TFAWS Interdisciplinary Paper Session

GT SUITE Fuel Cell Model Validation with Power Module Test Data

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Background

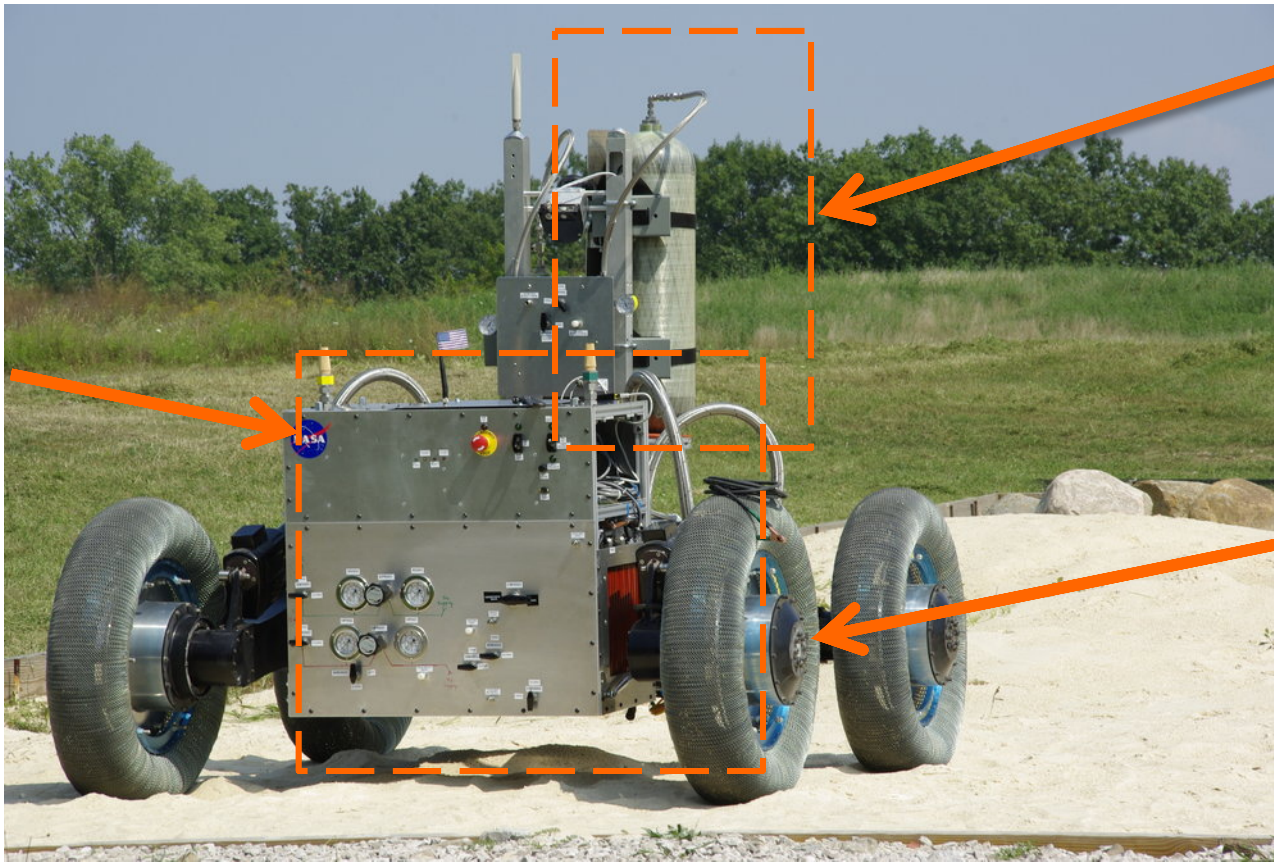
- AMPS fuel cell team has been building a regenerative fuel cell (RFC) model since 2017 that predicts various RFC performance parameters including system energy density, power density, and efficiency
  - Model is Excel based and while it works well for high level trade studies, a fluids/thermal model 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, a multi-physics transient modeling tool by Gamma Technologies
- 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

AMPS 1kW APWR NFT PFC Power Module 2015

Advanced Modular Power Systems 1 Kilowatt Advanced Product Water Removal Non-Flow-Through Primary Fuel Cell Power Module

