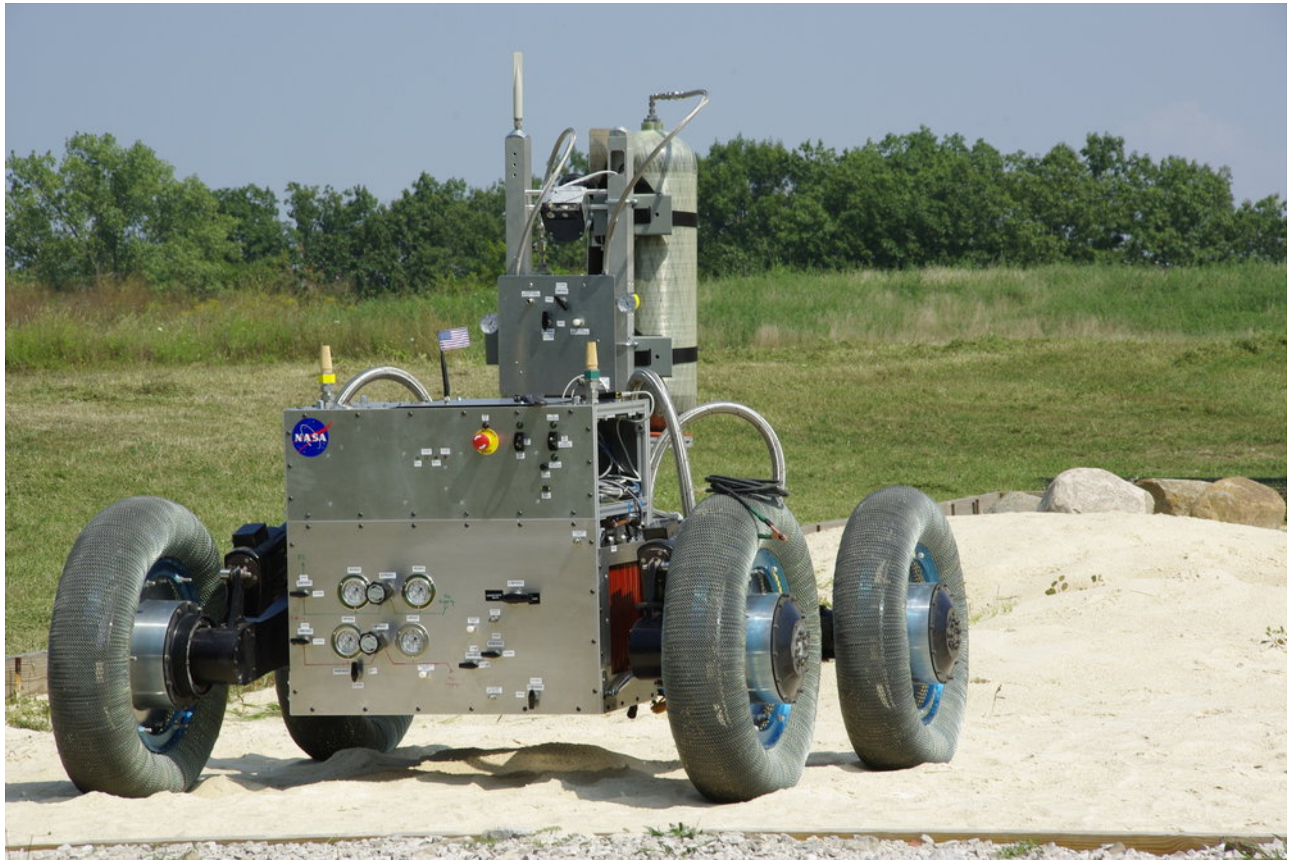
Fuel Cell Model Validation with Power Module Test Data



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Background

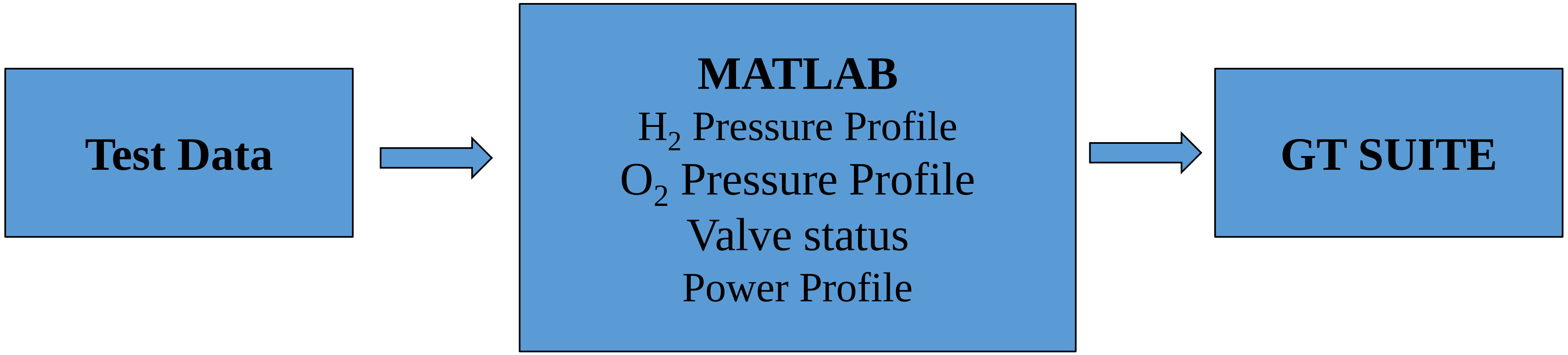
- AMPS fuel cell team at NASA Glenn Research Center has been building a regenerative fuel cell (RFC) model since 2017 that predicts various RFC performance parameters including system energy density, power density, and efficiency
  - Model is Excel based and while it works well for high level trade studies, a fluids/thermal model that could predict fluid transients was desired
- After discovering GT SUITE at TFAWS 2017, several engineers at NASA GRC participated in a free trial
- The AMPS project funded a 1 year trial of GT SUITE to determine the efficacy of using the program to model a transient non-flow through fuel cell system

