# Solid Oxide Fuel Cell

Final Project Report

#### **BRIGHAM YOUNG UNIVERSITY**

2016 Authored by: Daniel Carlson, Mark Redd

# **SOFC Final Project Report**

#### Abstract

Solid Oxide Fuel Cells are interesting options for power sources because of their high efficiency, low cost, low emissions, and fuel flexibility. These devices however, are not commercially viable because of their short lifetimes. Longer lifetimes are difficult to achieve because of the large mechanical strains on these devices due to their high temperature operation. This study utilizes the Campanari model implemented in APMonitor by Lee T. Jacobsen in order to adjust for power demand while maximizing cell lifetime. The cell lifetime is directly affected by large changes in temperature which causes micro cracking, damaging the cell. A controller that is configured to control the fuel flow rate intelligently can track power demand while maximizing SOFC lifetime.

#### Introduction

The model created to describe an SOFC is the focus of our study. This model was created by Ben Spivey, modified for AP monitor by Lee Jacobsen, and is based on the original model by Campanari. The model describes the interactions of the preformer, the ejector and the fuel cell. Our study focuses on changing the geometry of the fuel cell to model a planar fuel stack. We will then be able to compare our model to the data we have obtained from Pacific Northwest National Laboratories.

In this study, our initial focus was the degradation of the fuel cell due to large temperature gradients. These large thermal gradients generate thermal stresses in the SOFC which lead to fuel cell degradation and delamination. Our objective at the onset was to develop a controller to minimize these factors in order to increase the lifetime of the fuel cell. The goal of understanding this model is to develop controllers that extend the lifetime of the cell to more than 20,000 working hours which is considered the minimum lifetime to make the cell economically feasible for wide use.

Our initial goals included the following:

- Modify the model to match a planar stack geometry and verify its accuracy with data provided by PNNL.
- Estimate the effect of long term cyclic thermal stress on the rate of degradation, and delamination of the fuel cell.
- Develop optimized control methods that will maximize the life of the fuel cell.

As we became familiar with the original Spivey model and upon consulting with him, the scope of the project changed. The changes in the project helped us understand the large scope of our original goals.

#### Literature Review

Several literature sources helped us gain a qualitative understanding of the process. These included the results of Ben Spivey's model and the Campanari model papers.

The following was found from the literature:

- Jacobsen et al. gave us a good start understanding the process. The model is not particularly detailed in its description of the details of the model. From his paper we obtained a comprehensive first principles model of the process and a first understanding of its implementation in AP Monitor. The major improvements to the model from Spivey's model include order of magnitude faster computation time with the AP Monitor software.
- Spivey's dissertation gives a more complete explanation of the model as it is implemented in Simulink. This will form the basis for most of our modifications and frame work because of its inherent detail. The model was

repurposed for a tubular system and compared directly to the original Campanari model without obtaining new data.

• Campanari et al. published a description of the original model that was verified with data. Because this original model had a planar stack geometry, it will be useful in modifying the Jacobsen model in AP Monitor. We will use the data from Pacific Northwestern to verify our updated model. The data verification will be used in AP monitor with finite element analysis to verify the model and tune the model to best respond to available data.

#### **Model Description**

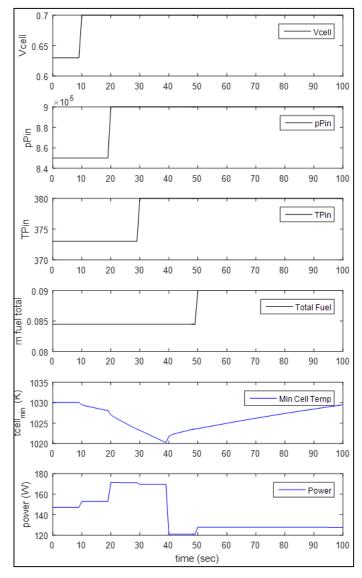
The inputs to the SOFC model are fuel pressure, fuel temperature, voltage, and system pressure. The model utilizes first principles equations to model Solid Oxide Fuel Cell behavior. Embedded in the model are equations to calculate the heat capacities of the different gases at different temperatures (in the form of Equation 3). An energy balance (Equation 1) is used to model the heat transfer behavior of the system, using the heat capacities, densities, temperatures, and thermal properties of the SOFC. The cell voltage is calculated from the temperatures of the SOFC as well as the pressures inside of it, using the electrochemical equations listed in equations 4-6. The kinetics of the reactions occurring within the SOFC are modeled using equations 7-10. The rate of the reaction is given by the Arrhenius equation.

