MODELING AND OPTIMIZATION OF FUEL CELL SYSTEMS FOR AIRCRAFT APPLICATIONS

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This research project is an extension of ongoing fuel cell simulation and system studies being carried out under NASA sponsorship as part of a URETI collaboration between Florida A&M University and Georgia Tech. The URETI on Aeropropulsion and Power is concerned, among other topics, with advancing the technologies needed to implement an all-electric aircraft, including, but not limited to, integration of fuel cells to airborne power systems.

The project is aimed at increasing the level of confidence and existing design know-how for the implementation of fuel-cells on aircraft. In this first year we have focused on a suite of studies related to the integration of fuel cells into aircraft and the optimization of fuel cell systems: 1. SOFC-gas turbine hybrid system for aircraft applications: modeling and performance analysis, 2. The optimal shape for a unit PEM fuel cell, 3. The Constructal PEM fuel cell stack design, 4. Optimization of the internal structure of an SOFC unit, and 5. The implementation of fuel cell based aero-propulsion systems into advanced power simulation environments (EMTDC, RTDS). In this executive summary we present the main aspects of these studies, a complete report (109 pages) is available to NASA.

Continuation of the above efforts will be complemented in 2006 with the characterization and optimization of regenerative fuel cell systems which are expected to provide renewable, regenerative, and relatively efficient means of sustainable energy onboard high altitude and space applications.

Study 1. SOFC-Gas Turbine Hybrid System for Aircraft Applications: Modeling and Performance Analysis

Abstract

There is a growing interest in fuel cells for aircraft applications [1-7]. Fuel cells when combined with conventional turbine power plants offer high fuel efficiencies. The feature of fuel cells (SOFC, MCFC) used in aircraft applications, which makes them suitable for hybrid systems, is their high operating temperature. Their dynamic nature, both electrical and thermodynamic, demands a dynamic study of the complete hybrid cycle. We developed a model for a SOFC/Gas Turbine hybrid system and implemented in Matlab-Simulink. Various configurations of the hybrid system are proposed and simulated. A comparative study of the simulated configurations is presented.
Components Models

Figure-1 illustrates the basic schematic of a hybrid system, which consists of a compressor, a fuel cell, a gas turbine, a combustor and heat exchangers.

We have developed and implemented into Simulink basic compressor, turbine, combustor, and heat exchanger models. The Pacific Northwest National Laboratory (PNNL) has developed and validated a single SOFC button cell model with experimental data [8]. The cell voltage is calculated based on deviations from the open circuit (current = 0) voltage, which is given by the Nernst equation. The deviations or overpotentials are accounted for as activation, concentration, ohmic, fuel leakage and internal current losses. Using the PNNL single cell model as a basis, we have developed a SOFC code for a stack that includes a thermal model, which predicts a 1D bulk temperature response (Fig. 2).

Figure-1 Schematic of a SOFC/gas turbine hybrid system

Figure 2 – SOFC stack temperature plot from start up at constant electrical load
Cycle Configuration

Modeling assumptions:

Compressor: Poytropic Efficiency: 85%; Compression Ratio: 2.3
Turbine: Poytropic Efficiency: 85%; Expansion Ratio: .43
Fuel: 97% H\textsubscript{2} + 3% H\textsubscript{2}O by moles
Air: 21% O\textsubscript{2} + 79% N\textsubscript{2} by moles
Design point: Sea level full power, temperature: 25\degree C, pressure: 1 atm

Configuration-1:

Figure-3 shows an schematic representation of the SOFC-GT hybrid system considered (configuration-1). Air is compressed by the compressor and sent to the air heat exchanger. From the fuel pump, compressed fuel stream (97% H\textsubscript{2} + 3% H\textsubscript{2}O by mole) enters the fuel heat exchanger. Air and fuel heat exchangers are sequentially fed by the hot exhaust from the turbine. Exhaust from the turbine preheats the air and fuel streams. After pre-heating, both the main streams of air and fuel enter the SOFC stack (air at cathode and fuel at anode). From heat exchangers, preheated streams of air and fuel are bypassed to combustor. The outputs of the fuel cell are electrical power and hot gases. The hot exhaust is sent to combustor where it is burnt with additional fuel and air (from the bypassed streams). The hot exhaust is fully expanded to almost ambient pressure in the turbine and power is extracted to run the electrical generator. The exhaust from the turbine enters the air and fuel heat exchangers.