Introduction

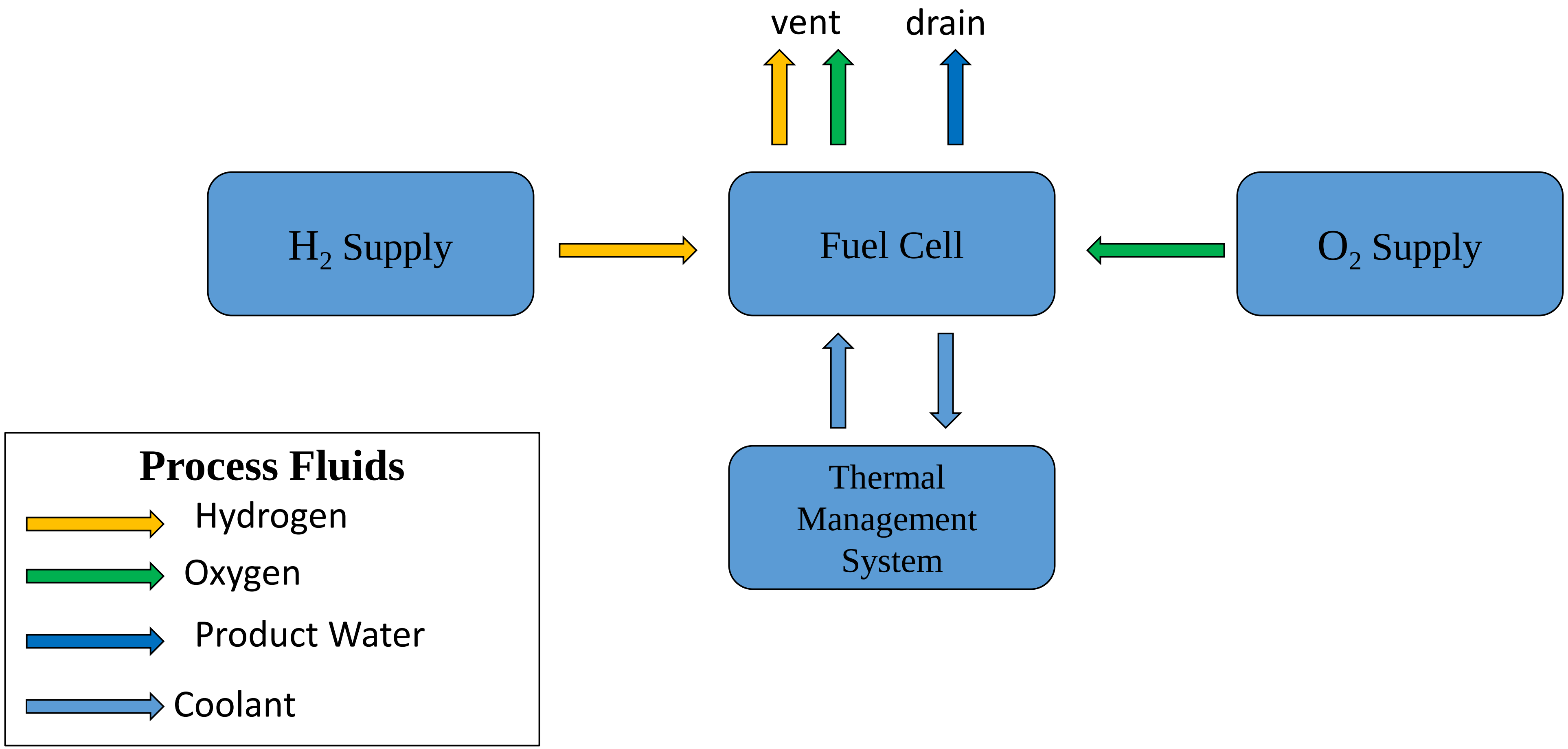
- A transient fuel cell model was created in GT-SUITE
- The purpose of the model was to verify GT SUITEs electrochemical and thermal/fluids performance results against actual test data of a Non-Flow-Through fuel cell system
- Test data from the AES Modular Power Systems (AMPS) fuel cell Power Module was used
  - Test data from Power Module Checkout Test on March 24, 2015

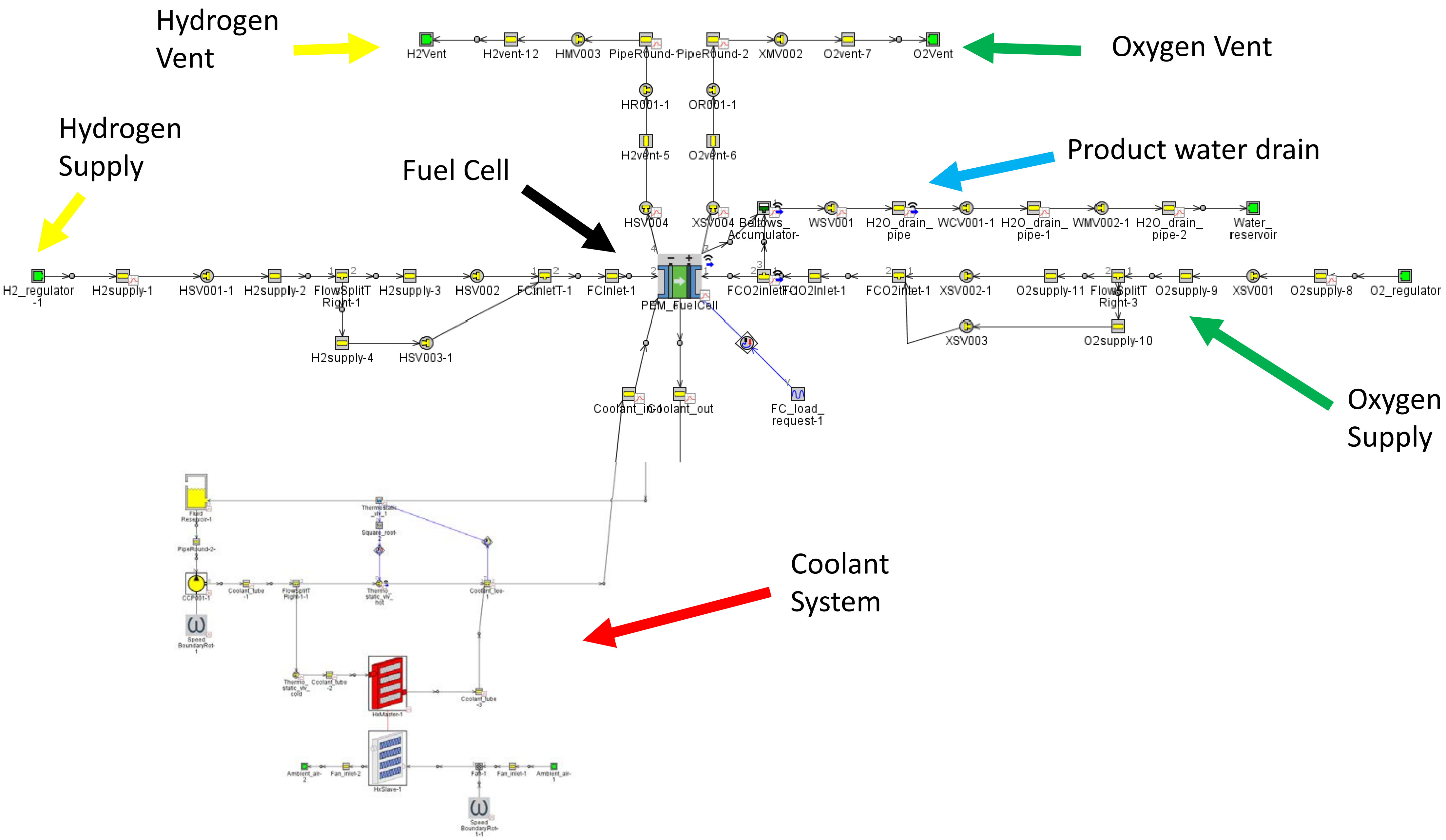
Data Processing for Model Inputs

- A MATLAB code was written to process the test data so that transient inputs could be incorporated into the GT model
  - Also so model results could be compared to test results
- Transient inputs include: valve status (open/closed), electrical load request, and input pressure



