TRANSIENT ANALYSIS OF A SOLID OXIDE FUEL CELL/ GAS TURBINE HYBRID SYSTEM FOR DISTRIBUTED ELECTRIC PROPULSION

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering

By

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I HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER MY SUPERVISION BY Venkata Adithya Chakravarthula ENTITLED Transient Analysis of a Solid Oxide Fuel Cell/ Gas Turbine Hybrid System for Distributed Electric Propulsion BE ACCEPTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF Master of Science in Mechanical Engineering.

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Gas turbine technology for aerospace applications are approaching limits in efficiency gains as increases in efficiency today occurs in very small increments. One limitation in conventional gas turbine technology is the combustion process, which destroys most of the exergy in the cycle. To address this limitation in a traditional Brayton power cycle, a hybrid system which is integrated with Solid Oxide Fuel Cell (SOFC) and gas turbine is developed. Hybrid systems involving fuel cells have better efficiencies than conventional power generation systems. Power generation systems with improved performance from low fuel utilizations and low maintenance costs are possible. The combination of a SOFC fuel cell with a gas turbine has shown higher efficiencies than conventional gas turbine systems due to the reduction of exergy destruction in the heat addition process. A one-dimensional dynamic model of a Solid Oxide Fuel Cell (SOFC) integrated with a gas turbine model to develop an efficient electrical power generation system for aviation applications is investigated. The SOFC - Combustor concept model was developed based on first principles with detailed modeling of the internal steam reformer, electrochemical and thermodynamics analysis is included. Initially, a detailed investigation of internal steam reformer kinetics is presented. The overall purpose of this thesis is to analyze the performance of the hybrid SOFC-GT system for both on-design and off-design operation in an aerospace application. Transient analysis is performed to understand the uncertainties in the SOFC temperatures and hybrid system; control and stability with sudden transient
changes of the system (rapid throttle changes, environment changes like climb). Finally, SOFC model integrated with a compressor and turbine model and investigation on the overall performance of the innovative hybrid thermodynamic cycle is presented. The SOFC hybrid system has a lower power density at sea level compared to a turbo-generator, but in a typical commercial flight the SOFC hybrid system outperforms the turbo-generator in both endurance and power-to-weight ratio at cruising altitude.
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\( p_o \) Standard reference pressure, atm

\( P_r \) Pressure ratio, dimensionless

\( \dot{Q} \) Heat, W

\( R_{\text{grain2neck},a} \) Ratio of anode grain contact neck length to grain size, dimensionless

\( R_{\text{grain2neck},c} \) Ratio of cathode grain contact neck length to grain size, dimensionless

\( R_{\text{pore},a} \) Average anode pore radius, micron

\( R_{\text{pore},c} \) Average cathode pore radius, micron

\( R_u \) Universal gas constant, J/mole-K

\( r_i \) Reaction rates for each gas species, kmol/s

\( T \) Temperature, K

\( V \) Volume, m\(^3\)

\( W \) Work, kW

\( x_i \) Gas species mole fraction, kmol

\( Y \) Altitude, ft

\( z \) Number of electrons transferred for each molecule of fuel

\( \alpha \) Symmetry coefficient, dimensionless

\( \delta_{\text{Electrolyte}} \) Electrolyte thickness, \( \mu m \)

\( \varepsilon_{\text{anode}} \) Anode electrode porosity, dimensionless

\( \varepsilon_{\text{cathode}} \) Cathode electrode porosity, dimensionless

\( \eta_{\text{Act},a} \) Anode activation polarization, V

\( \eta_{\text{Act},c} \) Cathode activation polarization, V

\( \eta_c \) Compressor design efficiency, dimensionless

\( \eta_{\text{Conc},a} \) Anode concentration polarization, V

\( \eta_{\text{Conc},c} \) Cathode concentration polarization, V

\( \eta_{\text{Ohm,elec}} \) Electrolyte ohmic polarization, V

\( \eta_{\text{Ohm,IC}} \) Interconnect ohmic polarization, V

\( \eta_T \) Turbine design efficiency, dimensionless
\( \mu \)  Fuel Utilization
\( \tau \)  Anode electrode tortuosity, dimensionless
\( \sigma \)  Leonard-Jones collision diameter, angstrom
\( \Omega \)  Diffusion collision integral, dimensionless
ACKNOWLEDGEMENTS

I have learned so much through this journey of pursuing an advanced degree in mechanical engineering. Through this process, I have enhanced my engineering, mathematical, and communication skillsets, thus growing as an engineer. I have encountered many people during this time whom have contributed a great deal to my education.

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nights and stressful times, they were always there for me. I couldn’t have asked for better support during my studies.
INTRODUCTION

The overall fuel efficiency of aircraft has increased over the last several decades, but it has begun to plateau. When analyzing an aircraft, the two major areas of losses is through drag and propulsion efficiency. Propulsion efficiency may be improved by driving the gas turbine to operate at higher pressures and temperatures within the engine core with material and design improvements. While this improves the thermal efficiency of the core, the propulsion efficiency of the turbofan engine increases as the fan pressure ratio (FPR) decreases Felder, Kim & Brown (2009). Thus, efficiencies are higher when the fan exhaust is lower both in velocity and temperature. This drives turbofan design to have a high-performance core at the highest operating pressure and temperature while having the fan at lower pressure ratios, lower velocities and higher mass flows resulting in high bypass ratios. From an exergy analysis, the same trend may be interpreted by analyzing the exergy losses within the wake of the aircraft Abbas & Riggins(2016). It has been shown that over 50 % of the exergy is destroyed within the wake of the aircraft. As stated by the Abbas, & Riggins (2016), the greater the dynamic thermal/fluid gradients between the propulsion exhaust and the ambient flow-field the greater the production of entropy generation and exergy destruction. Therefore to meet the NX-3 NASA goal of +70 % reduction in fuel and energy consumption in NASA’s Subsonic Fixed Wing project(Follen, Del Rosario, Wahls, & Madavan, 2011)(Follen, Del Rosario, Wahls, & Madavan, 2011), the trend in propulsion is to provide the required thrust, while minimizing the thermal/fluid gradients between the exhaust and ambient air.
There are geometric limitations in a conventional high bypass turbofan. Higher bypass ratios require larger diameter turbofans, which is limited structurally by the aircraft. If too large a diameter then the turbofan’s clearance with the ground during takeoff would diminish. Distributed propulsion provides the benefit of essentially a very high bypass fan flow with lower velocity and temperature exhaust relative to the ambient air without the need for large diameter inlets. Distributed propulsion also has aerodynamic benefits of boundary layer ingestion for drag reduction Goldberg et al. (2016). Distributed propulsion concepts have migrated towards distributed electric propulsion with electric driven fans. This arrangement would require electrical power production onboard an aircraft.

One option for the electrical power plant of the aircraft is a turbo-generator. Based on a first law analysis the turbo-generator efficiency when calculated will range from 30-35% for fuel-to-electricity conversion. Note from a second law exergy analysis 50-60% of the exergy destruction is within the wake of the vehicle. The exergy destruction within the combustor of the gas turbine based engine is 24-31% depending on the operating condition of the engine [Abbas, & Riggins(2016), Marley & Riggins (2011)]. Approximately 4% of the exergy destruction occurs within the inlet, compressor, and turbine. From a first law analysis, it may appear that a turbo-generator efficiency may be improved over time with advances in materials and component design, but in reality, 74-91% of the exergy is destroyed independent of the component and subsystem efficiencies.