$$\begin{split} \rho V c_{p,i} \frac{dT_{s,i}}{dt} &= hA \left( T_{s,surf,i} - T_{g,i} \right) + kA \frac{dT_{s,i}}{dx} + \\ \varepsilon F_i \sigma A \left( T_{s,opp}^4 - T_s^4 \right) + Q_{elec} \\ Q_{elec} &= \left( \frac{\Delta H_{f,H_2O(g)}}{nF} - V_{cell} \right) \cdot i \\ Q_{elec} &= \left( \frac{\Delta H_{f,H_2O(g)}}{nF} - V_{cell} \right) \cdot i \\ V_{cell} &= \alpha + \beta T + \gamma T^2 + \frac{S}{T^2} \\ V_{cell} &= V_{oc} - \eta_{act} - \eta_{conc} - \eta_{ohm} \\ V_{oc} &= V_{H_2}^0 + \frac{RT}{2F} \ln \left( \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right) \\ V_{H_2}^0 &= -\frac{\Delta G_0}{2F} + \frac{\Delta S_0}{2F} (T - 298) \\ (6) \\ CH_4 + H_2O \xrightarrow{r_{CH_4}}{K} CO + 3H_2 \\ CO + H_2O \xrightarrow{r_{shift}}{K} CO_2 + H_2 \\ CO_2 + H_2 \\ (8) \\ r_{CH_4} &= A \cdot \exp \left( -\frac{E_a}{RT} \right) p_{CH_4} \\ (9) \\ r_{shift} &= k \left( X_{H_2O} X_{CO} - \frac{X_{H_2} X_{CO_2}}{K_{eq}} \right) \\ (10) \end{split}$$

When we run a step test on the system (stepping each of the input variables), we are able to better observe the input-output relationships. This is shown in Figure 1.

We can see that when cell voltage and pressure are increased, the power output is increased. Increasing the temperature decreases the power, and increasing the fuel flow rate increases the power. It is important to note that the minimum cell temperature behaves opposite to power. As the power decreases, the minimum cell temperature increases, and viceversa.

This model is designed for the tube geometry of SOFC. Data for the planar geometry of SOFCs provided a basis for our estimation.





#### Estimation

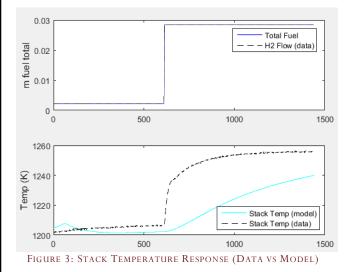
After consulting with Dr. Ben Spivey about the project we ccd hanged our focus from modifying the geometry of the model to using the existing model to match the physical data. Dr. Spivey advised us that changing the model was well beyond the scope of what we could do in a semester and suggested that we alter the model to favor a simplified "cell pile" model that does not consider geometry. After further consultation with Dr. Hedengren, we decided to take the current model and manipulate parameters to fit PNNL data.

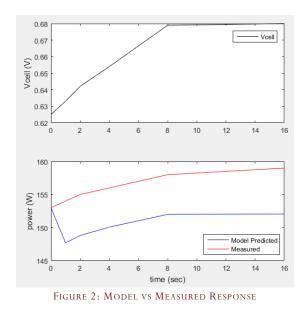
The PNNL data contains a slew of information, and multiple thermocouple readings across the SOFC. We took the average of the cathode temperatures as our cell temperature in the model. The fuel flowrate from the PNNL data is recorded in total SLPM, while the fuel flowrate in the model is reported in kg/s per cell. After converting he units, we were able to use these two data from PNNL and compare them to the model with time. An attempt was made to match the model to the experimental data to allow us to optimize the model and determine how the SOFC might be better operated to reach the required power while avoiding large temperature spikes.

The estimator's response to a change in the cell voltage did not exactly match the measured values as seen in Figure 1. This showed the sensitivity of the model to minor changes. In our analysis we were unable to find the error in our model and obtain acceptable parameters. The results are shown in Figures 2 and 3.