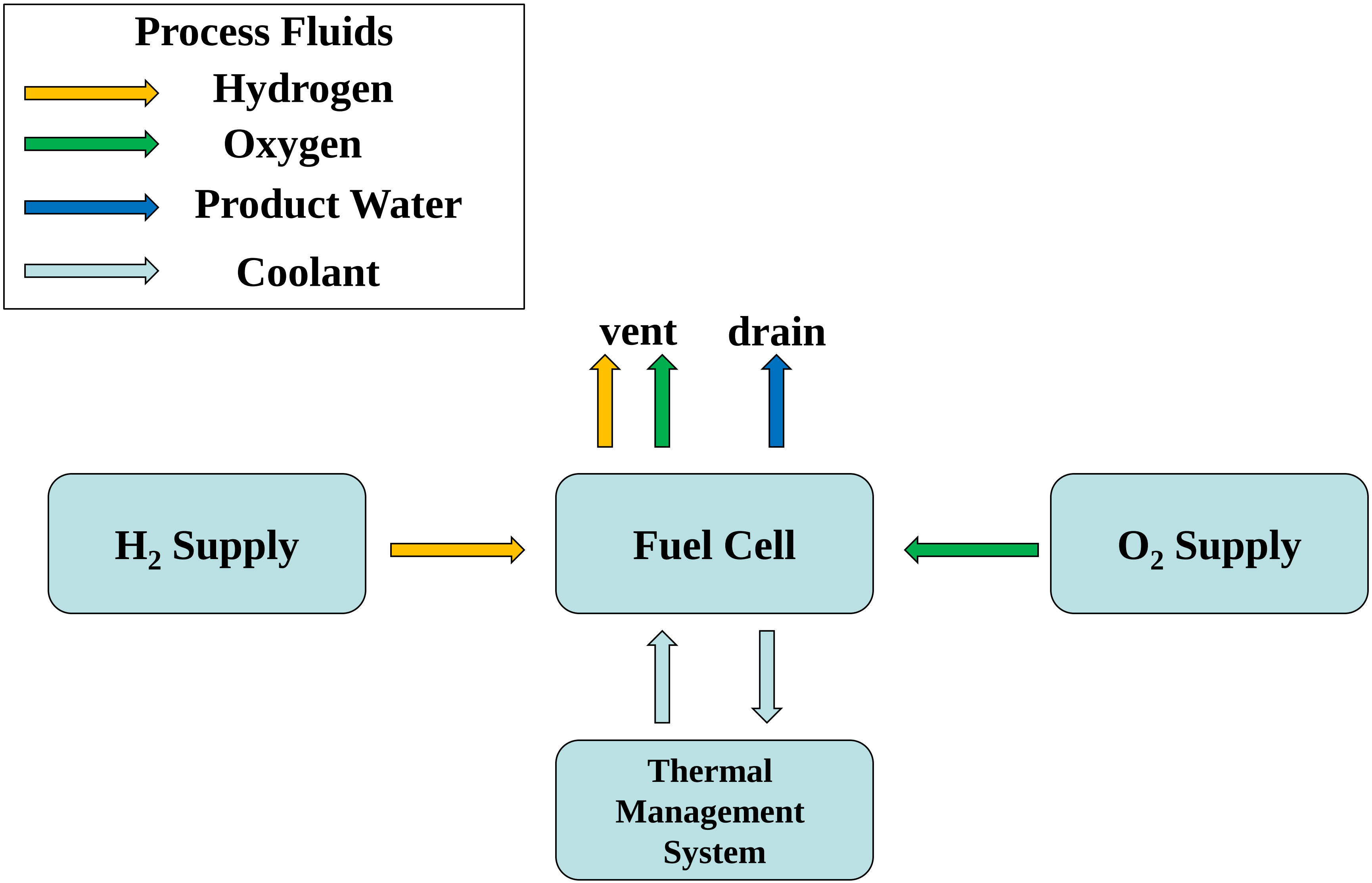


Reactant Supply Tanks

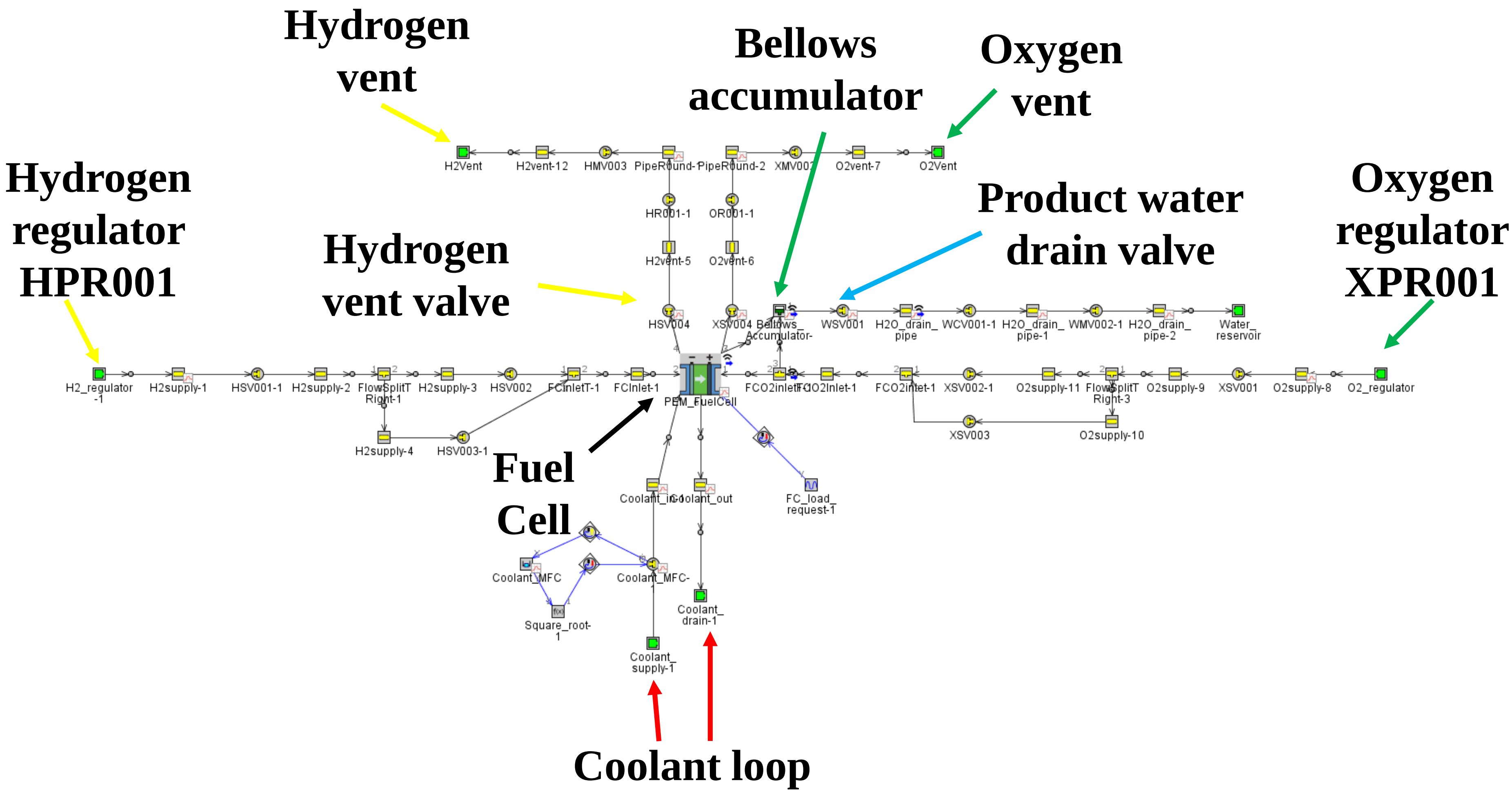
Power Module

Scarab Vehicle

Model Layout

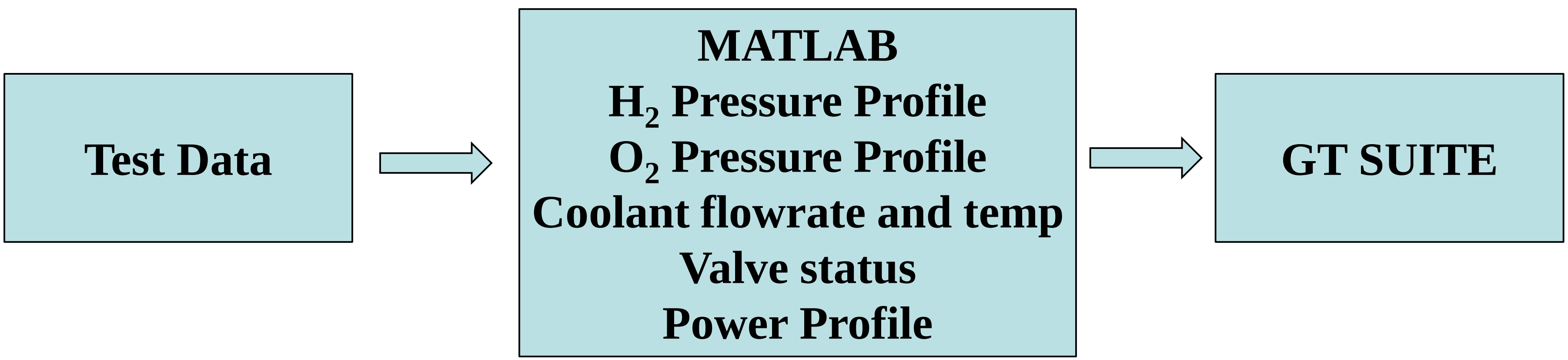


GT-SUITE Model



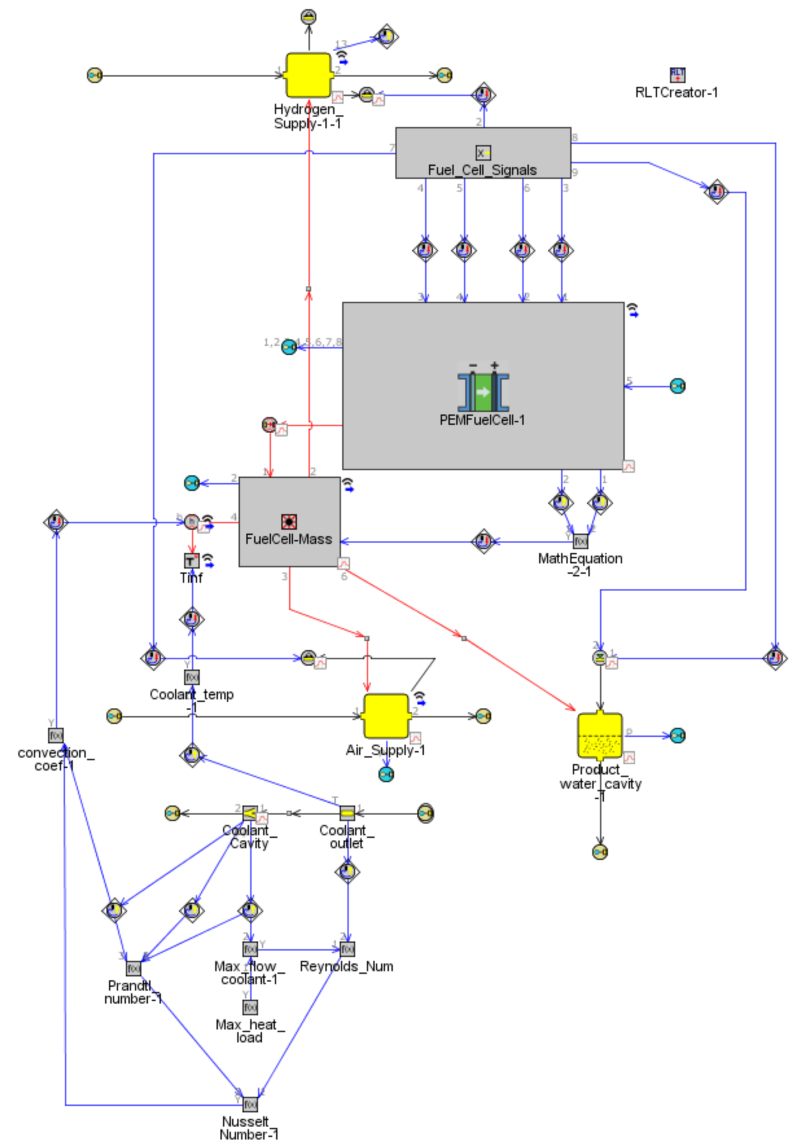
Data Processing for Model Inputs

- 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), coolant flow rate, electrical load request, and input pressure



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



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]

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

- 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]