To reach higher efficiencies, changes to the architecture for both power generation and propulsion is needed. As mentioned previously the exergy destruction in the wake may be reduced by a very high bypass turbofan engine or distributed propulsion through a series of distributed fans along the body of the aircraft. As for combustion, which corresponds
to the exergy destruction during power generation for the propulsion system there is very little room for improvement since the fuel is generally assumed to be 100 % burned. The chemical process of converting fuel to heat is a significant portion of the entropy generation thus exergy destruction. A recuperated cycle may be considered to regenerate some of the heat of the exhaust back into the system resulting reduced fuel burn. Pressure gained combustion is another concept for reducing the exergy destruction of the combustion process. Another option is the use of a high temperature fuel cell such as a solid oxide fuel cell (SOFC) in place of the combustor. The electrochemical oxidation process of the fuel is much lower in exergy destruction resulting in more efficient power generation on board of the aircraft.

In this thesis, the authors perform comparisons for both performance and efficiency of a SOFC–Gas turbine (SOFC/GT) cycle for power generation and a turbo-generator. To further analyze the behavior of the SOFC/GT cycle a transient cycle model was created. Results of the comparisons and transient simulations are presented.
BACKGROUND

Fuel cells are electrochemical devices which convert chemical energy into electrical energy. The fuel cells consist of three major components electrolyte and a pair of electrodes that act as anode and cathode. Fuel cells were first introduced to the world by British lawyer and physicist William Grove in 1839 who built a simple fuel cell using a beaker with a diluted acidic solution that served as the electrolyte (Grove 1839; Larminie 2003) and platinum rods as electrodes. These devices are known for their combustion less power generation devices. There are many types of fuel cells which are shown in Table 1

<table>
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<th>Table 1. Types of Fuel cells and properties</th>
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<tr>
<td>Fuel Cell Types</td>
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<tr>
<td>Direct Methanol Fuel cell (DMFC)</td>
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<td>Alkaline fuel cell (AFC)</td>
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<td>Phosphoric acid fuel cell (PAFC)</td>
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<td>Molten carbonate fuel cell (MCFC)</td>
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Figure 1 shows a detailed outline of different fuel cell’s electrolyte, ions flow through electrolyte and operating temperature. Solid Oxide Fuel Cell (SOFC) and Molten
Carbonate Fuel Cell (MCFC) are most suitable for power generation devices along gas turbines because of their operating temperatures. This thesis work SOFC is integrated with gas turbine engine to improve the over-all energy and exergy efficiencies. Investigations into SOFCs were started in mid-20th century and its benefits have matured with technology into the 21st century.

**Figure 1: Types of Fuel cell with outline of electrolyte transfer ions**

SOFCs are a highly attractive alternative electric power generation for various commercial sectors. They are known for high efficiencies, low emissions, low noise, reliability, and fuel flexibility therefore making them highly promising devices for future
energy conversions. SOFC’s can mainly be divided into two types depending on the geometry: planar and tubular. However, many research works are going on different configuration such as wave structured planar SOFC’s, hybrid of planar and tubular as mentioned by Buonomano et al (2015). Planar SOFCs are advantageous for their higher power density and simple manufacturing processes but lack mechanical strength and fuel flexibility. Tubular SOFC have higher mechanical strength therefore reliability and high-energy efficiencies with fuel flexibility. SOFCs consist of two porous ceramic electrodes (anode and cathode) and a solid ceramic electrolyte between the electrodes. A solid ceramic structure reduces corrosion problems and increases cell tolerance against high temperatures. Since SOFC’s can operate at high operating temperatures, hot exhaust gases can be utilized to drive Brayton or Rankine cycle. This ability of SOFC’s has attracted many researchers for development of SOFC hybrid systems. SOFC can be associated as pure power generation, cogeneration of power along with a gas turbine, Combined Heat, and Power generation (CHP), and Combined Cooling Heating and Power generation (CCHP).

SOFCs combined with gas turbine systems are a possible candidate as an efficient energy conversion device for the next generation. Consequently, a significant amount of research has been published investigating different aspects of this technology.

Daniel et al (2015) from University of Maryland, college park, has analyzed hybrid systems of SOFC’s integrated with gas turbine engines. They have integrated SOFC’s with three different gas turbine engine types’ turbojet, combined exhaust turbofan and separate exhaust turbofan. Catalytic partial oxidation is used to produce fuel (hydrogen) for the SOFC. Thermodynamic analysis is carried out for CPOx reactors, SOFC and three gas
turbines resulting in increased fuel efficiencies by 4% and 8% for 50kW and 90kW respectively hybrid power systems involving SOFC/ separate exhaust turbofan respectively. Similar results were shown for other gas turbine types. A parametric study on these hybrid systems show that the systems performance is dependent on operating fuel cell voltage, percent fuel oxidation, and SOFC assembly air flow. With these hybrid systems, fuel flow is reduced by 5% and electric power output is increased by ~500% without effecting TIT.

Zahar Hajabdollahi and Pei-Fang (2016) from Huazhong University of science and technology, Wuhan, China have worked on optimization of a cogeneration plant including gas turbine, SOFC, heat recovery steam generator(HSRG) as well as inlet cooling system. Individual mathematical models of each component were verified with the experiment data from literature and results were observed to be in ~2% range. A probability is carried by varying a system’s design parameters like compressor & turbine efficiencies, Turbine inlet temperatures(TIT), fuel mass flow rate etc.,. This study resulted in 5 optimum design points A-E. Point A shows maximum exergy efficiency of 0.4849 and worst total cost rate (TCR) i.e 1044$/hr, whereas point E shows minimum TCR (734$/hr) with a lower exergy efficiency of 0.4590. Remaining points shows moderate values of both objectives. Design points A and B include SOFC where other points do not include it. Thus, adding a SOFC system to the gas turbines increases exergy efficiencies where the TCR grows worst.

Barelli et al (2016) from University of Perugia, Perugia, Italy worked on SOFC/ GT system integrated in Micro- Grids. They stated that SOFC/GT hybrid system efficiency performance increases with a mean efficiency of 54.5% on daily basis and its short time response and a wide load perturbations as low as 42.8% of hybrid systems full power.
their research work, SOFC-GT hybrid systems dynamic model is created with control strategy to regulate the SOFC and GT systems to the load demand with safe SOFC operation. With drop in load demand, SOFC's efficiencies increases slightly by 2% for a load drop from 95kW to 62.5kW. This shows that SOFC-GT hybrid system with a well-established control strategy is one of the efficient power generation system for high load demand fluctuations.

Penyarat (2015) from King Mongkut's University of Technology North Bangkok, Thailand have worked on two different configurations of the SOFC-GT hybrid systems. For one of the configuration, fuel exchanger's hot stream is drawn from combustor and other from turbine exit. First configuration results in higher SOFC operating temperature and lower Turbine inlet temperature vice versa for the second configuration. First hybrid system's overall efficiencies are ~4.5% higher than second one. This is due to the higher operating temperature of SOFC system where as GT efficiency is higher in second configuration.

McLarty et al (2013) from University of California worked on integration of fuel cells with gas turbines. They have come up with molten carbon fuel cell and SOFC hybrid systems with Gas turbines. Steady state models for each hybrid systems are created and analyzed. Both the hybrid systems are assumed with cathode recirculation to increase the inlet air temperatures. These hybrid systems can produce up-to 1.2 MW electric power with LHV efficiencies higher than 70% and 75% respectively. This study shows that SOFC-GT hybrid systems are more efficient in terms of fuel LHV. McLarty et al also worked on dynamic models of the hybrid systems with additional control methods. These models results show that fuel cell hybrid systems response is better than individual sub systems.
(gas turbines, fuel cells etc...) over a larger operating envelope. The control methods include combined feed forward P-I and cascade control strategies which are capable of handling dynamic perturbations. These MCFC-GT and SOFC-GT could achieve 2:1 and 4:1 turndown ratio respectively with LHV efficiencies higher than 65%.