<table>
<thead>
<tr>
<th>Configuration-1</th>
<th>Configurations-2A, 2B</th>
<th>Configuration-3</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Configuration-1" /></td>
<td><img src="image2" alt="Configuration-2A, 2B" /></td>
<td><img src="image3" alt="Configuration-3" /></td>
</tr>
<tr>
<td>Figure 3. Hybrid SOFC/GT cycle configurations</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Configuration-2A:

The only difference between configuration-1 and configuration-2A is that in configuration-2A, there is no bypass stream from the air heat exchanger. Instead, soon after the compressor, one stream of compressed air is by passed to the combustor. The reason for this modification, which results in a performance improvement, is discussed in the later part when a comparative study is presented.

Configuration-2B:

Configuration 2B is the same as configuration 2A except that configuration 2B uses counter flow heat exchangers. The configurations discussed previously use parallel flow.
heat exchangers. The need of using counter flow heat exchangers and the advantages of configuration 2B over 2A are discussed in the comparative study.

**Configuration-3:**

All the compressed air is preheated by the turbine exhaust in the air heat exchanger and sent to the fuel cell. The fuel stream is heated by the hot cathode air coming out of the fuel cell and enters at the anode of the SOFC. After exiting the fuel heat exchanger, the cathode air stream enters the combustor. The anode exhaust of the SOFC is sent to the combustor where it reacts with additional fuel and cathode air from the fuel heat exchanger. The hot exhaust from the combustor is expanded in the turbine and mechanical power is extracted. Configuration-3 gives the best performance out of all the configurations considered in this study.

**Comparative Study**

Table 1 summarizes the results for the configurations discussed above.

<table>
<thead>
<tr>
<th></th>
<th>Config-1</th>
<th>Config-2A</th>
<th>Config-2B</th>
<th>Config-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel flow (g/s)</td>
<td>9.62</td>
<td>9.62</td>
<td>9.62</td>
<td>8.56</td>
</tr>
<tr>
<td>Air flow (g/s)</td>
<td>464</td>
<td>342</td>
<td>362</td>
<td>670</td>
</tr>
<tr>
<td>SOFC Temp (°C)</td>
<td>574</td>
<td>761</td>
<td>876</td>
<td>877</td>
</tr>
<tr>
<td>Turbine Inlet Temp (°C)</td>
<td>1442</td>
<td>1366</td>
<td>1370</td>
<td>1187</td>
</tr>
<tr>
<td>SOFC power (kW)</td>
<td>12</td>
<td>260</td>
<td>313</td>
<td>327</td>
</tr>
<tr>
<td>Turbine (kW)</td>
<td>157</td>
<td>114</td>
<td>119</td>
<td>189</td>
</tr>
<tr>
<td>Total power (kW)</td>
<td>169</td>
<td>374</td>
<td>432</td>
<td>516</td>
</tr>
<tr>
<td>Cycle efficiency</td>
<td>19%</td>
<td>32.5%</td>
<td>48%</td>
<td>64.5%</td>
</tr>
<tr>
<td>Exhaust Temp (°C)</td>
<td>779</td>
<td>734</td>
<td>645</td>
<td>312</td>
</tr>
</tbody>
</table>

From table-1, it can be seen that configuration-1 has the lower efficiency and configuration-3 the highest among the cases considered. Configuration-1 only gives ~19% efficiency and almost all the power is coming from the gas turbine. The low performance of configuration-1 can be attributed to the low operating temperature of the fuel cell stack. As we move from configuration-1 to 3, operating temperature improves and, hence, the performance of the fuel cell. The data show that in configuration-1, the air flow rate is very high through the parallel air heat exchanger because of the turbine inlet temperature limitations (maximum allowable was set to 1400°C) which results in lesser preheating of the streams entering the fuel cell. Therefore, the stack inlet temperature turns out to be very low which degrades the performance of the stack and consequently the entire hybrid system.

