum acceptable fuel cell temperature.

The available user controls are listed in Table B-1. Note that the imposed operating limits are set to match the limits of the adsorption data which forms the basis for the adsorbent models. This adsorption data was fit to the Modified Dubinin-Astakhov adsorption isotherm model as per Richard et al. (2009). Using the adsorbent model outside of these operating conditions could result in unrealistic results and/or model failure. Also note that for each set of user inputs, a pressure vessel is designed around the adsorbent and internal heat exchanger using the Hydrogen Storage Tank Mass and Cost Estimation Model ("Tankinator").

Additional inputs and system design functionality are available through the "Adsorbent System Design" button found on the main Framework GUI.

Table B-1: Description of the User Controls for the Adsorbent Hydrogen Storage Model

Parameter	Minimum value	Maximum value	Units	Description
Pi	$1.0x10^6$	$10.0x10^6$	Pa	Full tank pressure
P_FC	$0.5x10^6$	$0.5x10^6$	Pa	Empty tank pressure (pre-set to the fuel cell rail pressure)
Ti	77.0	300.0	K	Full tank temperature
Tf	77.0	320.0	K	Empty tank target temperature. This temperature should be set to Ti ≤ Tf ≤ Ti + 100 K
H2usable	0.5	12.0	Kg_{H2}	Usable hydrogen storage target
Type_Ads	1	2	-----	Type of Adsorbent: 1 – Powder MOF-5 using a HexCell heat exchanger 2 – Compacted MOF-5 using a MATI heat exchanger

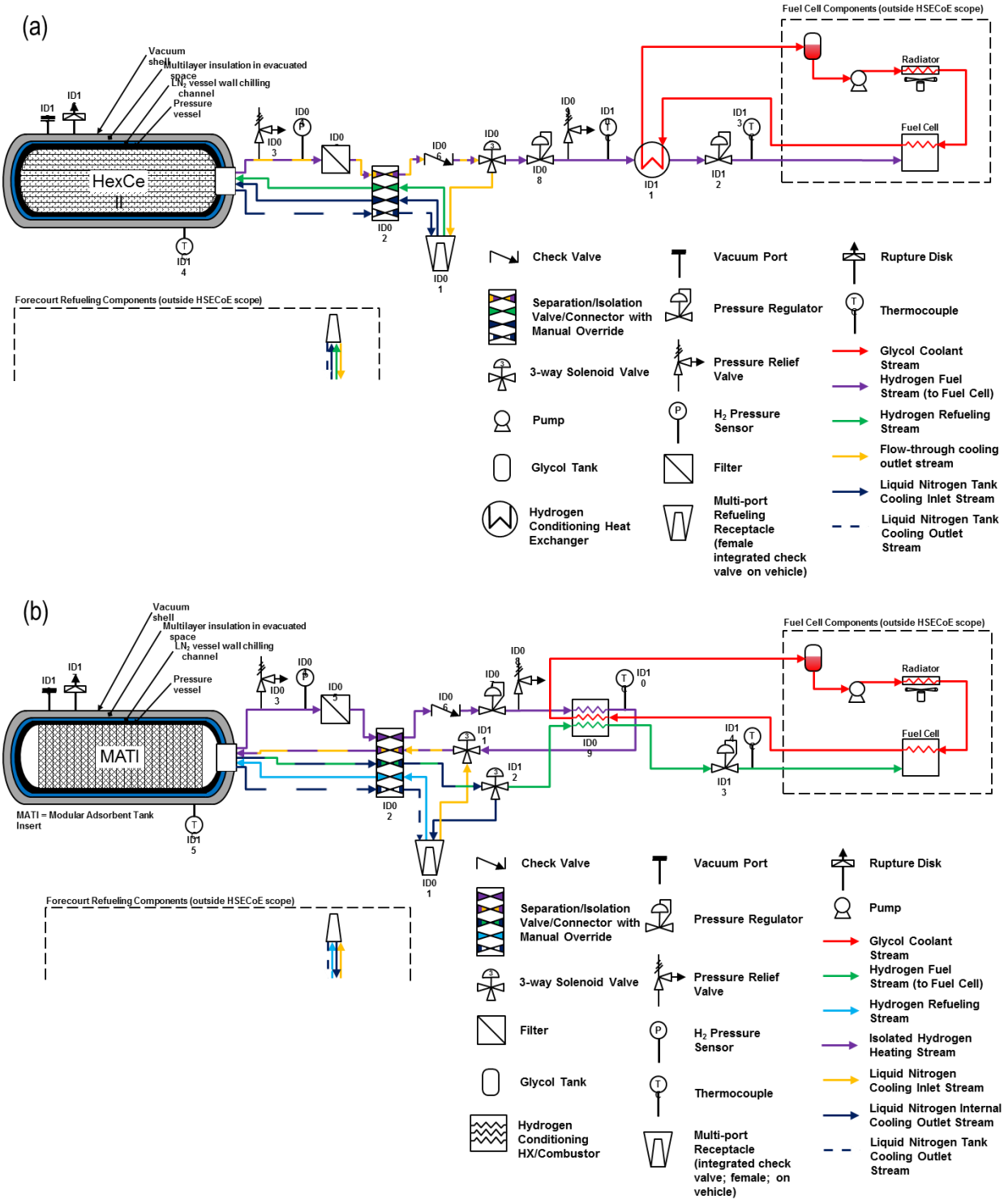

Figure 7: Schematics of the Cryo-Adsorbent Hydrogen Storage System Designs for a a) powder adsorbent (HexCell heat exchanger) and b) compacted adsorbent (MATI isolated-fluid heat exchanger).