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

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

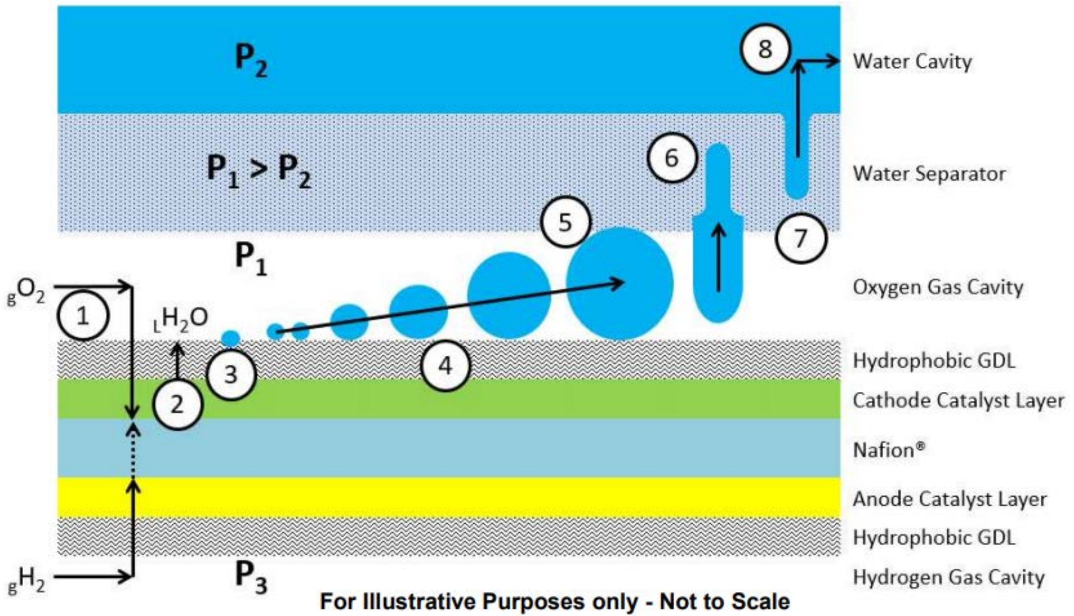
$$Nu = \frac{hL}{k} \quad (4)$$

  - 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

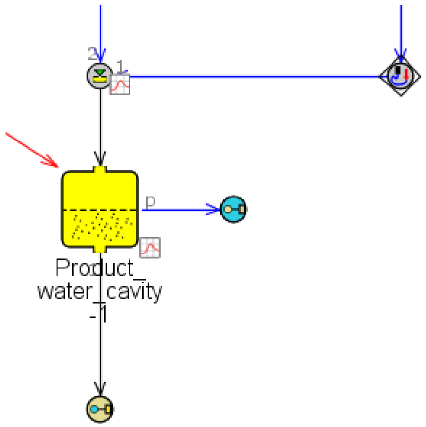
- In terrestrial fuel cells, product water is normally removed by flowing excess air through the oxygen cavity
- This is how the default GT SUITE fuel cell template is set up
- For aerospace fuel cells, pure oxygen is utilized and reactants are only moved through the stack at stoichiometric consumption 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].



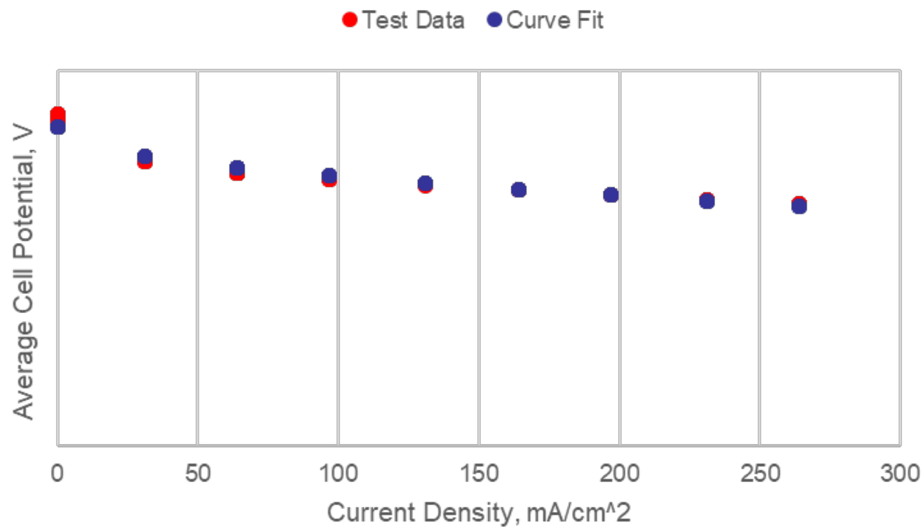
Product Water Cavity Continued

- 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



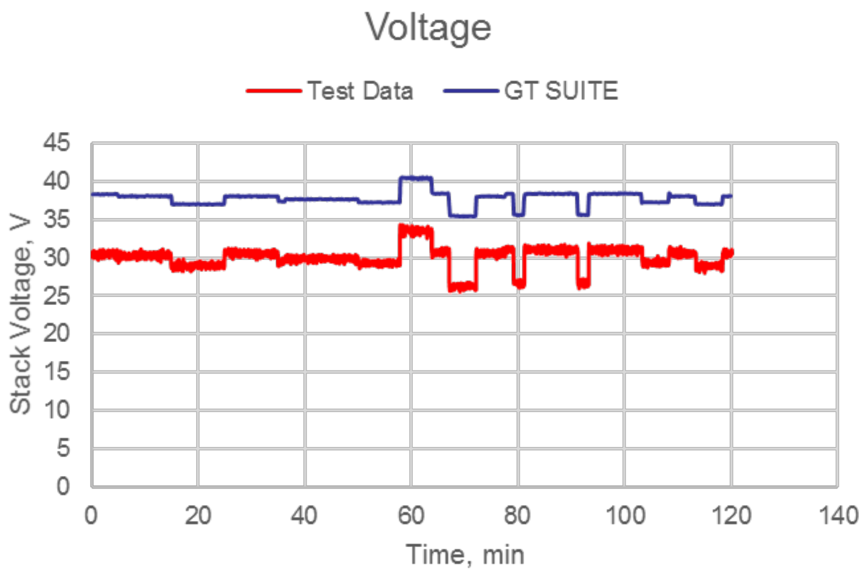
Fuel Cell Performance

- 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
- Note homogeneity is assumed across all cells in the model and therefore an average cell potential is used to account for differences between cells