Configuration-2A is an improved version of configuration-1. The entire stream coming out of the compressor is not sent to heat exchanger and preheated; instead air is bypassed to the combustor and only a partial stream enters the air heat exchanger. This
change improves the stack operating temperature because of enough preheating. The efficiency reached is 32.5%. The SOFC provides around 70% of the total power; a significant improvement from configuration-1.

Configuration-2B uses counter flow heat exchangers unlike configuration 1 and 2A. The SOFC’s operating temperature limits its performance. Low operating temperature was observed due to low preheating of fuel and air streams. The counter flow heat exchangers utilize the hot stream’s enthalpy in a more efficient manner and that explains the improvement of the SOFC’s performance from configuration 2A to configuration 2B.

Configuration-3 has the highest efficiency among the configurations studied. The cathode air is utilized to preheat the fuel stream. After preheating the fuel stream, the cathode stream is circulated back to the combustor. The compressed high temperature exhaust from the combustor is expanded in the turbine. The enthalpy of the exhaust leaving the turbine is high enough to give the required preheating to the air stream in the air heat exchanger. The exhaust from the air heat exchanger is released to the ambient. The efficiency obtained in this case is 64.5% and the power of the fuel cell is around 64% of the total power. The turbine inlet temperature and exhaust temperature are also found to be very low as compared to the other studied configurations.

**Results and Discussion**

The following flow sheet summarizes the results of the hybrid system at steady state and design condition. Temperature: 25°C, Pressure: 1 atm

**Table -2 Thermodynamic Analysis of Configuration-3**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Air</th>
<th>Fuel 1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>Fuel 2</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp (°C)</td>
<td>25</td>
<td>25</td>
<td>121</td>
<td>857</td>
<td>865</td>
<td>877</td>
<td>877</td>
<td>786</td>
<td>25</td>
<td>1187</td>
<td>897</td>
<td>312</td>
</tr>
<tr>
<td>Pressure (atm)</td>
<td>1</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>2.3</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
</tr>
</tbody>
</table>
Table 2 summarizes the steady state results of a hybrid system of 327 kW electrical and 189 kW mechanical output.

Table -3 summarizes the power outputs and efficiency of various components of the hybrid system. The fuel cell gives 327 kW of electrical power at steady state and the turbine gives ~189 kW of mechanical power. The steady state cycle efficiency is found to be 64.5% based upon the LHV of hydrogen fuel.

<table>
<thead>
<tr>
<th>Compressor</th>
<th>SOFC</th>
<th>Turbine</th>
<th>Cycle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (kW)</td>
<td>65</td>
<td>327</td>
<td>189</td>
</tr>
<tr>
<td>Efficiency</td>
<td>83.2%</td>
<td>66%</td>
<td>84%</td>
</tr>
<tr>
<td>Exit Temp</td>
<td>121°C</td>
<td>877°C</td>
<td>897°C</td>
</tr>
</tbody>
</table>

Studies 2 and 3: The Optimal Shape for a Unit PEM Fuel Cell and a PEM Fuel Cell Stack [9,10]