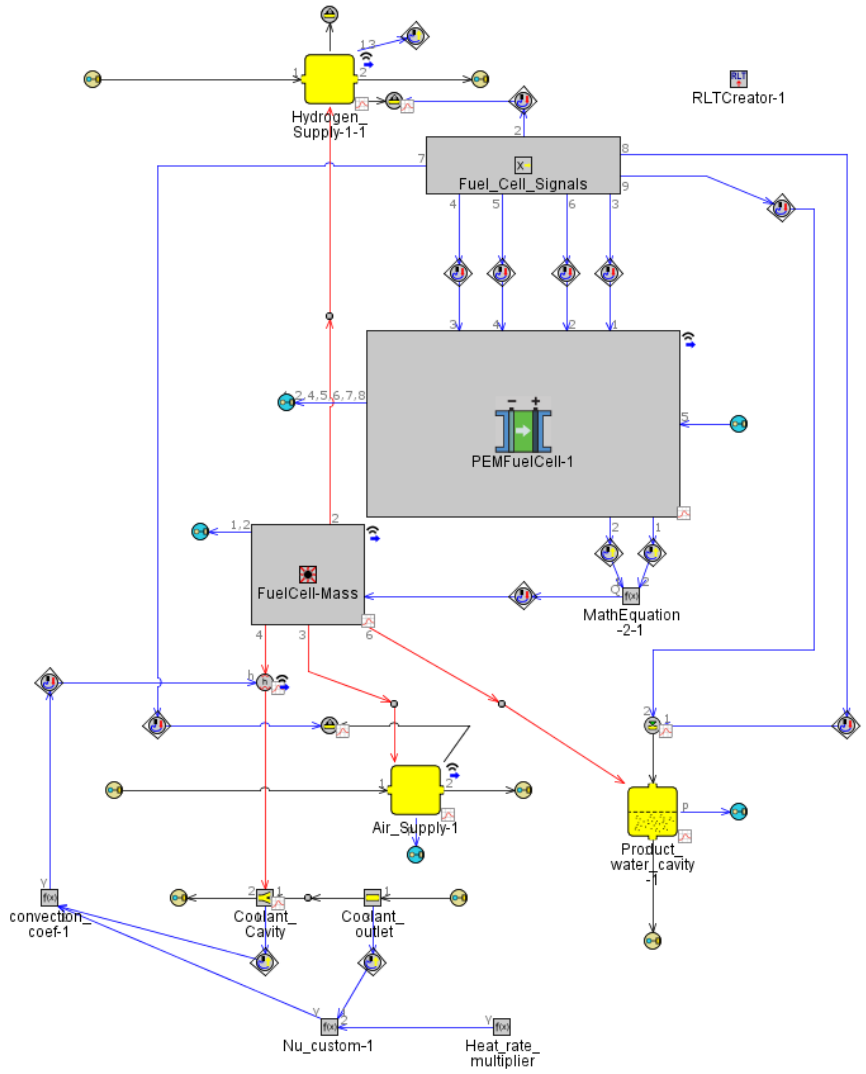
Model Layout




Hydrogen Vent
Oxygen Vent
Hydrogen Supply
Fuel Cell
Product water drain
Oxygen Supply
Coolant System
H2Vent
H2vent-12
HMV003
PipeRound-1
PipeRound-2
XMV002
O2vent-7
O2Vent
HR001-1
OR001-1
H2vent-5
O2vent-6
HSV004
XSV004
Bellows_Accumulator-
WSV001
H2O_drain_pipe
WCV001-1
H2O_drain_pipe-1
WMV002-1
H2O_drain_pipe-2
Water_reservoir
H2_regulator-1
H2supply-1
HSV001-1
H2supply-2
FlowSplitTRight-1
H2supply-3
HSV002
FCinletT-1
FCInlet-1
PEM_FuelCell
FCO2inletT
FCO2Inlet-1
FCO2inlet-1
XSV002-1
O2supply-11
FlowSplitTRight-3
O2supply-9
XSV001
O2supply-8
O2_regulator
H2supply-4
HSV003-1
XSV003
O2supply-10
Coolant_in
Coolant_out
FC_load_request-1

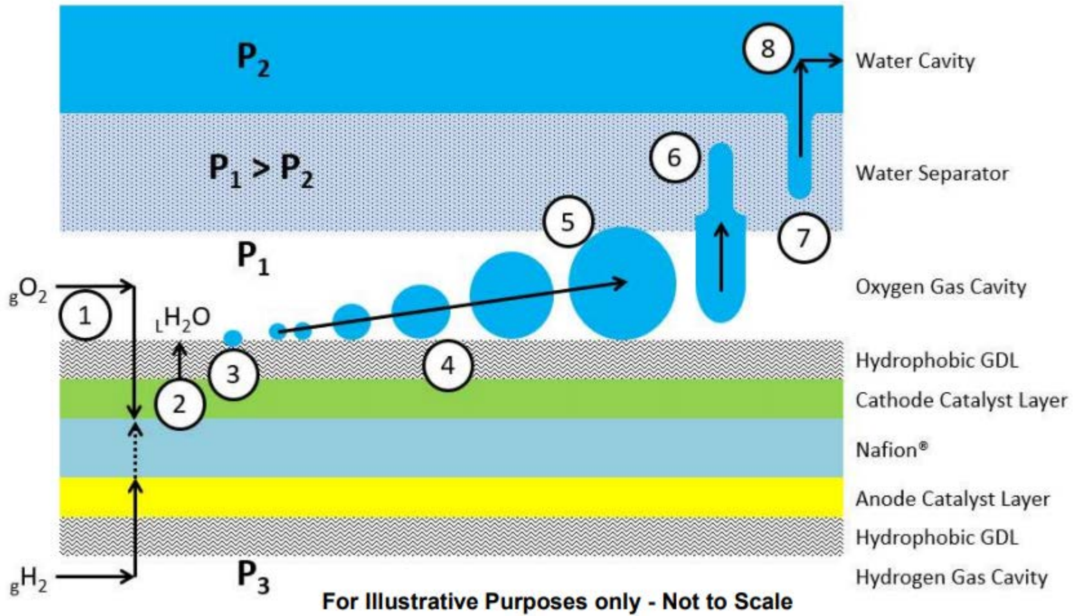
Custom PEM Fuel Cell Template

- Standard GT SUITE PEMFuelCellMT template with several modifications:
  - Fuel Cell Waste Heat Generated
  - Integral coolant cavity with heat transfer calculation
  - Discreet product water cavity
- PEM Fuel Cell Template within compound template calculates electrochemical performance of the fuel cell



Product water cavity

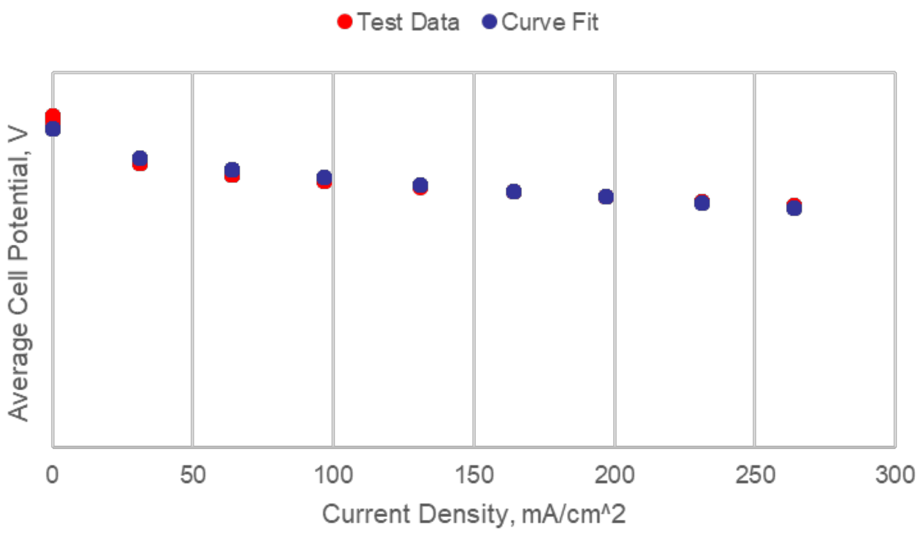
- In terrestrial fuel cells, product water is normally removed by flowing excess air through the oxygen cavity
- This is how the default GT SUITE fuel cell template is set up
- For aerospace fuel cells, pure oxygen is utilized and reactants are only moved through the stack at stoichiometric consumption rates
- Fuel cell stack used in Power Module testing has an Advanced Product Water Removal (APWR) capability with means of passively transporting product water into it’s own discreet cavity where it can be drained from the stack



Non-flow through fuel cell concept [3].