MODELING RESULTS

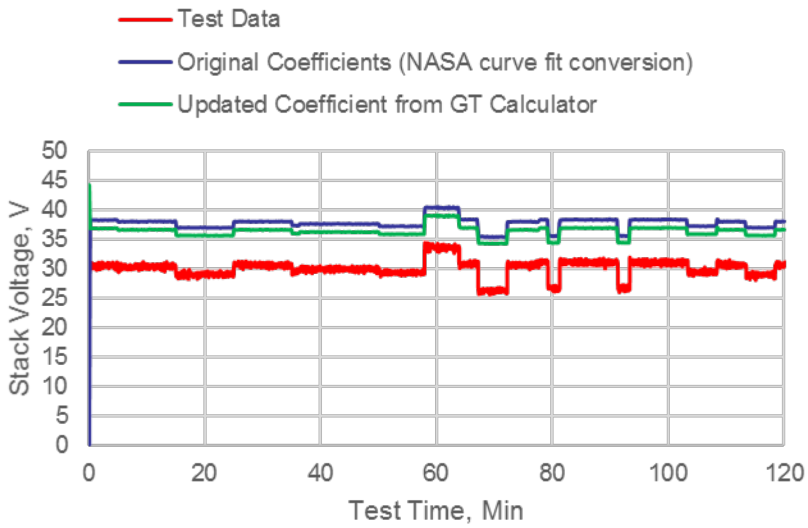
Electrochemical Performance



- Average cell potential from test data plotted against GT predicted stack potential divided by the number of cells
- GT SUITE over predicts cell potential by an average of 7.5 V (0.208 V/cell)
  - Very significant difference
- Power profile matches perfectly
  - Indicates current produced by the fuel cell was lower in the GT SUITE model
  - Fuel cells are current generating devices

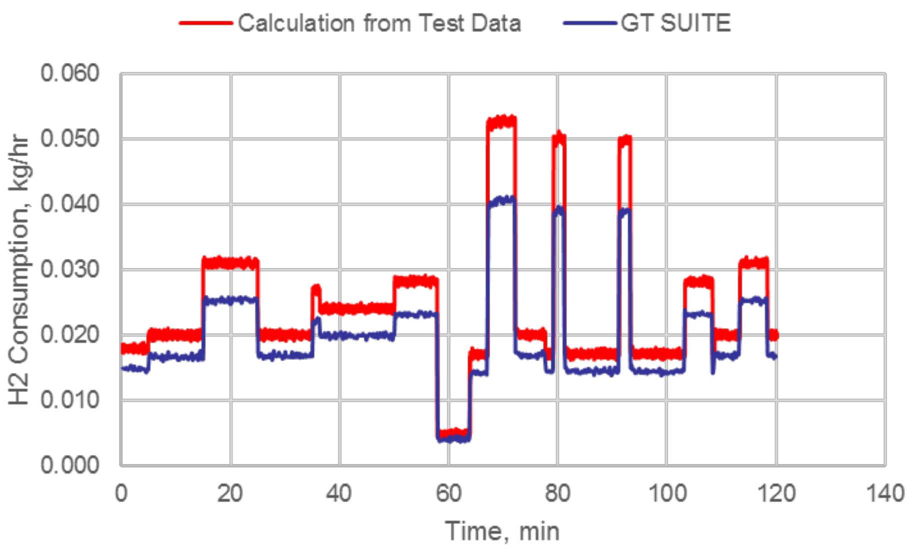
Electrochemical Performance Continued

- Contacted GT-SUITE support with discrepancy in cell voltages
  - GT engineers used in – house program to convert polarization curve to GT performance coefficients
  - GT coefficients resulted in marginal increase in accuracy
  - Both NASA and GT recognized that the theoretical open circuit voltage calculated is higher than in a real fuel cell stack
  - GT engineers actively working on update to adjust open circuit voltage for GT-SUITE version 2019
- Also possible that stack performance changed from December 2014 to March 2015
  - Average polarization data from multiple tests would be preferred



Reactant Consumption Rates

- Actual reactant consumption rates were calculated from power and voltage test data [4]
- Test calculations follow same trend as GT calculations, differences are due to higher voltage predicted by GT