Summary

A mathematical model and a structured procedure to optimize the internal structure (relative sizes, spacing) and external shape (aspect ratios) of a unit and stack PEM fuel cell and stack so that net power is maximized has been developed [9, 10]. Initially, the optimization of flow geometry was conducted for the smallest (elemental) level of a fuel cell stack, i.e., the unit PEM fuel cell, which is modeled as a unidirectional flow system and later the optimization of flow geometry was conducted for a PEM fuel cell stack. The polarization curve, total and net power, and efficiency were obtained as functions of temperature, pressure, geometry and operating parameters. The optimization is subjected to fixed total volume. There are three levels of optimization: (i) the internal structure, which basically accounts for the relative thickness of two reaction and diffusion layers and the membrane space, (ii) the external shape of the unit cell, which accounts for the external aspect ratios of a square section plate that contains all unit PEM fuel cell components. The available volume is distributed optimally through the system so that the net power is maximized. Temperature and pressure gradients play important roles, especially as the fuel and oxidant flow paths increase, and (iii) at the stack level, we optimized the external shape, which accounts for the external aspect ratios of the PEMFC stack. The flow components are distributed optimally through the available volume so that the PEMFC stack net power is maximized. Numerical results show that the optimized single cells internal structure and stack external shape are “robust” with respect to changes in stoichiometric ratios, membrane water content, and total stack volume. The optimized internal structure and single cells thickness, and the stack external shape are results of an optimal balance between electrical power output and
pumping power required to supply fuel and oxidant to the fuel cell through the stack headers and single-cell gas channels. It is shown that the twice maximized stack net power increases monotonically with total volume raised to the power 3/4, similarly to metabolic rate and body size in animal design.

**Elemental Fuel Cell**

Figures 4 and 5 illustrate the main geometric variables defining the external shape and the internal structure of a unit PEM fuel cell.

![Figure 4. Geometric variables defining the fuel cell external shape.](image)

Figure 4. Geometric variables defining the fuel cell external shape.
Figure 5. Internal structure of a unit PEM fuel cell and the control volumes selected for analysis

We have developed a mathematical model and a structured systematic procedure to optimize the internal structure (relative sizes, spacing) and external shape (aspect ratios) of a unit PEM fuel cell so that net power is maximized. The optimization is subjected to fixed total volume. The available volume is distributed optimally through the system so that the net power is maximized.

Figure 5 illustrates the seven control volumes selected in the analysis. The fuel channel (CV1), the anode backing layer (CV2), the anode reaction layer (CV3), the electrolyte (CV4), the cathode reacting layer (CV5), the cathode-backing layer (CV6) and the oxidant channel (CV7). Also shown are two end plates.

The length scale $V_T^{1/3}$ is dictated by the fixed total volume. This length scale is used for the purpose of nondimensionalizing all the lengths that characterize the fuel cell geometry,

$$\xi_j = \frac{L_j}{V_T^{1/3}}$$

where the subscript $j$ indicates a particular dimension of the fuel cell geometry.

Figures 6a and 6b illustrate the optimization of internal structure. The maximization of net power by varying the relative thickness of the reaction layers. It is assumed that the relative thickness of the electrodes and membrane are fixed. The optimal allocation of thickness results from the trade-off between two effects: activation polarization losses
and ohmic losses. As the relative thickness of the reaction layers $\xi_3 / \xi_x$ and $\xi_5 / \xi_x$ increase, the electrode wetted areas increase and the activation losses decrease. Here $\xi_x$ is $L_x / V_{x}^{1/3}$. On the other hand, the ohmic losses increase because the ionomer penetrates deeper into the electrodes, increasing electrical resistance.

The results of the internal structure optimization with respect to the average membrane water content, $\lambda = (\lambda_x + \lambda_z) / 2$, are shown in Fig. 6b, for two external shapes $\xi_y / \xi_x = \xi_z / \xi_x = 30$ and 50. The optimal internal structure $(\xi_3 / \xi_x = \xi_5 / \xi_x)_{\text{opt}}$ is independent of external shape for all tested water contents. As $\xi_y / \xi_x = \xi_z / \xi_x$ increases, the net power maximized with respect to $\xi_y / \xi_x = \xi_z / \xi_x$, $\hat{W}_{\text{net,m}}$, increases. The same effect is also observed as the water content increases. This again is due to smaller ohmic losses at higher water contents.