Fuel Cell Performance

- Fuel cell performance based on electrochemical coefficients input into GT SUITE
- Polarization curve from fuel cell test on December 17, 2014 was plotted and curve fit to generate performance coefficients
  - These coefficients resulted in poor performance agreement with test data
  - GT SUITE internally calculates reversible cell potential and without knowledge of this value it is difficult to accurately generate performance coefficients
  - GT engineers were able to use an internal program to generate higher accuracy coefficients
- Note homogeneity is assumed across all cells in the model and therefore an average cell potential is used to account for differences between cells



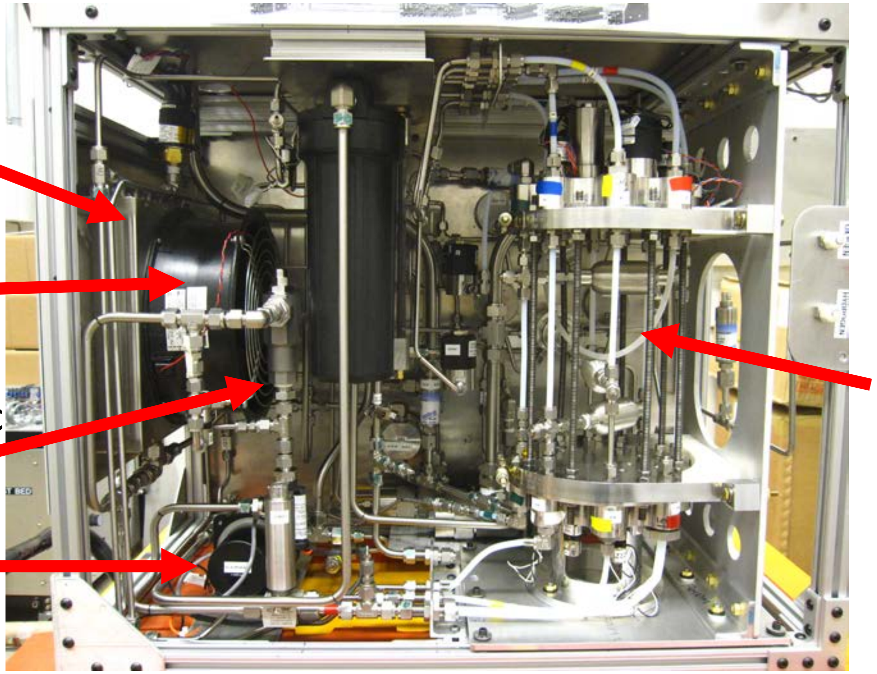
Coolant System

Heat Exchanger

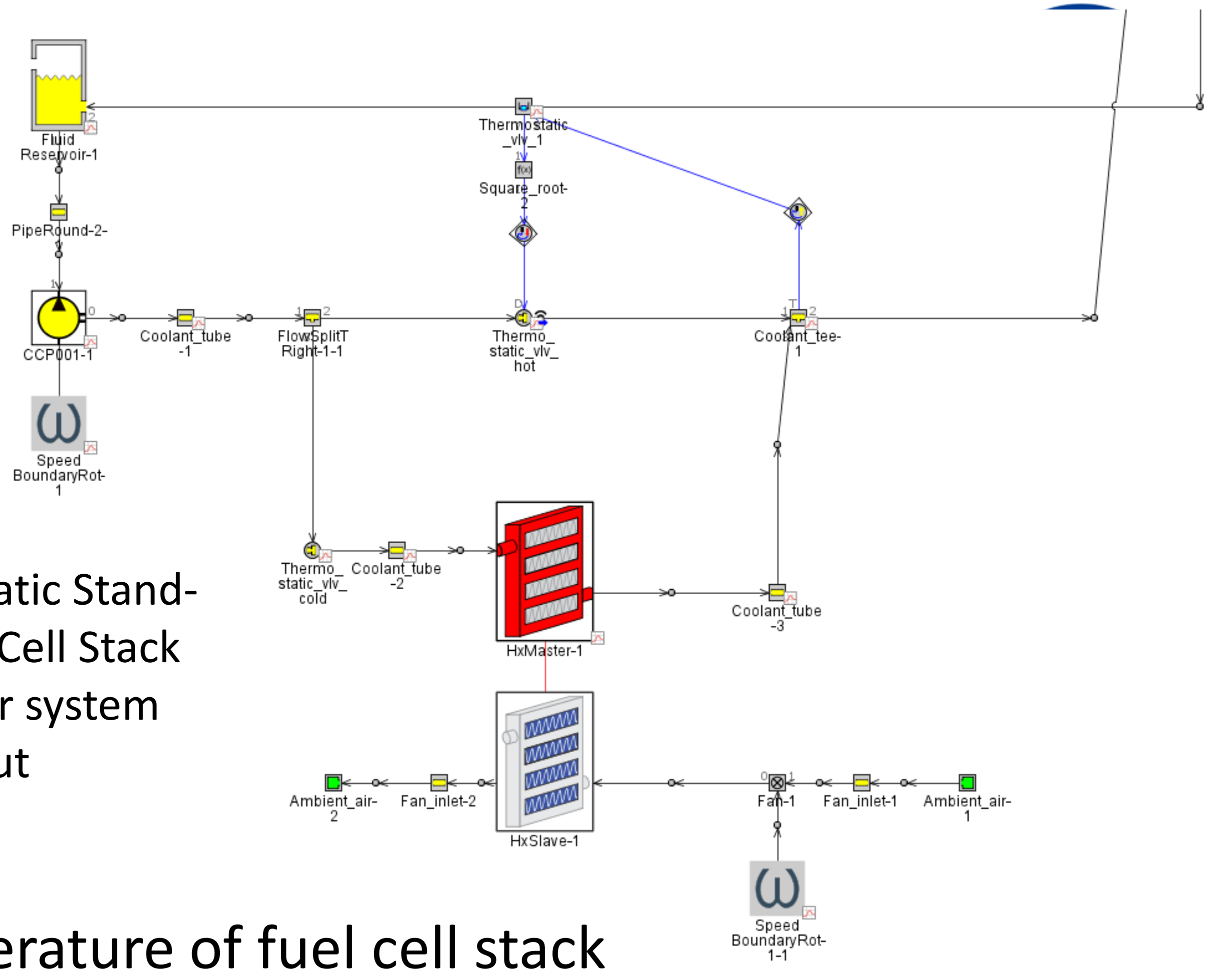
Heat Exchanger Fan