$$\dot{m}_{H2} = \frac{P_{ELE}}{2V_{CC}F}$$

$\dot{m}_{H2}$ = Hydrogen Consumption Mass Flow Rate, moles per second

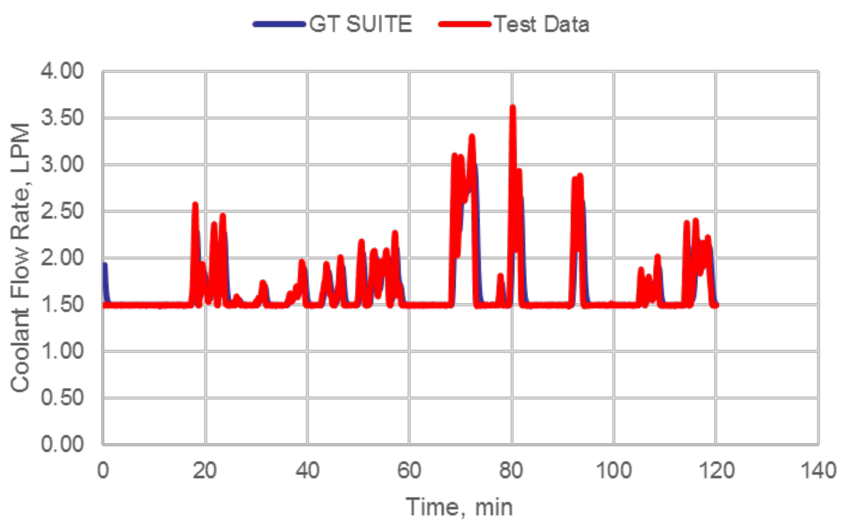
P_{ELE} = Electrical Power, Watts

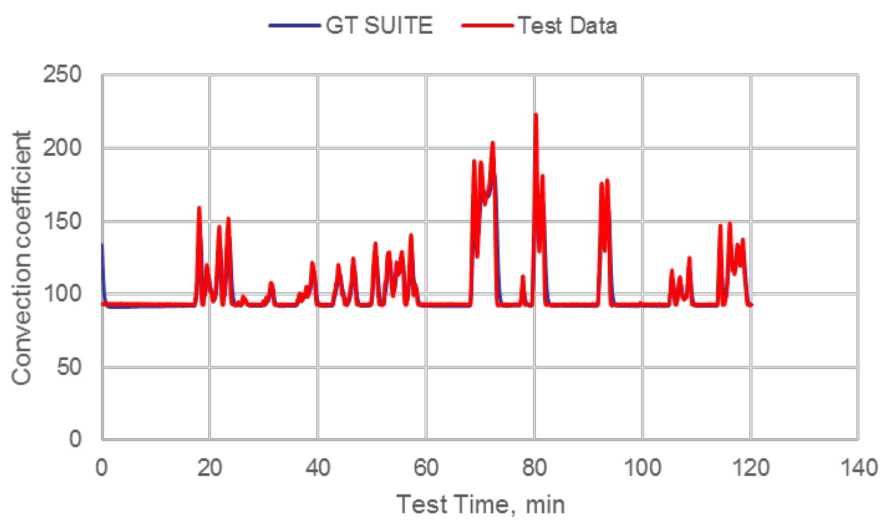
V_{CC} = Average Cell Potential, Volts

F = Faraday's Constant, 96,485 Coulombs per mole

Coolant Flow Rate and Convection Coefficient

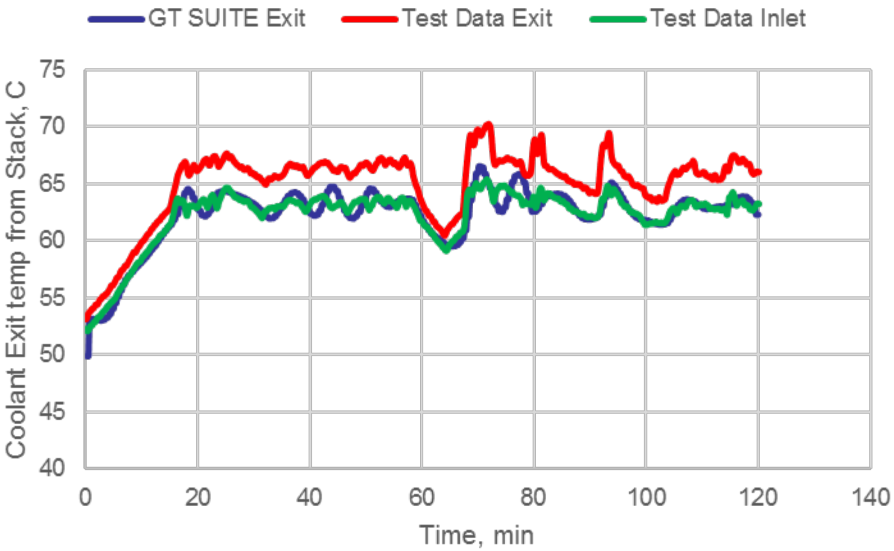
- PID controller nearly exactly matches commanded flow rate
  - The controller cannot always hit the peak flow rate when the coolant flow rate spikes but this is a minor difference
  - Matching flow rates result in GT SUITE convection coefficient matching well with that calculated from the test data
    - Recall Nusselt number equation was determined from test data and curve fit as a function of coolant flow rate

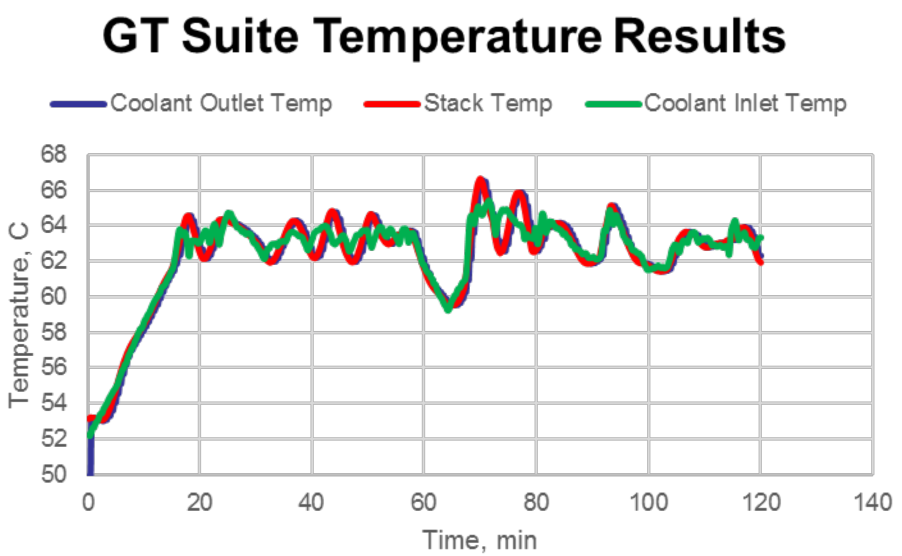




Stack Temperature

- Fuel cell temperature not directly measured during testing but the coolant exit temperature is assumed to be resemble the stack temperature (GT modeling results help confirm this)
- GT predicted exit coolant temperature is 1-2 ºC below the measured coolant exit temperature with temperatures very similar to the coolant inlet temperature
- Results indicate similar heat transfer between fuel cell and coolant for GT and testing result
  - Slight differences could be attributed to difference in waste heat generated (less waste heat predicted in GT SUITE simulation due to higher cell voltages)





Conclusion

- Several iterations of models were required to get the GT SUITE model of the Power Module running correctly
  - New user – GT support staff was very helpful
- Model accurately predicts thermal and fluidic performance of power module during testing
- GT SUITE electrochemical performance was much higher than actual test data
  - Cell voltage was consistently 0.21 V higher in model
  - GT engineers are aware of the discrepancy and actively working on a fix for the 2019 version of GT SUITE
- Forward work could include modeling entire system including pumps, heat exchangers, etc