An important conclusion is that $(\xi_3 / \xi_x = \xi_5 / \xi_x)_{\text{opt}}$ is nearly the same in Fig. 6b for all tested membrane water contents and external shapes. The optimal internal structure is relatively insensitive to changes in both $\lambda$ and $\xi_y / \xi_x = \xi_z / \xi_x$.

The fuel cell external shape optimization is illustrated in Fig. 7. Because the optimized inner parameters $(\xi_y / \xi_x, \xi_y / \xi_x = 0.01)$ are practically insensitive to changes in the external shape, the fuel cell external shape optimization procedure was conducted for a single internal shape structure defined by $(\xi_3 / \xi_x = \xi_5 / \xi_x)_{\text{opt}} = 0.01$.

Figures 7a and 7b show that for the optimized internal structure, and a given ionomer water content, the fuel cell net power maximized with respect to internal structure $(\hat{W}_{\text{net,m}})$ can be maximized further with respect to external shape at fixed volume $(\tilde{V}_T = 2.25)$. The existence of a net power maximum with respect to fuel cell external shape can be explained because $\hat{W}_{\text{net,m}} \to 0$ in the two extremes: (i) Small $\xi_y / \xi_x = \xi_z / \xi_x$ means that $\xi_x$ is large, $\hat{W}$ is small because of large flow resistances in the x-direction, $\hat{W}_p$ is small because of a small swept length $\xi_z$, therefore $\hat{W}_{\text{net,m}} \to 0$; and (ii) Large $\xi_y / \xi_x = \xi_z / \xi_x$ implies that $\xi_x$ is small, $\hat{W}$ is large because of small flow resistances in the x-direction and large wetted areas on the electrodes, $\hat{W}_p$ is also large because of a large swept length $\xi_z$ and small hydraulic diameters $D_h$, hence $\hat{W}_{\text{net,m}} \to 0$. There must exist an intermediate $\xi_y / \xi_x = \xi_z / \xi_x$ geometric configuration such that $\hat{W}_{\text{net,m}}$ is maximum. This configuration is a trade-off between electrical power output and pumping power to supply fuel and oxidant to the fuel cell.

The effect of unit fuel cell volume on the power extraction is reported in Figure 8. The fuel cell net power increases as $\tilde{V}_T$ increases. Additional results were produced to cover the entire range $1 \leq \tilde{V}_T \leq 10$, which led to the net power and external shape aspect
ratios plotted in Figure 8b as functions of $\tilde{V}_T$. The maximized net power increases monotonically with the total volume.

Figure 6. (a) The internal structure optimization according to Fig. 5 and the dependence on external shape and ionomer water content for $\zeta_1 = \zeta_7 = 3$, and (b) The results of the internal structure optimization with respect to average membrane water content, $\lambda$, for $\zeta_1 = \zeta_7 = 3$, and their dependence on external shape.
Figure 7. (a) The external structure optimization and the dependence on stoichiometric ratio for \( (\lambda_a, \lambda_c) = (16, 20) \), and (b) The results of the external structure optimization with respect to the stoichiometric ratios, \( \zeta_1 = \zeta_7 \), for \( (\lambda_a, \lambda_c) = (16, 20) \).
Figure 8. (a) The external structure optimization and the dependence on total fuel cell volume, for $\zeta_1 = \zeta_7 = 2$ and $(\lambda_a, \lambda_c) = (16, 20)$, and (b) The results of the external structure optimization with respect to total fuel cell volume, $\tilde{V}_T$, for $\zeta_1 = \zeta_7 = 2$ and $(\lambda_a, \lambda_c) = (16, 20)$. 
Optimization of PEM Fuel Cell Stack

The constructal development of the elemental fuel cell structure led to a new problem at larger scales: the optimization of a stack [10]. Essential new features are the manifolds used for fuel and oxidant distribution to the stack of unit cells connected in series, Fig. 9. 