Investigations on methane steam reforming started in mid-20th century. Xu and Froment (1989) conducted many experiments on this hydrogen production process and derived intrinsic rate equations for methane steam reforming process accompanied by water-gas shift equation on a Ni/MgAl₂O₄ catalyst. Ahmed and Fogre (2000) experimented on the fuel cell configuration and considered Ni-YSZ anode materials for the experiment. Two anode materials are used in the experiment. Anode A is like Xu and Froment (1989) study and Anode B is added with a basic compound (Ni-ZrO₂). Anode B showed increased methane conversion rates, steam dependencies and activation energies. Hou and Hughes (2001) considered Ni/α-Al₂O catalyst for the analysis and came up with different intrinsic rate equations and activation energies. These results can only be applied to the anode surfaces with similar catalyst. Campanari and Iowa (2004) and Qi et al (2006) used Ahmed and Fogre results for their analysis. Galluci et al (2004) and Oliveira et al (2009) used Xu and Froment results for their analysis. Oliveira et al (2009) also performed many experiments for different operating temperatures ranging from 773K to 890K derived effectiveness values of steam reforming equations. Effectiveness of steam reforming, water gas shift and over-all reactions are 0.32, 0.08 and 0.32 respectively. All the chemical reactions involved in the methane steam reformer are reversible reactions and operating temperatures decide the direction of reactions.
Other literature studies, Massardo & Lubelli (1999) developed four different hybrid cycle configurations of SOFC’s plus internal reforming integrated with gas turbines. Numerical thermodynamic models were modeled to understand the impact of anode and cathode inlet temperatures on thermos cycles. Campanari & Iora (2004) analyzed hybrid cycle of micro gas turbine integrated with SOFC. Hybrid cycles analysis results showed an overall electrical energy efficiency increased to 63% and when SOFC is used as CHP system, thermal efficiency increased to 86%. A similar study by Haseli (2008) on SOFC hybrid cycles, with on additional air and fuel recuperates increased energy and exergy efficiencies to 60.6% and 57.9% respectively. Mehrpooya et al (2014) compared cross and co-flow planar SOFC hybrid systems and observed that both the configuration delivered similar results. A further parametric analysis of the model resulted in increase in power output with inlet temperature and pressure of SOFC stack.
MATHEMATICAL MODELING

Mathematical models are enabling tools in the development of new technologies. One-dimensional mathematical model is developed based on the basic first principles. A hybrid thermo cycle is analyzed with following components: SOFC with internal steam reformer, compressor, and turbine Figure 2 shows the thermos cycle and flow of air and fuel through the system. This model has capabilities to simulate both steady state and transient behavior of the hybrid system for a wide range of operating conditions. Micro tubular SOFC’s with 4 mm diameter are assumed for the thesis. Depending on the required power output, these micro fuel cells are stacked together. A thorough thermodynamic and electro chemical analysis of a single fuel cell can be considered to understand the complete stack’s performance. Along with the performance analysis of the fuel cell, it is very important to understand the thermal gradients and species concentrations along the fuel cells, hence a single fuel cell is discretized into 10 nodes to understand this variation along the cell.

The following assumptions are considered for single cell:

1. No pressure losses along the node
2. Radiation losses are neglected
3. Equipotential cells.

Pressure losses along the fuel cell are very minimal (reasonable for micro cells) and can be assumed to be uniform along a single cell. SOFC tubes are stacked together, therefore, every tube is surrounded by the similar temperature tubes, which minimizes heat transfer
by radiation. However, tubes on the surface of stacks may be exposed to different temperatures and the system is assumed to be adiabatic.

**Figure 2: Schematic of SOFC-GT hybrid system.**

A counter-flow SOFC system is designed to integrate with the gas-turbine. Counter-flow SOFC system simplifies the thermo cycle by avoiding air recuperators and thus reduction in components, complexity and masss. High temperature air requirement of a SOFC system is achieved by burning the unutilized fuel from SOFC anode in the combustor to raise the air temperature from compressor exit temperature to the required cathode inlet temperature.

**A. Combustor Model:**

The combustor model is developed to capture the enthalpy and chemical species concentration changes due to the combustion of the unutilized fuel and/or exit products of the SOFC. This unutilized fuel from SOFC and air from compressor burns in the combustion chamber producing hot gases. The unutilized fuel is regulated to keep
combustion chamber’s overall temperature at 1043K. Equation 1 is used to calculate the combustor out temperature.

\[
\frac{dT}{dt} = \frac{1}{c_p \times C \times V} \left[ (N_{in} H_{in} + \Delta H_{comb} - N_{out} H_{out}) \right]
\]

1

Where, \( c_p \) is the specific heat at constant pressure, \( C \) is the chemical concentration of gas based on pressure and temperature \( C = \frac{P}{RT} \), \( N \) is the molar rates in and out, \( H \) is the enthalpy of the mixture in and out and \( \Delta H_{comb} \) is the heat produced in the combustion process.

B. Solid Oxide Fuel Cell Modeling:

As discussed earlier, a single solid oxide fuel cell is discretized along the cell length into 10 nodes and all the electrochemical and thermal properties were calculated at every node. SOFC modelling consists of two major parts: Electrochemistry and thermodynamic analysis. Electrochemistry in turn involves species conservation and voltage calculations.

1. Electrochemistry Model

Electrochemical model with dynamic internal reformer model is developed. Hydrogen and oxygen are the main reactants of the electrochemical reaction, there are different procedures to produce hydrogen. The most efficient way is from hydrocarbons using steam reforming process. When hydrocarbons react with steam in the presence of a catalyst (mostly nickel alloys), it generates carbon monoxide and hydrogen. For this thesis work, liquid natural gas (LNG) is considered as the fuel and hydrogen is produced from steam reforming process. The following are the chemical reactions of steam reforming process.
\[
\begin{align*}
\text{CH}_4 + \text{H}_2 \text{O} &\rightleftharpoons \text{CO} + 3\text{H}_2 & \text{2} \\
\text{CO} + \text{H}_2 \text{O} &\rightleftharpoons \text{CO}_2 + \text{H}_2 & \text{3} \\
\text{CH}_4 + 2\text{H}_2 \text{O} &\rightleftharpoons \text{CO}_2 + 4\text{H}_2 & \text{4}
\end{align*}
\]

Change in enthalpies for the reaction's 2, 3 and 4 at room temperature are \(\Delta H_{298}^\circ = 206 \text{ kJ/mol, } \Delta H_{298}^\circ = -41 \text{ kJ/mol and } \Delta H_{298}^\circ = 165 \text{ kJ/mol} \) respectively. Reactions 2 and 4 are endothermic in nature whereas reaction 3 is exothermic. Xu and Froment (1989) conducted many experiments to estimate the kinetics of methane steam reforming process and developed following reactions rate equations as shown in Equation 5.

\[
\begin{align*}
\frac{r_1}{k_1} &= \frac{p_{\text{CH}_4}p_{\text{H}_2 \text{O}} - p_{\text{H}_2}^{0.5}p_{\text{CO}}}{p_{\text{H}_2}^2} \\
\frac{r_2}{k_2} &= -\frac{p_{\text{CO}}p_{\text{H}_2 \text{O}} - p_{\text{CO}_2}}{p_{\text{H}_2}} \\
\frac{r_3}{k_3} &= -\frac{p_{\text{CH}_4}p_{\text{H}_2 \text{O}}^2 - p_{\text{H}_2}^{1.5}p_{\text{CO}_2}}{p_{\text{H}_2}^3}
\end{align*}
\]

where,

\[
\begin{align*}
\text{DEN} &= 1 + K_{\text{CO}}p_{\text{CO}} + K_{\text{H}_2}p_{\text{H}_2} + K_{\text{CH}_4}p_{\text{CH}_4} + K_{\text{H}_2 \text{O}} \frac{p_{\text{H}_2 \text{O}}}{p_{\text{H}_2}} \\
k_i &= A_i \exp\left(-\frac{E_i}{RT}\right) \quad \text{i= Reactions 1, 2 and 3} \\
K_j &= A_j \exp\left(-\frac{\Delta H_j}{RT}\right) \quad \text{j= CH4, CO, CO2, H2, H2O}
\end{align*}
\]
Using the above kinetic reaction rate equations, methane steam reforming chemical reactions rates are calculated based on operating conditions. Experimental values for the kinetic and adsorptions parameters are shown in Table 2 and Table 3.