References

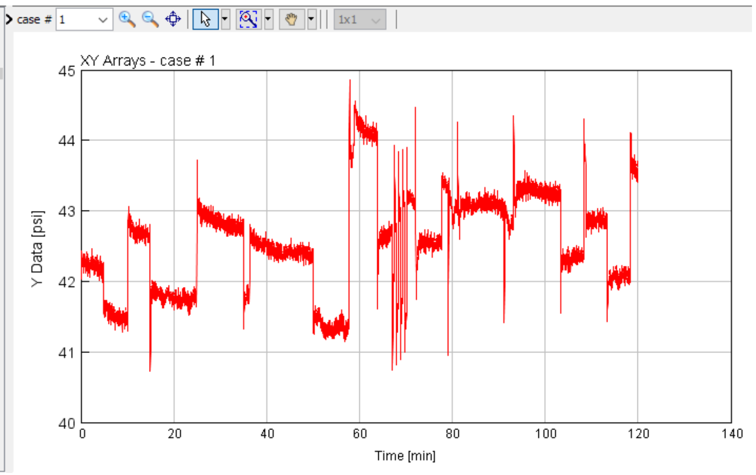
1. Wang, Chao-Yang. “Fundamentals for Fuel Cell Engineering.” 2004.
2. Incropera, DeWitt, Bergman and Lavine. *Fundamentals of Heat and Mass Transfer.* Wiley 2013.
3. Bennet, Edwards, Guzik, and Jakupca. “Non-Flow Through Fuel Cell Power Module Demonstration on the Scarab Rover.”
4. Jakupca, Ian. “Basic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

BACKUP

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

Attri...	Time	Y Data
0	min	psi
1	0.0	42.027
2	0.016666651	42.032
3	0.033333302	42.063
4	0.049999952	42.101
5	0.066666603	42.083
6	0.083333254	42.226
7	0.099999785	42.147
8	0.116666675	42.224
9	0.133333445	42.228
10	0.149999976	42.295
11	0.166666746	42.261
12	0.183333278	42.277
13	0.199999928	42.386
14	0.216666579	42.436
15	0.233333349	42.289
16	0.25	42.239
17	0.266666651	42.333
18	0.283333302	42.242
19	0.299999952	42.26
20	0.316666722	42.317
21	0.333333254	42.261



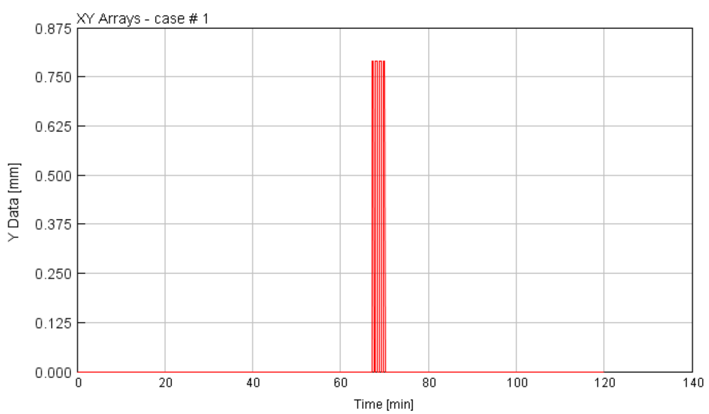
$$V_{OC} = \frac{-\Delta \bar{g}_f}{2F} = \frac{(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{H_2} - 0.5 \cdot (\bar{g}_f)_{O_2}}{2F}$$

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

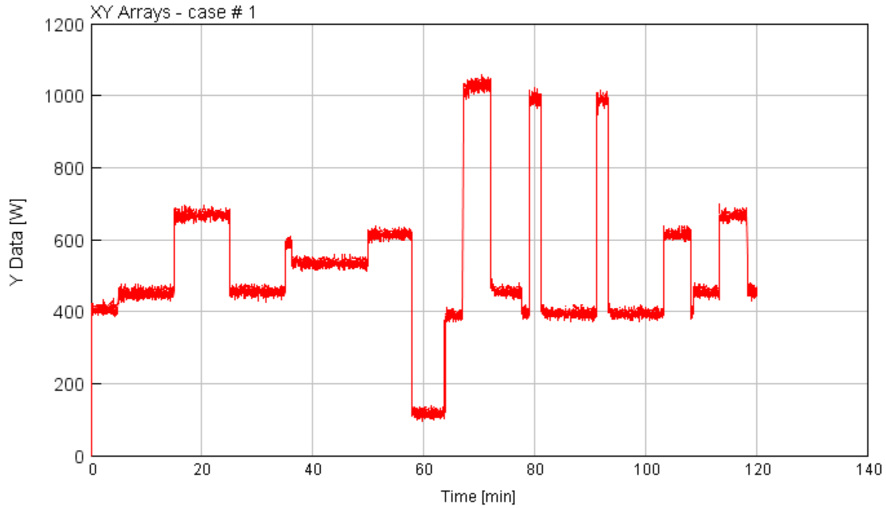
0	min	mm
1	0.0	0.0
2	0.016666651	0.0
3	0.033333302	0.0
4	0.049999952	0.0
5	0.066666603	0.0
6	0.083333254	0.0
7	0.099999785	0.0
8	0.116666675	0.0
9	0.133333445	0.0
10	0.149999976	0.0
11	0.166666746	0.0
12	0.183333278	0.0
13	0.199999928	0.0
14	0.216666579	0.0
15	0.233333349	0.0
16	0.25	0.0
17	0.266666651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



Electrical load

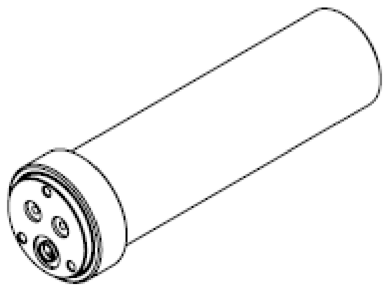
- Power demand as function of time input into GT-SUITE
  - Used same load request as that during testing of power module
- Must be within performance capability of fuel cell
- Only 2-hour load profile segment of total test day was used to reduce computational time