Figure 9. External geometry of the fuel cell stack

Figure 10. Scaling of optimized fuel cell stack
The constructal optimization of a PEMFC stack was conducted for maximizing the stack net power output. The procedure started with the construction of a mathematical model for fluid flow, mass and heat transfer in a PEMFC stack, which takes into account spatial temperature and pressure gradients in a single PEMFC, pressure drops in the headers and all gas channels in the entire PEMFC stack. The single PEMFC internal structure has an optimal allocation, and total thickness being such that wetted area in the reaction layers and electrical resistance are optimally balanced for maximum electrical power, and maximum global stack net power. Additionally, a three-dimensional flow space with the dimensions $L_x$ and $L_y$ in the plane perpendicular to $L_z$ was considered and the total volume was fixed (Fig. 9). The new degrees of freedom, i.e., the aspect ratios $L_z/L_x$ and $L_y/L_x$, allowed for the optimization of the PEMFC stack external shape, in addition to the single PEMFC internal structure and total thickness. As a result, an external shape was found such that electrical and pumping power are optimally balanced for maximum PEMFC stack net power. Dimensionless optimization results were presented graphically for the sake of generality.

A parametric analysis investigated the effect of stoichiometric ratio, $\zeta$, membrane water content, $\lambda$, and total PEMFC stack volume on the optima found. For the set of parameters given by Table 1, the optimal PEMFC stack external shape was shown to be "robust" with respect to the analyzed parameters, i.e., $1.5 \leq \zeta_1 = \zeta_1 \leq 3$, $12 \leq \lambda \leq 21$, and $0.1 \leq V_T \leq 1.16$, and the twice maximized stack net power increases monotonically with total volume, i.e., $\tilde{W}_{\text{net,mm}}$ increases approximately as $V_T^{3/4}$, similarly to metabolic rate and body size in animals [10]. This is an important finding for the purpose of “scaling up” or “scaling down” PEMFC stack design.

Fundamentally, it was shown that electrical and fluid flow trade-offs exist, and that from them results the single cell internal structure and total thickness, and the PEMFC stack external shape—the relative sizes and spacings—of flow systems, in accordance with other features of constructal design [11]. In practice, such trade-offs must be pursued based on models that correspond to real applications. The maxima found are sharp, stressing their importance for practical design, and therefore must be identified accurately in the quest for increasing the stack net power efficiency, approaching the actual PEMFC first-law efficiency level. The constructal design results reported in this study demonstrate clearly that in a PEMFC stack, gas supply causes pressure drops that induce considerable power consumption. Those facts need to be taken into account by modeling or experimentally analyzing the entire PEMFC stack, in practical fuel cell design.

**Study 4. Preliminary Results on the Internal Structure of an SOFC Unit**

This section presents our preliminary results on the optimization of the internal structure of an unit solid oxide fuel cell (SOFC). This research effort will be continued during our second year in the program.

**Introduction**

The internal structure, which accounts for the thickness of the two electrodes and the electrolyte, and the flow channels geometry, is being optimized. The model is developed using a control volume approach, in which, all relevant thermal and electrochemical interactions between adjacent elements are accounted for in as similar
fashion to our previous work on PEM fuel cells. The optimized internal structure results from optimal balances between the thickness of anode and cathode, channel shoulder aspect ratio, and the number of fuel and oxidant channels. The optima found are sharp and therefore, important to be identified in actual SOFC design.

**Thermodynamic Model**

The main features of a single SOFC are shown in Fig. 11. The fuel may be pure hydrogen, or a diluted hydrogen mixture generated from a hydrocarbon reformation process. For simplicity, the model is based on the assumption that the fuel stream is pure hydrogen, and that the oxidant is pure oxygen.