Thermostatic Valve

Coolant Pump



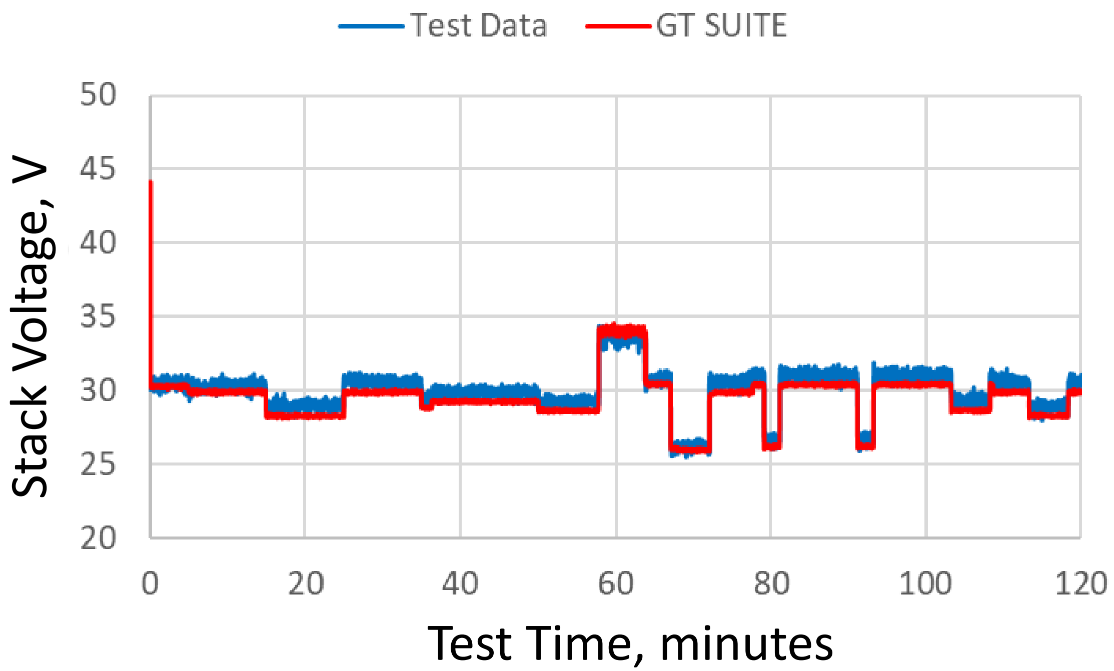
Pneumatic Stand-In Fuel Cell Stack used for system checkout



- Deionized coolant loop used to control temperature of fuel cell stack
- Tube-fin heat exchanger with fan used to reject heat generated by fuel cell
- Thermostatic valve regulates coolant inlet temperature to 65 °C
- Pump speed controlled as a function of stack temperature
- Heat exchanger, fan, thermostatic valve, pump, and reservoir modeled individually as components of coolant system

MODELING RESULTS

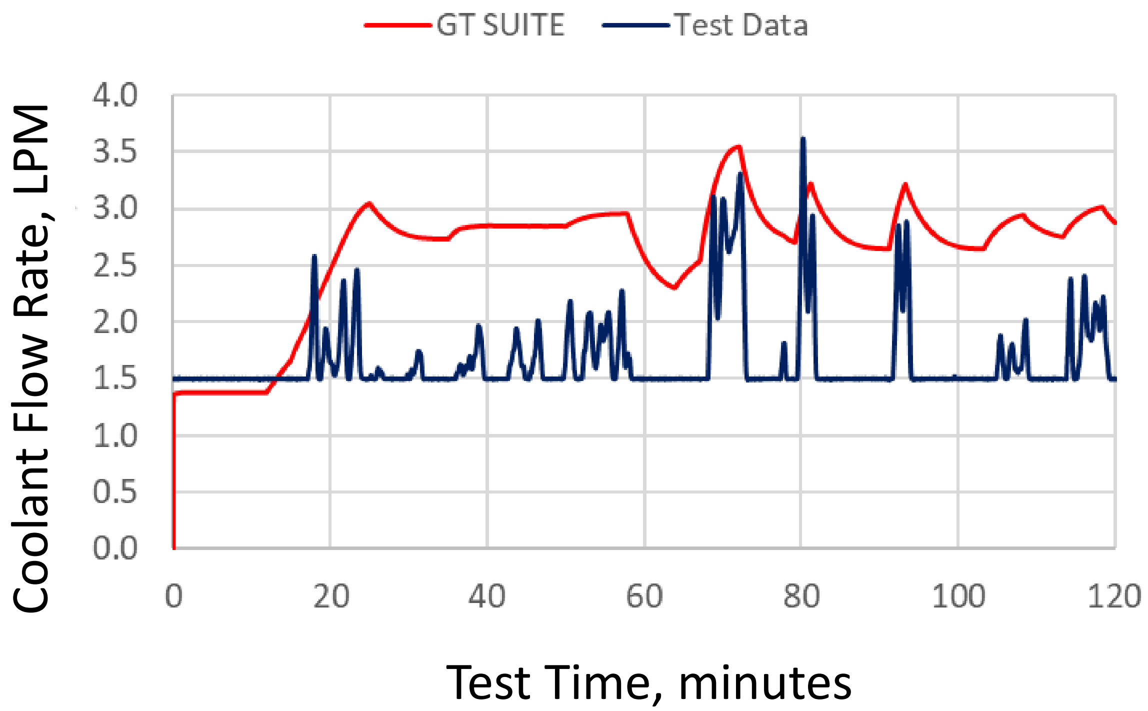
Electrochemical Performance



- Excellent agreement between average cell potential from test data and predicted stack voltage from GT SUITE
- Fuel cell meets power demand and also has excellent agreement with requested power load (and therefore current)