**Table 2. Kinetic parameters Xu and Froment (1989)**

<table>
<thead>
<tr>
<th>Reaction No.</th>
<th>( A_i ) \ [ mol.MPa^{0.5} (g_{cat})^{-1} h^{-1} ]</th>
<th>( E_i ) \ [ kJ mol^{-1} ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.336.10^{15}</td>
<td>240.1</td>
</tr>
<tr>
<td>2</td>
<td>1.955.10^{7}</td>
<td>67.13</td>
</tr>
<tr>
<td>3</td>
<td>3.226.10^{14}</td>
<td>243.9</td>
</tr>
</tbody>
</table>

**Table 3. Adsorption parameters Xu and Froment (1989)**

<table>
<thead>
<tr>
<th>Species</th>
<th>( A_j ) \ [ Mpa^{-1} ]</th>
<th>( \Delta H_j ) \ [kJ mol^{-1} ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>8.23.10^{-4}</td>
<td>-70.65</td>
</tr>
<tr>
<td>H2</td>
<td>6.12.10^{-8}</td>
<td>-82.9</td>
</tr>
<tr>
<td>H2O</td>
<td>1.77.10^{-5}</td>
<td>88.68</td>
</tr>
<tr>
<td>CH4</td>
<td>6.65.10^{-3}</td>
<td>-38.28</td>
</tr>
</tbody>
</table>

Hydrogen produced in the methane steam reforming process reacts with the catalyst on the anode side and splits into hydrogen ions and 2 electrons whereas the oxygen molecules on the cathode side goes through reduction reaction and splits into oxygen ions and 4 electrons. These oxygen ions travel through the ceramic electrolyte of the SOFC to oxidize the hydrogen ions on the anode side. Meanwhile the electrons on the anode side
and cathode side are collected by the electrodes and transferred through interconnects to the load.

Cathode Reduction Reaction:

\[
\frac{1}{2} O_2 \leftrightarrow \frac{1}{2} O_2^- + 2e^- \quad 6
\]

Anode Chemical Reaction:

\[
H_2 - 2e^- \leftrightarrow H_2^{2-} \quad 7
\]

Overall Electro-Chemical Reaction:

\[
H_2 + \frac{1}{2} O_2 \leftrightarrow H_2O \quad 8
\]

2. Species Conservation:

SOFC electrochemistry is very important in understanding the performance of the fuel cell. There are many reactions that happening simultaneously at very high temperatures. Some of the reactions are endothermic and some of them care exothermic. Fuel cell performance and reliability depends on the chemical species concentration along the cell. A general species conservation equation is given by Equation 9

\[
N_{total} \frac{d\chi_i}{dt} = N_{in} \chi_{i \_in} - N_{out} \chi_{i \_out} + R\chi_i \quad 9
\]

where \( \chi_i \) is the respective species concentration with \( i = \text{CH}_4, \text{CO}, \text{CO}_2, \text{H}_2, \text{H}_2O, \text{N}_2 \) & \( \text{O}_2 \), and \( R \) represents the reaction rates of the chemical reactions in which individual species are involved. The reaction rate in Equation 9 includes both the electrochemical and internal steam reforming reaction rates. The change in mole fractions of species due to the electrochemical and steam reforming reactions is calculated based on the chemical reaction equations (Equation 10).
A negative sign before the reaction rate indicates that the species is consumed during the process and a positive sign before the rate indicates that the species is formed during the process.

3. Voltage Calculations:

Ideal cell voltage or open circuit voltage from an electrochemical reaction is known as the Nernst potential and is given by the Nernst equation. The Nernst equation is derived from the Gibbs free energy where $\Delta G$ is related to voltage ($E$) by

$$ \Delta G = -nFE $$

where $n$ is number of electrons transferred, $F$ is faraday’s constant (96485 C/mol e$^-$) and $E$ is the potential. Equation 12 is known as Gibbs law at standard conditions.

$$ \Delta G_o = -nF E_o $$

For non-standard conditions, the change in Gibbs free energy is related to standard conditions by,
\[ \Delta G = -\Delta G_0 + RT \ln \left( \frac{P_{H_2}P_{O_2}^{0.5}}{P_{H_2O}} \right) \]

Using equation 12 and 13, the Nernst potential for the electrochemical reaction (Equation 14) is given by,

\[ E_{\text{NERNST}} = -\frac{\Delta G_0}{nF} + \frac{RT}{nF} \ln \left( \frac{P_{H_2}P_{O_2}^{0.5}}{P_{H_2O}} \right) \]

where \( R \) is universal gas constant, \( T \) is operating temperature, \( n \) is the number of electrons transferred (\( n=2 \) for current analysis) and \( p \) subscript is the partial pressure of \( H_2, O_2 \) and \( H_2O \). The reversible \( E_{\text{ernst}} \) is not possible because of irreversibility’s related to activation, concentration and ohmic polarizations. Hence the final voltage calculations involve these losses and is given by Equation 15

\[ V_{FC} = E_{\text{NERNST}} - V_{\text{act}} - V_{\text{ohmic}} - V_{\text{Conc}} \]

\[ a. \ Activation \ Loses: \]

Energy used to start the chemical reaction is called the activation energy. This phenomenon to start an electro chemical reaction drops the voltage and is called as activation loss. These losses are seen on both anode and cathode sides of fuel cell. However, oxygen reduction reaction rates are much slower than hydrogen oxidation rates. Hence the reduction of oxygen shows higher activation losses. Butler-Volmer has given an equation to calculate this loss.

\[ V_{\text{act}} = \frac{RT}{2F} \ln \left( \frac{j}{j_0} + \sqrt{1 + \left( \frac{j}{2j_0} \right)^2} \right) + \frac{RT}{4F} \ln \left( \frac{j}{j_0} + \sqrt{1 + \left( \frac{j}{2j_0} \right)^2} \right) \]

From equation 16, the first part resembles the oxidation of hydrogen reaction where 2 electrons are being transferred (\( n=2 \)) where the second part resembles the reduction of
oxygen where 4 electrons are being transferred \((n=4)\). Activation losses are the dominant losses of all fuel cell losses.

**b. Ohmic Losses:**

Ohmic losses occur due to the resistance of the components towards the transfer of ions and/or electrons. This loss is generally observed in the components like electrolyte, interconnects, electrodes. This resistance of components causes a voltage drop and can be calculated using Ohms law as shown in Equation 17.

\[
V_{\text{ohmic}} = R_{\text{ohmic}} J \tag{17}
\]

\[
R_{\text{ohmic}} = \sum_{n=1}^{4} \delta_n A_n \exp\left(\frac{B_n}{T}\right) \tag{18}
\]

where \(\delta\) is the thickness of the respective component, \(A_n \exp\left(\frac{B_n}{T}\right)\) is the corresponding material resistivity and constants \(A\) and \(B\) are listed in Table 4. Cathode and Anode material resistivity’s are very minimal compared to the electrolyte and interconnects and hence neglected from calculations.