#### Results

When we perform a step test by adjusting the fuel flow rate, we can see that our model reacts much slower than the data (see Figure 2)



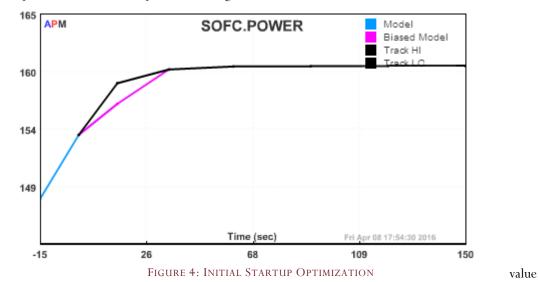


The stack temperature responds much faster to an increase in  $H_2$  flow rate than our model indicates. This could mean that our model needs further adjustment (a faster response---faster gain) in order to accurately match the PNLL data. The tubular SOFC model as it stands may have differences from the planar stack used in PNNL data. For the scope of the project however, we are assuming the differences are negligible.

## **Optimization and Control**

From these failures we found the model to be more complex than originally anticipated and beyond the scope of our project. Upon finding this our focus shifted to understanding the model through experimentation of the parameters concerned. The optimization performed focused on stepping down the fuel cell in the event of a shutdown. The objective here is to minimize damage to the cell through sudden large temperature changes. From the literature large temperature changes are cited as the cause of significant micro cracking and delamination. An initial optimization from startup is shown in figure 4.

The model is specifically designed to simulate these conditions. By setting our time horizon to a sufficiently long run we successfully dropped power to below 100 W output before cutting fuel and air to the cell. This procedure is found in Figure 5.



From these results we expect the fuel cell to be in such a state that temperature will have a sufficiently low time derivative

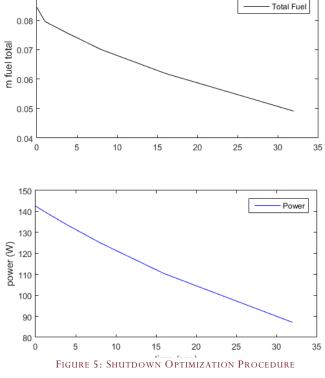
while power drops. Having a low temperature gradient will prevent internal cracking of the ceramic interior of the cell. We changed parameters in the MATLAB script to have an initial power output of 153 Watts and ramp slowly down to below 90 Watts. This method

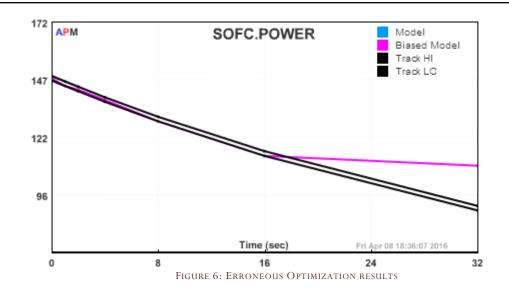
was repeated until desired results were produced.

#### Results

The objective is a control file that controls the model with the intent to create a shutdown sequence that will maximize shutdown speed while protecting the fuel cell. In our attempts to produce these results the model showed a propensity to crash and fail in the optimization. Time horizons consequently were kept to minimum values to avoid crashes.

Furthermore, the output files from such failures were successful up to such a time as they went outside the dead band. An example of this is shown in Figure 6.





At length we were able to produce results that converged in a shutdown procedure. This began with a step down in fuel that is shown in Figure 7. This test showed promise so more alterations to the code were performed. The next test was to perform estimation that gradually reduces the fuel input on a defined trajectory and attempting to follow it down. The results are shown in Figure 8. As can be

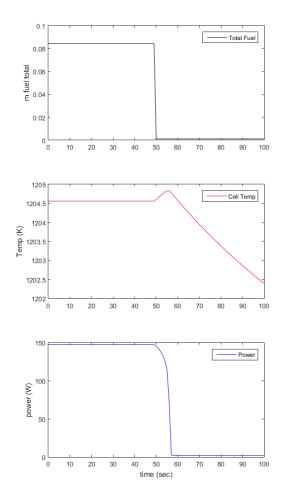


FIGURE 7: STEP DOWN SHUTDOWN TEST

seen from the power trajectory plotted with x's, the power does not follow the trajectory after the 8 seconds. This was determined to be due to constraints placed on fuel control. The code was modified further to improve this error. This is shown in Figure 9.