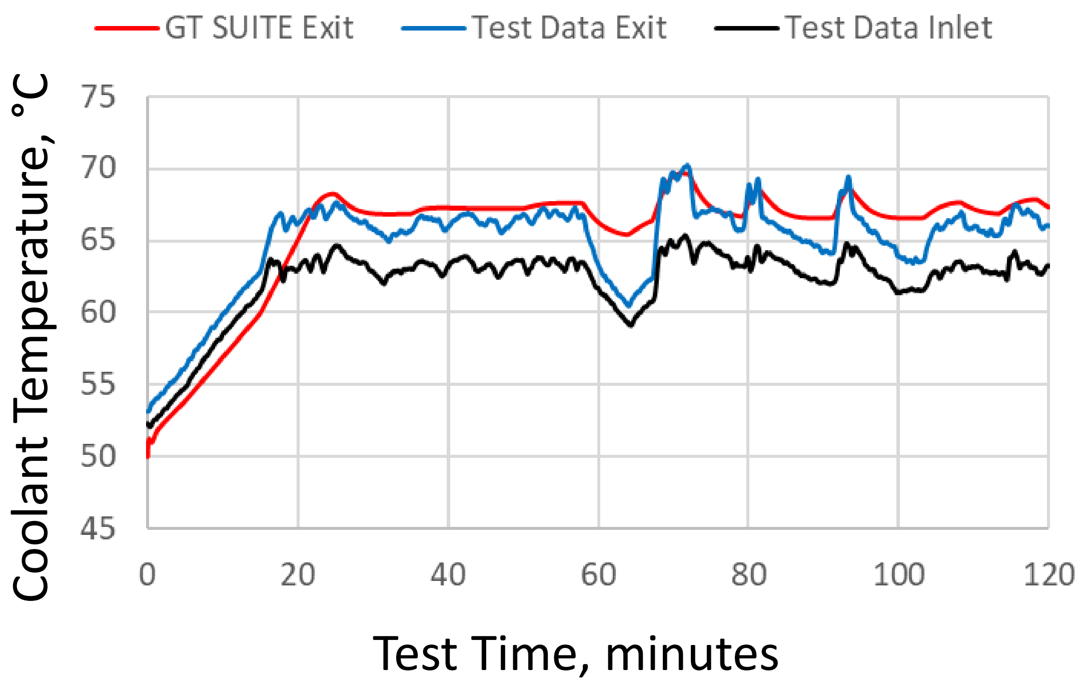
Coolant Flow Rate

- The GT model controlled pump speed based on the fuel cell stack temperature
- In actuality, the Power Module controlled pump speed based on both the coolant outlet temperature and temperature difference between coolant inlet and outlet
- Forward work remains to revise the pump control logic in the GT model to more closely match the real-world controls
  - Coolant flow rate matches trends in data well



Temperature

- Fuel cell temperature not directly measured during testing but the coolant exit temperature is assumed to resemble the stack temperature
- GT predicted exit coolant temperature agrees well with measured exit coolant temperature
  - Average deviation of 1-2 °C above the measured coolant exit temperature with temperatures
- Results indicate similar heat transfer between fuel cell and coolant for GT and testing result



Conclusion

- Model accurately predicts thermal, fluidic, and electrochemical performance of Power Module during testing
  - Modeling results vs test data presented for several key performance parameters
  - Adjustment of pump speed control logic is required for better coolant flow rate agreement
  - Successful validation of modeling approach against test data
- GT SUITE “Flow-Through” fuel cell template can be converted into a “Non-Flow-Through” fuel cell for aerospace fuel cell modeling
- Several other parameters have interesting results but were not presented due to time constraints
  - Product water cavity control, reactant consumption rates, heat exchanger performance

Acknowledgements

- Thank you to the NASA Advanced Exploration Systems (AES) AMPS program for funding this work and to the AMPS fuel cell team for a successful demonstration of the Power Module on the Scarab Rover
  - Karin Bozak, Monica Guzik, Ian Jakupca, Phillip Smith, Hank Kacher
- Thank you to GT support engineers Jake How, Tom Wanat, and Jonathan Harrison for technical support while building the model

Backup Slides

Stack Heat Generation

- The thermo-neutral voltage (V_{TN}) is the theoretical cell voltage where no waste heat would be produced during the redox reaction
  - In reality the cell voltages will always be lower than the V_{TN} and the waste heat generated is directly proportional to this difference [1]

$$Q = (V_{TN} - V_{cell}) I_{stack} n_{cells} \tag{1}$$

- GT SUITE calculates a waste heat load that is slightly less than Equation 1 so a MathEquation template was used to calculate the waste heat generation and the default GT source heat was deleted
- The waste heat that is generated needs to be removed via the thermal control system, in this case a deionized water cooling loop

Coolant Cavity

- Coolant cavity plus inlet and outlets were added to the fuel cell template
- Original GT fuel cell template has temperature control via PID controlled convection coefficient based off target temperature
- Wanted to have heat rejection reflect coolant conditions (flow rate, velocity, temp, etc)
- Finding a correlation for heat transfer through intricate coolant cavities was difficult
  - Complex geometry and flow path
  - Calculated Nusselt number as a function of coolant mass flow using the test data [2]

$$Q_{out} = \dot{m}_{coolant} c_p \Delta T_{coolant} \quad (2)$$

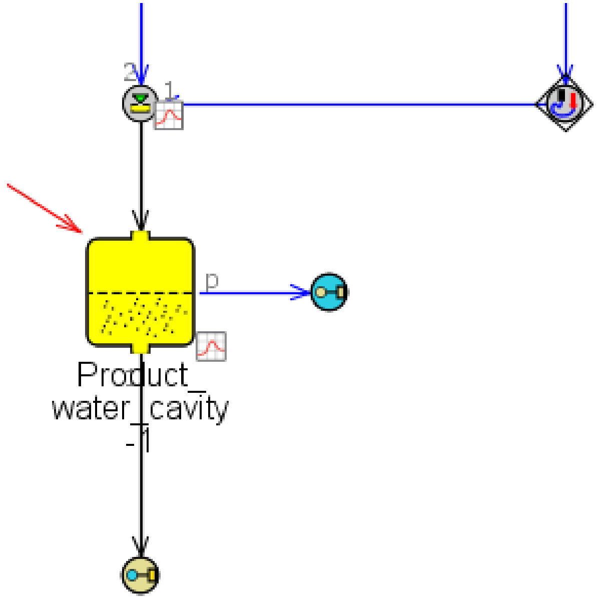
$$h = \frac{Q_{out}}{A(T_{FC} - T_{coolant})} \quad (3)$$

$$Nu = \frac{hL}{k} \quad (4)$$

  - Fuel cell temperature (T_{FC}) assumed to be coolant exit temperature
  - Linear correlation between Nu and ṁ was obtained and used in the model

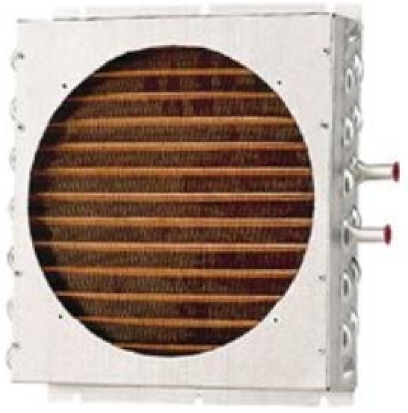
Product Water Cavity Continued

- GT SUITE calculates the stoichiometric amount of water produced
- A flow volume was inserted into the custom PEMFuelCell template and an injector was used to flow water into the cavity at the rate of production
- A CompoundPortConn was used to drain water from the stack
- Originally the model failed to converge using this technique due to a poor selection of fluid database
  - “H2O” from the FluidLiqCompressible database worked whereas the “FluidLiqIncompressible” and “FluidNASA-LiqGas” databases resulted in convergence issues