**Table 4. Ohmic loss Constant Parameters**

<table>
<thead>
<tr>
<th>Components</th>
<th>(A(\Omega \text{-m}))</th>
<th>(B(\text{m}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrolyte</td>
<td>2.94E-05</td>
<td>1.05E+04</td>
</tr>
<tr>
<td>Interconnector</td>
<td>1.20E-03</td>
<td>4.69E+03</td>
</tr>
</tbody>
</table>

c. **Concentration losses:**

The concentration losses/mass transport losses are due to the overflow of reactants over the electrode surfaces. From Faraday’s law of electrolysis, transferred charge and
molar fluxes are directly proportional to the current density. At high current densities, molar fluxes increase, increasing concentration of species on the electrode surfaces. This in turn increases the partial pressures of the reacting species which effect the voltage calculations, Equation 14. Concentration losses can be calculated using Equation 19.

\[ V_{conc} = \left( \frac{1}{1 + \alpha} \right) \frac{RT}{nF} \ln \left( \frac{j_L}{j_L - j} \right) \]

where \( \alpha = 1 \) for anode and \( \alpha = 0.5 \) for cathode. \( J_L \) is the limiting current density where reactants concentration reaches zero and is given by Equation 20

\[ j_L = \frac{DCn_eF}{t} \]

where \( D \) is the diffusivity, \( C \) is the concentration and \( n_e = 2 \) for the anode and 4 for the cathode. However, most of the fuel cells doesn’t operate at higher current densities due to higher losses.

\[ \text{Figure 3: Fuel cell’s Voltage vs Current Density Curve.} \]

Figure 3, shows current density vs Voltage plot or well known as V-J plot. Ideal voltage is the maximum voltage that can be attained by a fuel cell at standard day
conditions. Zero current voltage or Nernst potential is the maximum voltage that can produced by a fuel cell for zero loading (when no current is drawn from fuel cell). With the increase in the current density the voltage starts dropping due to the three polarizations discussed above. Initially, activation polarizations reduce the fuel cell voltage to initiate the electro-chemical reactions. This voltage loss decreases exponentially with the increase in the current density. With further increase in the current density, fuel cell components start resisting the electron motion. Thus, the ohmic polarization reduces the fuel cell voltage. Since the ohmic polarization equation is linear in nature, the drop is also linear with current density. Any further increase in the current density, the concentration of the species increases and thus increasing concentration polarization. This loss is a logarithmic decrement and thus fuel cell voltage drops drastically with further increase in the current density.

Power produced by the fuel cell is the product of the voltage and current. From Figure 3, the second axis represents fuel cell power density. With the increase in the current density, power density increases initially and starts decreasing with the polarization losses reducing the voltage drastically. SOFC attains maximum power densities typically at a voltage of 0.5V. Due to the presence of catalyst on the surface of the cell, electrochemical reactions are assumed to be happening on the surface of the cell. Hence, for all the voltage calculations cell temperatures at individual nodes were used.

C. Thermodynamic Model:

Thermodynamic model is developed based on first law of thermodynamics. SOFC performance depends on the voltage fluctuations which in turn depends on the temperature gradients (From the previous section). Hence it is very important to understand the
temperature profile along the tube. High temperature gradients reduce the reliability of the fuel cell. Electrochemistry of the fuel cell involves many reactions some of which produces heat and some consume it. In this paper, a one dimensional dynamic thermodynamic model is developed to calculate the temperature profiles of fuel/ products on Anode side, fuel cell wall temperature (catalyst is available on the wall and all the reactions happen on wall) and hot gases through the cathode side.

Figure 4: Thermodynamic models for the anode, tube, and cathode.

This thermodynamic model is similar to combustor model discussed in section 2-A. The only different would be the species concentration also depends on the reaction rates of the chemical reactions. This chemical reaction rates vary along the cell causing uneven heat distribution. In addition to the chemical reactions, heat due to voltage losses also effect the tube surface temperatures. The air thermodynamic model is like the fuel with additional
heat transfer from the surroundings. Figure 4 shows the three thermodynamic models used to calculate fuel, wall, and air temperatures. Equation 21 is the general form of energy conservation for air and fuel temperatures.

\[
\frac{dT_{\text{air/fuel}}}{dt} = \frac{1}{cp \times C \times V} \left[ N_{\text{in}} H_{\text{in}} + hA(T_{\text{out}} - T_{\text{tube}}) - N_{\text{out}} H_{\text{out}} \right] \tag{21}
\]

where \(N_{\text{in}},\) and \(N_{\text{out}},\) are the molar rates of the fuel or hot gases passing in and out of a control volume, \(H_{\text{in}}\) and \(H_{\text{out}}\) are their enthalpies, respectively. Equation 22 is the general form of energy conservation for tube temperatures.

\[
\frac{dT_{\text{tube}}}{dt} = \frac{1}{c_p \times c \times V} \left[ \Delta H_{\text{chem}} + \Delta V_{\text{losses}} + hA(T_{\text{out}} - T_{\text{air/fuel}}) \right] \tag{22}
\]

where tube temperature calculations involve heat (\(\Delta H_{\text{chem}}\)) from chemical reactions and voltage losses (\(\Delta V_{\text{losses}}\)).

**D. Turbo-Generator Model:**

![Turbo-Generator schematic](image)

**Figure 5: Turbo-Generator schematic.**

A simple turbo-generator model, with compressor, combustion, turbine, and generator is analyzed to understand the over-all system’s performance enhancement because of the
integation of SOFC. Figure 5 shows the turbo generator systems schematic. This turbo-generator is more like an industrial engine. Combustor model of the turbo-generator is similar to the combustor model of the SOFC system.

1. Compressor Model

Compressor model is based on the isentropic efficiency equation and compressor performance maps designed to meet the SOFC’s pressure and flow requirements. Pressurized SOFC’s are proven for their better performance than ones which operate at atmosphere conditions. With altitude pressure and temperature drops, it is important to maintain the stable SOFC inlet conditions throughout the mission profile.

\[ T_{\text{out}} = T_{\text{in}} \left(1 + \frac{1}{\eta} \left( \frac{P_{\text{out}}}{P_{\text{in}}} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right) \]  

Where \( \eta \) is the compressor efficiency and its value was assumed to be 0.8. Equation 23 is used to calculate the exit temperature of the air. Enthalpy change across the compressor can be calculated using the inlet and exit temperatures of the air. This enthalpy difference is the work required to compress the air from atmospheric conditions to combustor inlet conditions.

2. Turbine Model

A dynamic turbine model is developed based on the isentropic efficiency and ideal gas equations. In any thermodynamic cycles, pressures are calculated from the outlet of system to inlet of system i.e is from nozzle’s outlet to nacelle’s inlet whereas all other parameters are calculated vice versa. Pressure changes across the turbine are calculated based on the inflow rates and outflow rates of the turbine. Inflow rates are the gas mass flow rates from
SOFC and outflow rates are calculated from the turbine performance maps (maps are sized to match the system requirements). These performance maps assume that the turbine exit is connected to an ideal nozzle which means the exhaust flows to atmosphere. Hence the exit pressure of the turbine is always atmosphere pressure.

\[
T_{out} = T_{in} \left(1 + \eta \left(\frac{P_{out}}{P_{in}} \right)^{\frac{γ-1}{γ}} - 1\right)
\]

Equation 24

where \( η \) is the turbine efficiency and its value was assumed to be 0.8. Equation 24 is used to calculate the exit temperature of the gas. Enthalpy change across the turbine can be calculated using the inlet and exit temperatures of the gas. This enthalpy change is nothing but the work extracted from the hot gases. This work extracted is transferred through the single shaft connected to compressor and generator.
PROPULSION ARCHITECTURE COMPARISONS

A simple enthalpy balance analysis is carried out to understand the performance of SOFC-GT hybrid system over GT system. Two thermodynamic cycles are compared in this analysis. Cycle 1 is simple Brayton cycle consists of compressor, combustor & turbine, as shown in Figure 5 and Cycle 2 is hybrid system where SOFC-Combustor replaces combustor of cycle 1 as shown in Figure 2. Both cycles were analyzed for cruise condition (i.e. at 3500ft.). The cruise condition assumptions are shown in Table 5. Table 6 presents the assumptions made for the analysis.