#### Discussion

Our controller adjusts the fuel flowrate in order to slowly lower the power output to zero. We first ran an estimator to find the values for the total air flow and cell temperature that would best match our data (seen in Figure 10).

Once we had determined these values (which are Fixed Variables—constant over the entire time horizon) we were able to then use our controller to change the values for fuel flow rate to simulate a shutdown procedure (lowering the power output to zero) while maintain a small temperature gradient to minimize damages to the fuel cell.

Our results are not optimal--the model does not converge past a certain time horizon, so operating the controller has proved difficult. We were able to lower the power from 150W to about 90W, but the controller failed with longer time horizons. We are unsure if the failure to produce results on longer time horizons was a failure of the controller or of the SOFC APM model we have.

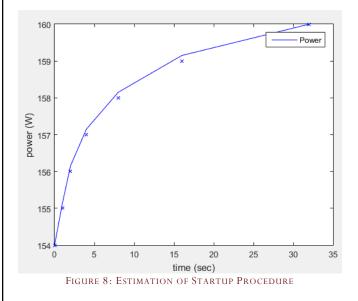
The best option seen to successfully converge while dropping the power of the model is to use the step down method. This is not optimal however because the temperature change is too drastic. Micro cracking and delamination will occur. This is thus far best mitigated by slow fuel flow changes.

#### **Conclusions and Future Work**

There remains a great deal work on the project. Future work may include determining how to get the system to converge to a solution on longer time horizons. Much of the analysis is theoretical in nature and is not validated by data. The utility of this model can only be validated by real data. There are also many projects that may come from this work including the following:

- Changing geometry to fit planar data for model validation
- Estimating model parameters to more closely fit data for tubular systems
- Simplifying and removing superfluous info from the APM model to improve usability
- Optimization of the validated model to maximize the lifetime of SOFCs

Initially we set out to achieve these goals but the scope of each of these were too large for the limited time that we had to complete the project. However we were able to understand the workings of the fuel cell and perform some preliminary analysis of the model. We recommend a longer time to be able to fully explore the aspects of the model and its potential.



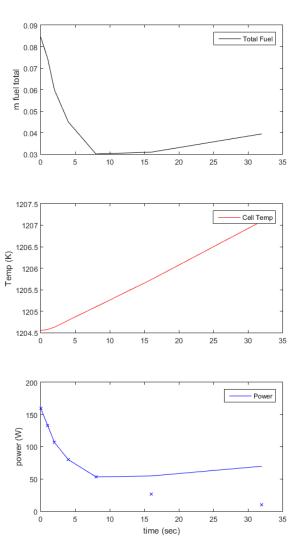


FIGURE 9: ADJUSTED CONTROL WITH POWER TRAJECTORY

## References

- Jacobsen, L.T.; Spivey, B.J.; Hedengren, J.D., "Model predictive control with a rigorous model of a Solid Oxide Fuel Cell," in American Control Conference (ACC), 2013, vol., no., pp.3741-3746, 17-19 June 2013
- Kevin Lai, Brian J. Koeppel, Kyoo Sil Choi, Kurtis P. Recknagle, Xin Sun, Lawrence A. Chick, Vladimir Korolev, Moe Khaleel, "A quasi-two-dimensional electrochemistry modeling tool for planar solid oxide fuel cell stacks", Journal of Power Sources, Volume 196, Issue 6, 15 March 2011, Pages 3204-3222 (<u>http://www.sciencedirect.com/science/article/pii/S0378775310021142</u>)
- Mike Powell, Kerry Meinhardt, Vince Sprenkle, Larry Chick, Gary McVay, "Demonstration of a highly efficient solid oxide fuel cell power system using adiabatic steam reforming and anode gas recirculation", Journal of Power Sources, Volume 205, 1 May 2012, Pages 377-384.
- Spivey, Benjamin J. Dynamic Modeling, Model-Based Control, and Optimization of Solid Oxide Fuel Cells. Diss. U of Texas at Austin, 2011. N.p.: n.p., n.d. Print.
- Campanari S., Iora P., "Comparison Of Finite Volume SOFC Models For The Simulation Of A Planar Cell Geometry", Fuel cells: from fundamentals to systems, Volume 5, Issue 1, February 2005, pp. 34-51, DOI: 10.1002/fuce.200400057