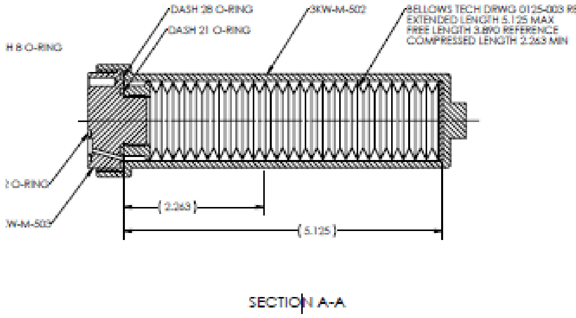
The "load profile" is intended to simulate power demands from the Scarab rover over a 2 hour period



Bellows accumulator

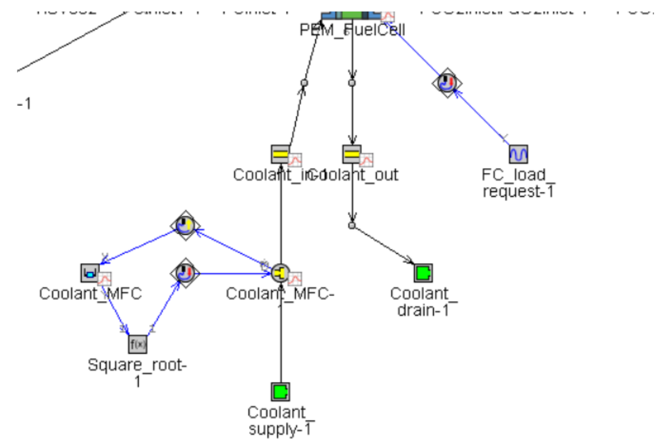
- Massless membrane connects product water drain to oxygen cavity
- Since data was not collected on status of water drain valve, bellows was used for water drain control
- When volume of water in bellows exceeded limit, drain valve was opened for 30 seconds by setting the RLT interval to 30 s in GT SUITE

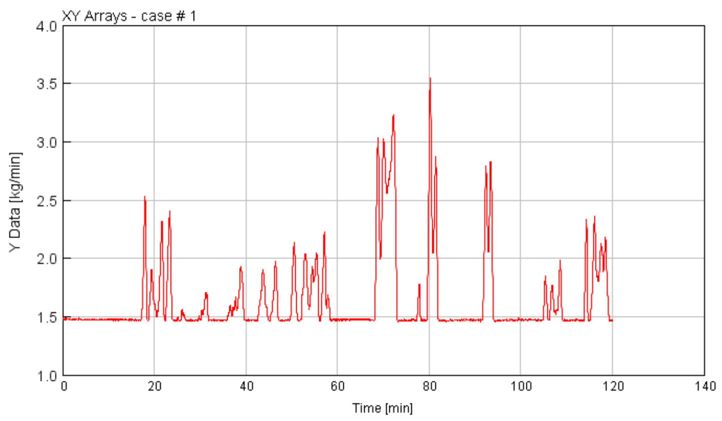




Coolant loop

- Deionized water coolant used
- “High” (30 psia) pressure supply and “low” (14 psia) drain with PID control of valve (orifice) adjusting mass flow
- Gains calculated in spreadsheet using GT SUITE tutorial
- Coolant mass flow rate data was collected from the power module and used as the set point for the mass flow controller
- Coolant inlet temperature to the fuel cell was also recorded during the test and used as the boundary condition for the inlet flow
- Future work will include modeling the entire coolant system including pump and heat exchanger





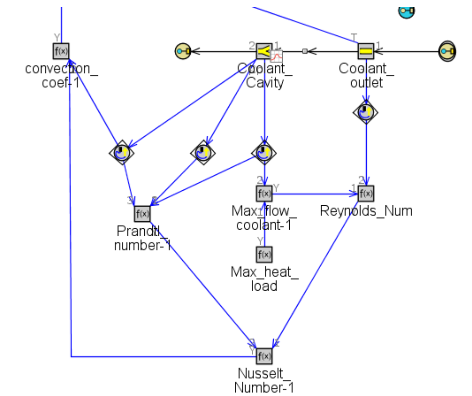
Coolant set point for PID controller

Stack-Coolant Heat Transfer

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

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

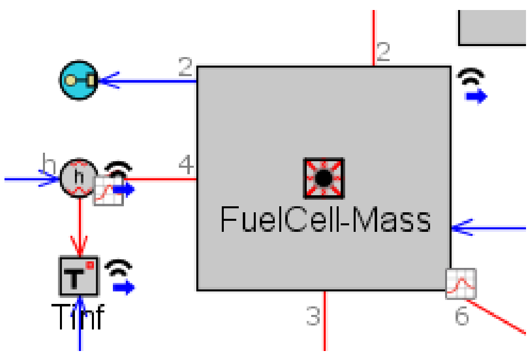
  - where A is the active area



- 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:

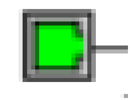
$$Q = hA_{HX}(T_{FC} - T_{coolant}) \quad (8)$$

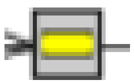
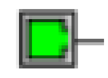
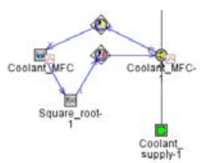
- Q is then added as a heat source to the coolant stream to reflect the heat exchange

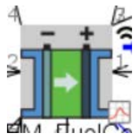


GT Templates Used

Component	GT SUITE Template Used	Description
Supply pressure regulator	End Environment	Species, time-dependent pressure and temperature defined
Valve	Orifice	Orifice diameter equal to actual PN from BOM; can be transient for vent valves
Tubing	Pipe round	Diameter + length specified
Ambient environment	End Environment	1 atm; 22 C
Coolant mass flow controller	Orifice with PID controller	Actively controls orifice diameter to obtain specified mass flow rate
Bellows Accumulator	Accumulator	Massless membrane separates O_2 and H_2O
Fuel Cell	PEMFuelCell with custom modifications	GT template includes electrochemical equations, custom fluidic balance of plant modifications





Fuel Cell Performance [5]

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.