Table 5. Assumption for flight condition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Altitude</td>
<td>35000</td>
<td>ft</td>
</tr>
<tr>
<td>Mach No.</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Inlet Pressure</td>
<td>23.88</td>
<td>kPa</td>
</tr>
<tr>
<td>Inlet Temperature</td>
<td>218.2</td>
<td>K</td>
</tr>
</tbody>
</table>

Similar compressor and turbine properties are assumed for both the cycles. Exit temperatures of these components are calculated using the isentropic efficiency equation. Inlet and exit temperatures of the components (compressor and turbine) are used to calculate change in specific enthalpies. From the first law of thermodynamics, net work performed is equal to change in enthalpy (assuming systems are adiabatic). Hence the
change in specific enthalpies is nothing but work required or work extracted per unit mass of air from the component in an adiabatic environment.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>TG</th>
<th>SOFC-GT</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressor efficiency</td>
<td>0.8</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Compressor Pressure ratio</td>
<td>42.1</td>
<td>29.3</td>
<td></td>
</tr>
<tr>
<td>Turbine Inlet Temperature</td>
<td>1573</td>
<td>1093</td>
<td>K</td>
</tr>
<tr>
<td>Turbine Efficiency</td>
<td>0.8</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Methane LHV</td>
<td>50</td>
<td>50</td>
<td>MW/Kg</td>
</tr>
</tbody>
</table>

Table 6. Cycle assumptions

Turbo-generator’s combustion process calculates the amount of fuel (methane) required to raise unit mass of air from compressor exit temperature to the turbine inlet temperature. Change in specific enthalpy across the combustion chamber is the total energy per unit mass of air available for the system. In Cycle 2, SOFC-GT hybrid, the combustion process is different because of its electrochemical reaction. To minimize the concentration and activation polarizations, SOFC exit gas’s minimum oxygen percentage should be greater than 12%. Overall chemical reaction is balanced to achieve this 12% oxygen at the exhaust of SOFC system. Fuel-to–air ratio is calculated based on balanced chemical reaction. Available total energy per unit mass of air can be calculated using methane’s LHV and fuel-to-air ratio. Electric power produced by the SOFC system is the difference between total energy available and heat required to raise the unit mass of air from compressor exit temperature to turbine inlet temperature. This simple approach of calculating the SOFC
power from an energy balance is used because in the configuration being studied the SOFC power is limited by the oxygen at the exit of the stack.

Table 7. Analysis results of cycles 1 and 2 on a unit kg air basis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>TG</th>
<th>SOFC-GT</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel-to-air ratio</td>
<td>0.0241</td>
<td>0.0236</td>
<td></td>
</tr>
<tr>
<td>Total Energy</td>
<td>1.205</td>
<td>1.180</td>
<td>MW</td>
</tr>
<tr>
<td>Total Power</td>
<td>0.544</td>
<td>0.818</td>
<td>MW</td>
</tr>
<tr>
<td>Cycle Efficiency</td>
<td>45.1%</td>
<td>69.3%</td>
<td></td>
</tr>
</tbody>
</table>

Table 7 shows, cycle efficiency is increased by ~24%. Electrical efficiency of the SOFC alone is 55.1%. The lower electrical efficiency is due to the absence of air preheater or recuperator when compared with the earlier models from the literature. Weight comparison analysis is made to understand the effect of SOFC. NASA subsonic fixed wing project has stated that it requires 30MW of power to drive the distributed electric fans as mentioned by Felder, Kim & Brown (2009). Air mass flow rates for the TG and SOFC-GT are 55.2 kg/s and 36.7 kg/s respectively, where fuel flow rates are 1.33 kg/s and 0.87 kg/s respectively. SOFC/GT air mass flow rate are about \( \frac{2}{3} \) of the TG air mass flow rate. This indicates that size of the SOFC-GT should be \( \frac{2}{3} \) of the TG. A smaller nacelle (inlet) would result in reduced drag, which is not be considered in this study. A non-cryogenic generator with an efficiency is 95% assumed for both systems.

Figure 6 shows TG’s and SOFC/GT’s weight comparison with cruise flight time. Dry weight of the SOFC/GT system is calculated using the initial Simulink analysis. The power to weight ratio of the SOFC system from the analysis is 2kW/kg. TG system’s dry weight
is obtained from the NASA’s blended wing aircraft’s assumptions. Only the factor that varies with the cruise flight time is the amount of fuel required. From the Figure 6, it is evident that TG system is suitable for the short distance flight hours (<3hrs). For long-distance flight hours (>3Hrs.), SOFC/GT hybrid power system is more gravimetrically efficient considering the weight of the fuel needed for flight.

Figure 6: The cycle weight ratios including fuel as a function of flight time.

Figure 7 shows power to weight comparison of two cycles with altitude. Based on the sea-level weight estimates from NASA NX-3 blended wing aircraft’s data, dry weights of SOFC-GT and Turbo-generator systems are calculated. Power to weight ratios were extrapolated for different altitudes and were shown in the Figure 7. Turbo-generator’s power to weight is higher than SOFC-GT system at sea-level. With altitude SOFC-GT power to weight ratio values are constant whereas the turbo-generator’s values are linearly dropping to 1/3rd of the sea-level ratios. This drop in TG’s power to weight ratio is due to the drop in the density of the air. SOFC-GT system’s power to weight ratio remains constant because SOFC power is maintained with constant inlet conditions which means
gas turbine components in the SOFC-GT system change shaft speed with the altitude to provide constant inlet conditions. This would result in max shaft speed reached at max altitude.

Figure 7: Power to Weight ratio comparison for SOFC/GT and TG

Figure 8: Fuel mass difference and operational cost analysis.
Figure 8 shows the fuel mass difference of TG and SOFC-GT systems and operational cost difference per flight time. As per US Energy information administration, natural gas cost for commercial sectors is \$3.91/1000 cubic ft. (oct. 2016). This data is used to calculate the operational cost (fuel cost) of the both the systems. According to the analysis, SOFC-GT reduces 14Mgs of weight and saves \$4300 for every 8hrs. flight time over TG system. Thus, the SOFC-GT system may be costly initially due to high manufacturing costs but this can be compensated by the low operational cost.

Other than weight, manufacturing, material, and maintenance are three important factors of gas turbine engines. With SOFC on board, maximum TIT reduces to as low as 1093K (820C). High temperature resistant materials are not required and blade cooling problems are reduced which in turn reduces the manufacturing costs (due to less complex blade geometries). SOFC are known for their reliability and low maintenance hence less maintenance cost compared to the conventional gas turbines. The emissions would dramatically be reduced for the SOFC system with power, lower carbon dioxide emissions due to higher efficiencies, lower NOx emission due to reduced operating temperature of the system and lower CO emission due the catalyst naturally contained within the SOFC materials. SOFC/GT hybrid system is heavier than TG but its advantages like low emissions, high efficiency and reduced drag outweighs the weight of the system.
DYNAMIC SIMULATION OF SOFC-GT MODEL

A dynamic SOFC-GT model is developed in MATLAB-Simulink environment. This model is developed with the capability to simulate the transient behavior of the SOFC-GT system. These simulations help in understanding the system’s behavior to the dynamic load perturbations and the stability of the model. This ability to operate dynamically under designed conditions is a crucial feature for power generation systems of the aircraft. A simple commercial flight envelope is chosen for the analysis which is shown in Figure 9.

![Commercial Flight Envelope and Power Requirement](image)

**Figure 9: Commercial Flight Envelope with Power Requirement vs Time.**

Typical flight envelopes consist of a take-off time of 15-20 minutes depending on the size of the aircraft. This 15-20 minutes’ take-off time is for the engine that are idling during boarding meaning the engine is still at higher temperatures and can reach the operating temperatures faster than the engine which is shut-down. Completely shut-down engine’s warm-up to take-off time will be higher due to the core of the engine being at
ambient temperatures and warming up to the take-off operating temperature will take time depending up on the size of the engine. A transient analysis of SOFC-GT hybrid engine which is completely shut-down is considered and analysis is carried from warm-up to climb (35000ft.) of the flight envelope.

A. Control and stability of hybrid systems

A control strategy is developed to maintain the SOFC-GT hybrid system within acceptable operational conditions. Any delay in the response could severely damage or even crash the system. As mentioned by Barelli et al (2016), SOFC system over the years developed into a dynamically stable system. Its transient response is one of the key requirements of power generation systems for maximizing the performance of SOFC-GT system and as a promising technology for the efficient power generation.