![Image of SOFC internal structure and control volumes](image)

**Figure 11.** The internal structure of a single SOFC and the control volumes selected for the optimization study.

The fuel cell is divided into six control volumes that interact energetically with one another. The fuel cell also interacts with adjacent fuel cells in a stack. The stack is assumed well insulated from the ambient. The bipolar plate (interconnect) has the function of allowing the electrons produced by the electrochemical oxidation reaction at the anode to flow to the external circuit or to an adjacent cell. The control volumes (CV) are the solid bipolar plate (CV1), the fuel channels (CV2), the anode layer (CV3), the electrolyte layer (CV4), the cathode layer (CV5), and the oxidant channels (CV6).

The model consists of writing the conservation equations for each control volume, and the equations accounting for electrochemical reactions, where reactions are present. The reversible electrical potential and power of the fuel cell are then computed (based on the reactions) as functions of the temperature and pressure fields determined by the model. The actual electrical potential and power of the fuel cell are obtained by subtracting from the reversible potential the losses due to surface overpotentials (poor electrocatalysis), slow diffusion and all internal ohmic losses through the cell (resistance of individual cell components, including electrolyte layer, interconnects and any other cell components through which electrons flow). These are functions of the total cell current (I), which is directly related to the external load (or the cell voltage). In sum, the total cell current is considered an independent variable in this study.
Shape Optimization and Results

The main geometric features of the single SOFC considered in this study are: the external dimensions \((L_x, L_y, \text{ and } L_z)\), the individual layer thickness \((L_i)\), fuel and air channels shoulder thickness \((L_t)\) and width \((L_{ch})\), and the number of channels embedded in the bipolar plate \((n_{ch})\).

Figure 12a shows the single SOFC polarization curve and the comparison of each potential loss calculated by the model. The largest loses are the activation loses, for \(0 < i < 2.7 \text{ A/cm}^2\). The results illustrate the importance of improving electro catalysis in fuel design, either by increasing wetted surface area and/or operating temperature, or by the utilization of improved new materials.

![Figure 12a](image)

**Figure 12** (a). Polarization curve. (b). Anode supported SOFC power density curves for different cathode thickness.

The effect of cathode thickness in an anode supported SOFC is illustrated in Fig. 12b. The separation of power density curves at the high working current density region illustrates that the cathode thickness affects considerably the fuel cell performance. Fig. 12b also shows that very large or very small cathode thickness does not benefit SOFC power density. Such behavior is explained physically by analyzing two extremes: i) for large cathode thickness, \(L_5\), the activation overpotentials decrease due to large wetted areas, but both ohmic (due to the large thickness) and concentration (due to large oxidant path to the reaction site) overpotentials increase and decrease the power density, \(P_w\); and ii) for small cathode thickness, both ohmic resistance (due to small thickness) and concentration (due to shorter oxidant path to reach the reaction site) overpotentials decrease, but the activation potential will be large due to lack of reaction area (poor electrocatalysis), so power density, \(P_w\), decreases at this extreme too. Therefore, there must be an intermediate optimal thickness between the two extremes that maximizes power density.
The investigation of the existence of the optimal cathode thickness was conducted in Fig. 12b. For three values of $L_5$, in the range [50, 600] $\mu$m, a maximum power density was found with respect to current density. The largest value of the maximum power density was observed for the intermediate value of the cathode thickness, i.e., $L_5=150 \mu$m, demonstrating the existence of an optimal design for the studied single SOFC. Similar studies are being conducted for cathode supported SOFCs and for anode thickness variations.