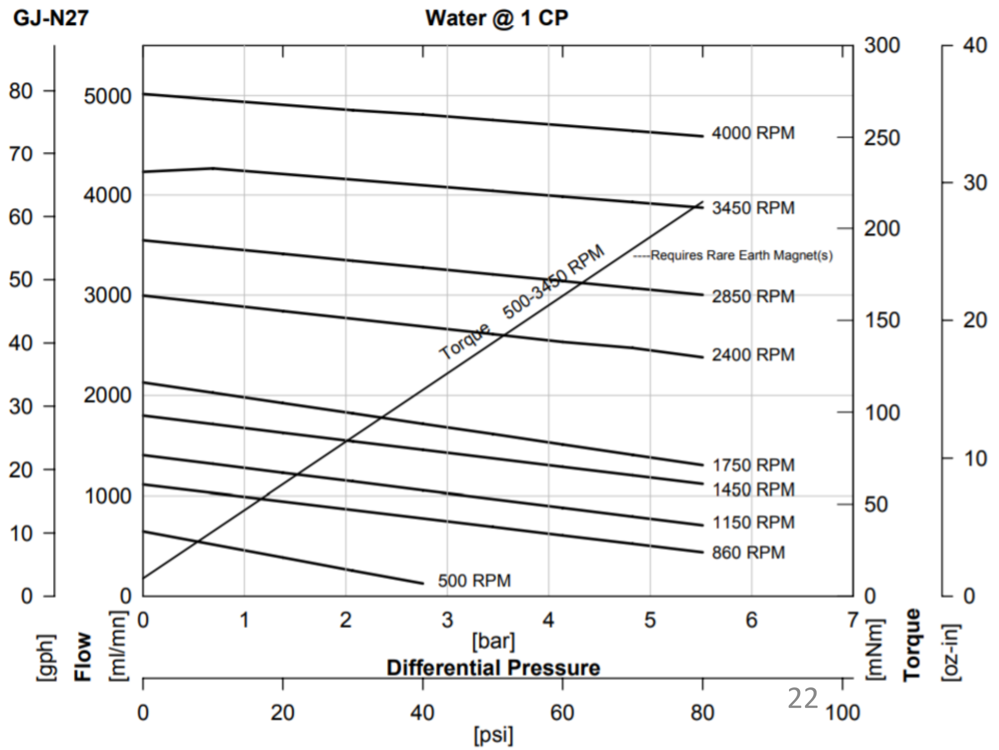
Heat Exchanger and Fan

- Lytron Direct Model 4310G10 Stainless Steel tube-fin heat exchanger
- Deionized water flows through multiple passes of tubes cooled via air flow from a Comair Rotron Caraval DC fan
- Heat exchanger geometric, heat transfer, and performance data input into GT SUITE
- Fan performance (air flow and pressure) also input into model



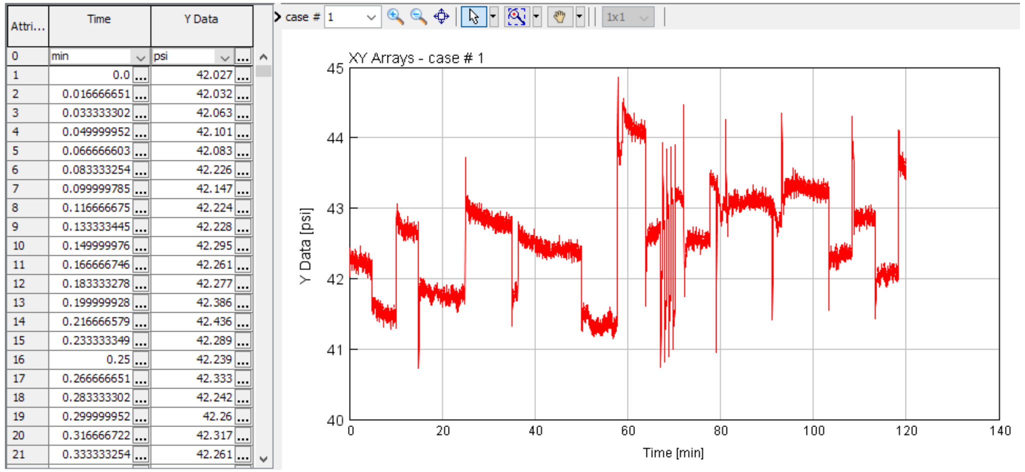
Pump

- Micropump GJ Series external gear pump
- Flow range: 0.15 to 6.8 LPM
- Pump speed controlled via feedback of fuel cell stack temperature
  - If T_{stack}<60 °C, speed = 1200 RPM
  - If 60 °C < T_{stack} < 80 °C, speed varied linearly from 1200 to 4000 RPM
  - If T_{stack}>60 °C, speed = 4000 RPM



Regulated pressure

- Test Data from stack hydrogen and oxygen input as time variant pressure
- Simulates pressure downstream regulators (HPR001 and XPR001)
- Pressure and temperature affect electrochemical performance



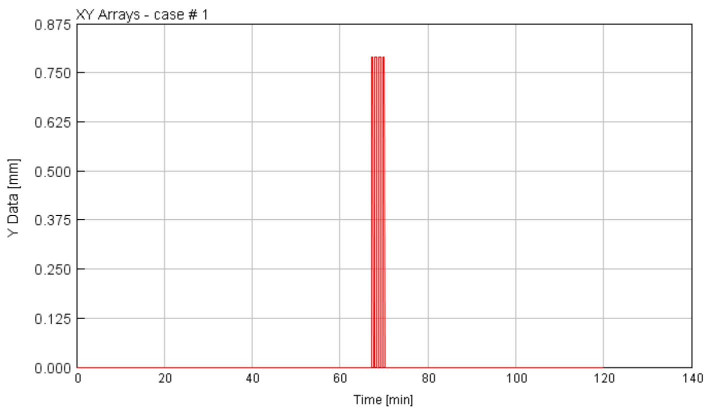
$$V_{OC} = \frac{-\Delta \bar{g}_f}{2F} = \frac{\left(\bar{g}_f\right)_{H_2O} - \left(\bar{g}_f\right)_{H_2} - 0.5 \cdot \left(\bar{g}_f\right)_{O_2}}{2F}$$

Gibbs free energy is function of inlet pressure, temperature [1]

Venting

- Vent valve orifice diameter controlled based on actual venting during test
- Several vents initiated at a test time of around 70 minutes
- Flow restrictors were needed in the vent line in the model as in the real life system to limit the flow rate during vents and prevent sonic flow in the vent lines

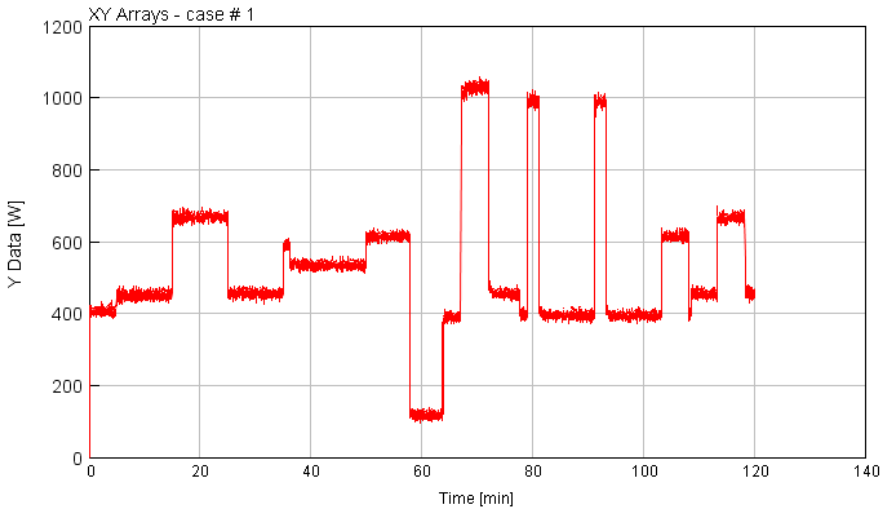
0	min	mm
1	0.0	0.0
2	0.016666651	0.0
3	0.033333302	0.0
4	0.049999952	0.0
5	0.066666603	0.0
6	0.083333254	0.0
7	0.099999785	0.0
8	0.116666675	0.0
9	0.133333445	0.0
10	0.149999976	0.0
11	0.166666746	0.0
12	0.183333278	0.0
13	0.199999928	0.0
14	0.216666579	0.0
15	0.233333349	0.0
16	0.25	0.0
17	0.266666651	0.0
18	0.283333302	0.0
19	0.299999952	0.0
20	0.316666722	0.0
21	0.333333254	0.0