Roberts (2005) mentioned that a load following SOFC-GT system introduces much complexity and hence it is important to approach the load demands creatively. Flight envelope shown in Figure 9 shows the constraints on SOFC-GT system that dictate the time and power requirement along the flight traveling time. In SOFC-GT hybrid system, power is produced by the both individual systems (i.e. SOFC and gas turbine) and gas turbine engine’s power generation is heavily dependent on the SOFC. Power extracted by the gas turbine is based on the SOFC exit temperature and pressure. The total power produced by the hybrid system can only be controlled by the power demanded from the SOFC. Hence controlling the operating conditions of the SOFC should produce a controlled and stable power generation system.

These controls should be robust and should have capabilities of handling many disturbances. A thorough modeling effort is necessary for analyzing the dynamic behavior
of SOFC-GT hybrid systems. A complete flight envelope consists of warm-up to take-off phase, climbing phase, cruise phase and decent phase. Commercial flights have two climb phases, initial climb, and climb. Per US standards, flight take-off speed is limited under 10,000 ft. for example below 250 kt CAS to control the noise alleviations in airports. Considering a completely shut-down SOFC-GT system, SOFC’s tubes must warm-up to operating temperatures (>1113K) and stabilize to provide the constant power output throughout the operation cycle flow chart of warm-up to take-off process is shown in Figure 10.

![Flow Chart](image.png)

**Figure 10: Warm-up to Take-off flow chart.**

For better performance and reliability of the SOFC system power density of the system is limited to 0.5W/cm². Depending on the power requirement, number of fuel cells required
can be calculated based on the power density value. For example, 1MW power output requires ~100,000 fuel cells of 4mm dia. Shut-down SOFC temperatures will be at ambient and combustor exit hot gases are used to raise the temperature of fuel cells.

State flow models were developed to employ the control and stability strategies. Two chart models were included one chart model for the warm-up to take-off Phase and second chart model for the climb Phase. Warm-up to take-off Phase chart is based on the fuel cell
temperature and current drawn from fuel cell. Climb Phase chart is based on the flight time and controls the altitude in turn the environment pressure and temperatures. Flow charts representing the above two phases are shown in Figure 10 and Figure 11.

Along with the above chart models, PID controllers were included in the model to get a smooth response for the disturbances caused along the flight envelope. Following PID controllers were included in the model:

1. Fuel cell’s maximum temperature changes with the air mass flow rate which depends on the shaft’s RPM. Hence, the RPM is manipulated to keep the fuel cell’s temperatures within a desired operating temperature.

2. Shaft’s RPM is calculated by balancing the power extracted from turbine, power consumed by the compressor and power transferred to generator. Altering the power transferred to and from the motor/generator can control the shaft’s RPM. Hence, a controller was set-up to control the RPM based on compressor, generator, and turbine loads.

3. Another controller was set-up to match the shaft’s RPM set point (from 1st PID controller) by controlling the power transferred to the generator.

4. Combustion chamber’s temperature depends on the unutilized fuel from the SOFC’s Anode side. Hence, the fuel flow is manipulated to control the combustion temperature.

5. During the warm-up of the fuel cell, a controller is set-up to increase the fuel cell’s current linearly such that fuel cell operates at maximum performance point (Voltage=0.5V) Figure 12: PID controller’s schematic diagrams.
Figure 12 shows all the controller’s schematics. All the controls were experimented for various load perturbations to understand the robustness of the model.

![PID controller's schematic diagrams](image)

**Figure 12: PID controller’s schematic diagrams.**

**B. Simulation Results:**

The above developed SOFC-GT model is analyzed for the flight envelope shown in the Figure 9. Analysis parameters are shown in Table 8.

**Table 8. Simulation parameters for SOFC-GT hybrid propulsion system**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>value</th>
<th>Units</th>
</tr>
</thead>
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<tr>
<td><strong>Inlet Chemical Species Mole Fractions</strong></td>
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<td></td>
</tr>
<tr>
<td>Methane</td>
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<td></td>
</tr>
<tr>
<td>Hydrogen</td>
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<td></td>
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<tr>
<td>Steam</td>
<td>0.00%</td>
<td></td>
</tr>
<tr>
<td>Nitrogen</td>
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<td></td>
</tr>
<tr>
<td>Oxygen</td>
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</table>
SOFC Single Cell

<table>
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</thead>
<tbody>
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<tr>
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</tr>
<tr>
<td>Mass per unit cell</td>
<td>0.005 kg</td>
</tr>
<tr>
<td>Number of cells per 1MW</td>
<td>100,000</td>
</tr>
</tbody>
</table>

Gas turbine Components

<table>
<thead>
<tr>
<th>Compressor efficiency</th>
<th>0.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbine efficiency</td>
<td>0.8</td>
</tr>
<tr>
<td>Turbine Inlet temperature</td>
<td>1093 K</td>
</tr>
<tr>
<td>Combustion chamber min. temperature.</td>
<td>1043 K</td>
</tr>
</tbody>
</table>

Transient behavior of the SOFC-GT model is captured for the warm-up to cruise condition of the flight envelope. Following methodology is employed to capture this transient behavior.

Warm-up to Take-off Phase:

Initially compressor is rotated at 110kRPM by an external generator/motor to provide hot compressed air to the combustion chamber. Fuel is added to combustion chamber to increase the SOFC inlet temperature to 1113K. Hot inlet air is passed through the fuel cells to increase its temperature. Minimum temperature of the fuel cell is monitored. When fuel cell’s minimum temperature reaches to 923K or 650C, current can be collected from the fuel cell. Ceramic material can only transfer ions efficiently and other electrochemistry and reformation reactions become stable for fuel cell temperatures higher.
than 923K. Hence, current collection from a cooler fuel cells (<923K) results in voltage crash and/or slow reformation. Load/current is linearly increased till the fuel cell’s power density reaches 0.5W/cm² or till the maximum load point of fuel cell. Fuel cell temperature takes 15 mins to stabilize and the SOFC-GT system is ready for take-off.

Climb Phase:

As discussed before, there are two climb phases involved in this phase. This phase in the model is completely dependent on the altitude variation. Warm-up to take-off is designed for 50mins (Shut-down engine takes more time), initial climb to 10,000ft. is designed for 5min, a small maneuver for 5 mins with 75% power utilization, final climb from 10,000ft. to 35,000ft. for 10 mins and cruise at 35,000ft for 3hrs. with 50% power utilization.

![Figure 13: Transient Analysis Mission Profile.](image)

Simulation results for the mission including warm-up to take-off, climb and cruise is presented in the thesis. Analysis mission profile along with power requirement is shown in Figure 13.
Figure 14 to Figure 24 shows the simulation results of the SOFC-GT dynamic model. Figure 14 shows the current and voltage variation with time. As per the earlier discussion, current cannot be collected from the fuel cell until the minimum temperature reaches to 923K. Voltage value starts dropping with the fuel cells temperature. Voltage drops further when current is gradually drawn from fuel cell due to polarization losses. Power required is obtained by controlling the current collected and all other controllers respond accordingly to maintain the SOFC safe and efficient. Voltage value is completely dependent on the fuel cell temperatures, gas composition and current. With the drop in the current, fuel utilization decreases and this increases the cathode inlet temperature (since the unutilized fuel maintains the combustor temperatures). Fuel flow decreases to maintain both limits (current and combustor temperature). This changes thermodynamics of systems and fuel cell temperature drops increasing voltage.

![SOFC Tube Voltage and Current](image)

Figure 14: Voltage and current variation along the mission profile.
Figure 15: Temperature distribution through the Single fuel cell.