**Preliminary Conclusions**

The preliminary results of this effort showed that the internal structure of a single SOFC could be optimized so that electrical power density is maximized. This was demonstrated at the most elemental level, by constructing a model for fluid flow, mass and heat transfer in a single SOFC, which takes into account spatial temperature gradients. Two geometric degrees of freedom have been considered to be optimized, i.e., the anode thickness, $L_3$ and the cathode thickness $L_5$, other degrees of freedom currently under investigation are the channel shoulder aspect ratio, $L_t/L_{ch}$, and the total number of reactant channels, $n_{ch}$. The optima found are sharp and therefore, important to be identified in actual SOFC design. In the present study the variation of power density in the studied ranges of $L_5$ was of 11%.

In principle, the optimization performed in this study can be extended on a hierarchical ladder to large and more complex SOFC systems, to explore multi-scale packing that use the available volume for optimal performance.

**Study 5. Implementation of Fuel Cell Based Aeropropulsion Systems into Advanced Power Simulation Environments (EMTDC, RTDS)**

This effort focuses on the development and implementation of a SOFC model into an advance electrical power system simulator (e.g., EMTDC, RTDS). Electro-magnetic transients in DC, or EMTDC, is the solution engine of PSCAD (power system simulator). PSCAD/EMTDC has sophisticated algorithms specific to power electronics and an extensive library of electrical power system components.

The starting point is the SOFC model described in the SOFC/GT hybrid (Study 1) of this report, which accounts for thermal transients but not for electrical ones. The electrical response of a fuel cell model should accurately be captured before it is implemented into a power simulator such as EMTDC.

Using EIS (electrical impedance spectroscopy) data, an equivalent fuel cell electrical circuit, Fig.13, can be deduced [13].

![Figure 13- Sketch of an equivalent electrical circuit of a FC for transient analysis.](image-url)
As applied to fuel cells, the capacitor in the electrical circuit of Fig. 13 is responsible for the dynamic effect experienced correlating to the activation and concentration overpotential changes [14]. A wide range of suggested values exist for the capacitance in the equivalent circuit due to each fuel cell’s unique characteristics [13]. The fuel cell capacitance effects were incorporated in the steady state electrochemical model and implemented in EMTDC to create an electrical transient model. An EMTDC simulation illustrating the effects of the fuel cell capacitance is depicted in Figure 14. As oppose to seeing an instantaneous rise in the voltage as the load is immediately changed from .1 ohms to .2 ohms, we can observe the fuel cell’s 1st order response.

![Figure 14 - Single SOFC voltage response to a load resistance step up input (~ .7 milliseconds)](image)

Fig. 15 illustrates how the electrically enhanced model allows us to observe the overshoot phenomena in the solid oxide fuel cell’s transient power response. The spike seen in the power plot is directly related to the current response. An accuracy test was performed to insure that the spike was not being caused by an inadequate numerical time step. In addition to the electrical transient SOFC model described above, a PEMFC, boost converter, and inverter model components exist and are available as part of collaboration efforts with NASA URETI (Table 4).
<table>
<thead>
<tr>
<th>Table 4 – Fuel Cell Electrical Power System Components</th>
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</thead>
<tbody>
<tr>
<td><strong>Fuel Cell</strong></td>
</tr>
<tr>
<td>Inputs</td>
</tr>
<tr>
<td>Flow rate, capacitance # of cells, Physical geometry (area, thickness) Temperature (SOFC) and pressure</td>
</tr>
<tr>
<td>Voltage Current</td>
</tr>
<tr>
<td>PEMFC and SOFC models</td>
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</tbody>
</table>

The items listed in table 4 were integrated to form a preliminary arrangement of power systems components (Figs. 16 and 17). A super-capacitor energy storage component is also readily available. Currently, we are also investigating using batteries as energy storage components and focusing on dynamic loading simulations that may be typical in aircraft applications. Furthermore, we are looking to combine the unsteady electrical model with the transient thermal model. The thermal model operates on a much larger timescale than the electrical model; however, the RTDS simulator is capable of simulating systems with very different timescales.

Figure 16 – EMTDC assembly of SOFC, boost converter, and inverter component models
Figure 17 – EMTDC assembly of a complete PEM fuel cell electrical power system

References