Electrical load

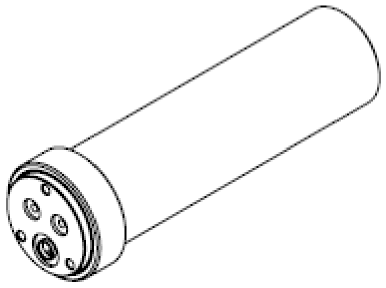
- Power demand as function of time input into GT-SUITE
  - Used same load request as that during testing of power module
- Must be within performance capability of fuel cell
- Only 2-hour load profile segment of total test day was used to reduce computational time

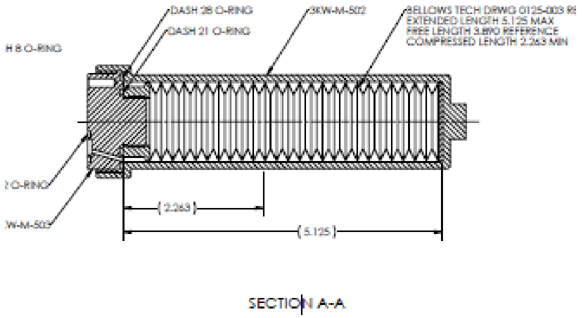
The “load profile” is intended to simulate power demands from the Scarab rover over a 2 hour period



Bellows accumulator

- Massless membrane connects product water drain to oxygen cavity
- Since data was not collected on status of water drain valve, bellows was used for water drain control
- When volume of water in bellows exceeded limit, drain valve was opened for 30 seconds by setting the RLT interval to 30 s in GT SUITE





Stack-Coolant Heat Transfer

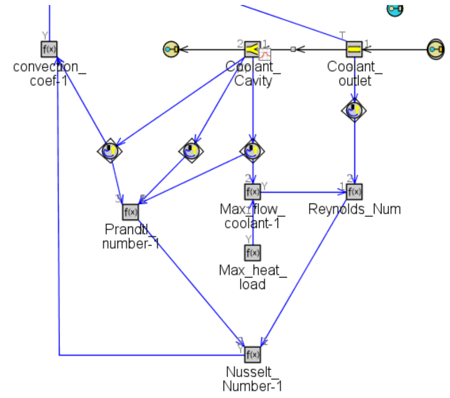
- The heat transfer area is calculated per knowledge of the stack design

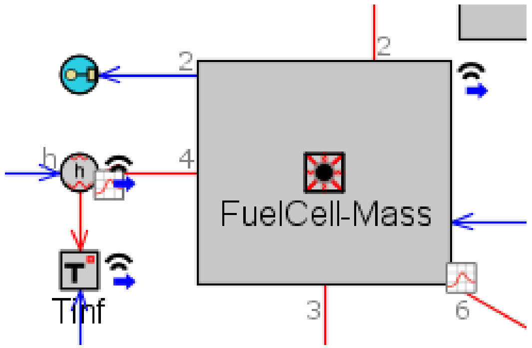
$$A_{HX} = 2(n_{cells} + 1)A \qquad (7)$$

  - where A is the active area
- Thermal mass used for fuel cell heat transfer calculations and represents FC temperature
  - Stainless steel material properties chosen as endplates are 316 SS
- Heat transfer from fuel cell to coolant is:

$$Q = hA_{HX}(T_{FC} - T_{coolant}) \qquad (8)$$

- Q is then added as a heat source to the coolant stream to reflect the heat exchange





Fuel Cell Performance []

Open Circuit Voltage (Defined by the Gibbs free energy of formation of the reaction)

$$V_{OC} = \frac{-\Delta \bar{g}_f}{2F} = \frac{(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{H_2} - 0.5 \cdot (\bar{g}_f)_{O_2}}{2F}$$

Activation Losses (Defined by the Tafel equation)

$$V_{act} = \frac{R_{gas} \cdot T}{2 \cdot \alpha \cdot F} \cdot \ln\left(\frac{i}{i_0}\right)$$

Mass Transport (Concentration) Losses

$$V_{mt} = -C \cdot \ln\left(1 - \frac{i}{i_l}\right)$$

Ohmic Losses

$$V_{ohm} = I \times R$$

Fuel Cell Operating Voltage

$$V_{cell} = V_{OC} - V_{act} - V_{mt} - V_{ohm}$$

V_{OC}:	Open circuit voltage
$\Delta \bar{g}_f$:	Gibbs free energy of formation of the fuel cell reaction. The Gibbs free energy of formation is calculated using physical properties of the species entering the reaction.
$(\bar{g}_f)_i$:	Gibbs free energy of formation of specie i
F:	Faraday's Constant
V_{act}:	Activation voltage loss. Over potential related to the reaction kinetics.
R_{gas}:	Universal gas constant
T:	Fuel cell operating temperature
α:	Charge transfer coefficient. Parameter that is involved in the change of the rate of the electrochemical reaction
I:	Fuel cell current
i:	Current density. Current per active unit area of a cell defined by I / Aa, where Aa is the active cell area (area over which reaction occurs in a single cell).
i_0:	Exchange current density. The current density at which the activation losses begin to become non-zero. For hydrogen fuel cells the exchange current density at the cathode is much smaller than at the anode and the anode activation losses are negligible.
V_{mt}:	Mass transport (concentration) voltage loss. This voltage loss is caused by the change in the concentrations of the reactants at the surface of the electrodes.
C:	Mass transport loss coefficient. For a PEM fuel cell this coefficient is equal to (Rgas * T) / 2F for the anode side and (Rgas * T) / 4F for the cathode side. However, a single coefficient accounting for losses at both electrodes is used for simplicity.
i_l:	Limiting current density. The current density at which the fuel is consumed at a rate equal to its maximum supply rate. When the limiting current density is reached at one electrode, no matter what the limiting current density is for the other electrode the fuel cell voltage drops to zero.
V_{ohm}:	Ohmic voltage loss. This voltage loss is caused by the electrical resistances of the fuel cell components and the resistance to the flow of hydrogen ions through the polymer electrolyte.
R:	Overall cell resistance. Lumped resistance term accounting for both the total electrical resistance and the resistance to ion flow.

References

1. Wang, Chao-Yang. “Fundamentals for Fuel Cell Engineering.” 2004.
2. Incropera, DeWitt, Bergman and Lavine. *Fundamentals of Heat and Mass Transfer.* Wiley 2013.
3. Bennet, Edwards, Guzik, and Jakupca. “Non-Flow Through Fuel Cell Power Module Demonstration on the Scarab Rover.”
4. “PEMFuelCell_MT - Proton Exchange Membrane Fuel Cell with Mass Transfer (Compound).” GT SUITE Help File.