Figure 16: Current distribution through the Single fuel cell.
Figure 15 shows the temperature distribution through the single fuel cell. Temperature profile varies with the change in cathode inlet temperature. During warm-up phase, hot combustion exit gases at 1113K enters cathode side of the fuel cell and starts warming up the fuel cell surface to the operating temperatures. Cathode inlet side of fuel cell warms-up faster than the anode inlet side due to the heat transfer from low fuel inlet temperatures. Thus the cathode inlet temperature reaches higher temperatures initially. Fuel cell temperature raises gradually in about 15 mins (time mostly depend on the surface area of the fuel cells and the mass flow rates of hot gases). Combustor temperature will be dropped to 1043K once the fuel cell minimum temperature reaches 923K to maintain the temperature gradients of fuel cell in limits. During the acceleration phase of the fuel cell, fuel cell temperature gradients are effected by the steam reforming and electro chemical reactions. Due to the endothermic nature of the methane steam reformation reaction, it reduces the cell’s anode inlet temperatures. Heat required by the methane steam reformation process is dependent on its reaction rates and methane availability. Once methane concentrations reduce which means produced hydrogen is available for electro chemical process. As shown in Figure 17, methane concentration decreases exponentially towards the cathode inlet, thus slowing down the methane steam reformation reaction rates and less heat is consumed form fuel cell and also temperature increases due to the heat produced by the water gas shift and electro chemical reactions. Levels of hydrogen decreases from 30% of the fuel cell is due to high electro-chemical reactions thus explaining high steam levels towards the end of fuel cell. Thus high temperature point will be at the location where steam reformation reaction slows down (maximum methane is converted to hydrogen and CO₂) and electro-chemical reaction rates increases. Fuel cell
cathode inlet temperatures are mostly controlled by the combustor exit temperature and combustor exit is maintained at 1043 K. This explains the low temperatures at anode inlet and cathode inlet of fuel cell.

**Figure 17: Species Mole Fractions Variation through fuel cell.**

Figure 16 shows the Current distribution through the single fuel cell. Current distribution varies depending on the gas composition and temperatures. As mentioned in the above sections, all nodes are assumed to be equipotential and voltage calculations depend on the current (i.e chemical compositions) and fuel cell temperatures. Due to the variation in the fuel cell’s temperatures, voltage values cannot be same through the fuel cell. As shown in Figure 3, increasing current values will decrease voltage values. Hence the current produced by individual nodes varies through the fuel cell to keep all the nodes at same voltage levels.
Figure 18: Fuel cell’s maximum and minimum temperatures.

Figure 18 shows the maximum and minimum temperature variation through the mission profile. Maximum temperature of the fuel cells is well maintained within the limits to avoid damages due to cells. As mentioned earlier SOFC’s electrolyte material is not a good ionic conductor for temperatures below 923K. Hence monitoring the fuel cell’s minimum temperature is important for better performance. Figure 19 shows the cathode inlet and outlet temperatures. The temperature profile shows that fuel control system is more stable and able to control the cathode inlet temperature well within the limits. Cathode exit temperature or turbine inlet temperature is crucial in the turbine performance. Figure 19 also shows that the TIT is responding smoothly with SOFC system. Figure 20 shows the fuel flow controller and fuel utilization is always below 80%.
Figure 19: SOFC’s cathode inlet and exit temperature’s.

Figure 20: Fuel Flow and Utilization plot for 0-5000 secs.
Figure 21: Compressor Maps with SOFC-GT operating profile.

Figure 21 shows the compressor map and the operating range of the SOFC-GT system over the mission profile. Red line in the plot indicates the surge line and any operation beyond surge line makes compressor stall. Blue line in the plot shows the operation of the SOFC-GT system with mission profile. Red circled point is the cruise operation point. From the Figure 21, it is evident that the compressor operation is in the safe region of the map. Compared conventional engines that operate at higher speeds and produce a high noise pollution. With this hybrid systems, noise alleviations in the airports can reduced. Figure 22 shows the SOFC power output and the over all-efficiency of the SOFC- GT system with the mission profile. SOFC-GT is \(~51\%\) efficient during take-off and its efficient increase with the altitude. During cruise, power requirement is dropped to \(50\%\) and efficient increased to \(~64\%\).
Figure 22: Power and Over-all efficiency variation with mission profile.

From the above simulation results it is evident that SOFC-GT hybrid system’s response to the load perturbations is sufficient to maintain stable operation and provides the power required more efficiently than the conventional gas turbine. Thermodynamic model of the SOFC-GT system is well developed and temperature fluctuations caused due to the load perturbations are controlled by the robustness of control and stability system.

Figure 23 shows the current and voltage variation for the warm-up to take-off phase of the mission and Figure 24 shows the fuel cell’s maximum and minimum temperatures variation for the warm-up to take-off phase of the mission. From the both the figures, current collection from the SOFC is started when fuel cell’s minimum temperature reached 923K. Current collection from the fuel cell drops voltage rapidly because of the activation, ohmic, and concentration polarizations.
Figure 23: Voltage and current vs Time for Warm-up to take-off.

Figure 24: Fuel cell’s Max & Min Temperatures for Warm-up to take-off.
Zahra Hajabdollahi and Pei-Fang Fu (2016) stated that SOFC system more efficient in terms of rate of exergy destruction. According to their study, rate of exergy destruction of turbo-generator model is ~2.5MW and SOFC is ~0.5MW. SOFC-GT configuration developed in this thesis is a simple system without any air/fuel recuperators that make the system more complex and heavy. Hence, SOFC-GT hybrid system has its advantages as well as disadvantages. Some of the disadvantages are 1) initial manufacturing cost of SOFCs are high, 2) SOFC’s power density is lower compared to Turbo-generator’s and hence occupies more volume, & 3) Lower power density also end in higher surface area which takes more time to warm-up. But as a hybrid system, it is more efficient in terms of performance and reliability. This system is developed to withstand various disturbances caused due to sudden load demand changes or environmental changes.
CONCLUSION

A dynamic Simulink model of an innovative cycle consists of solid oxide fuel cell and gas turbine engine is modeled and analyzed for its transient behavior over a commercial flight’s mission profile. Mission profile consists of warm-up to take-off, take-off to climb and cruise phases. A shut-down SOFC-GT system is considered for the analysis (all the components are at room temperature). To increase the temperatures of the fuel cell external generator or battery power on board is used to rotate the compressor at high speeds to raise the temperatures of the fuel cells and other components. SOFC takes ~15 mins to raise to the minimum operating temperature. Current is gradually increased until the power density reaches 0.5w/cm². A sudden increase in the current during the warm-up may results in high temperature gradients and material damage. It takes another 10mins to reach the operating power density. SOFC system performance also depends on the thermodynamic and species concentration dynamics. For the better performance and the reliability of SOFC, stability controllers are included in the model to drive the system to high performance point. When the system reaches the high-performance point then it is ready for the take-off.

Fuel flow controller is designed to keep the combustion chamber temperature higher such that it won’t flameout. It also takes care of fuel utilization demand to provide steady power output. Fuel cell’s temperature profiles are monitored through the system to understand the gradients along the fuel cell. Controllers are set-up to keep the temperature
gradients in limit and maximum temperature difference is below 100K during the operation. Chemical stability of the SOFC is dependent on the temperature gradient along the fuel cell. Thus, the fuel flow controller and maximum temperature controller takes care of the chemical stability of SOFC.

A simple enthalpy comparison of SOFC-GT and turbo-generator presented in the thesis shows that SOFC-GT system is more efficient in terms of system’s weight. SOFC-GT system is ~24% more efficient than turbo-generator model considered for the thesis. SOFC-GT hybrid system developed in this thesis is more economical in terms of maintenance and fuel consumption. Integration of the SOFC with the gas turbine reduces the size of the gas turbine components because of lower mass flow rates and compression pressure ratios. This reduction in the size of the gas turbine reduces both weight and drag. With the lower turbine inlet temperatures, turbine manufacturing becomes less complex and economical. An efficient and stable solid oxide fuel cell and gas turbine system is developed and is tested for transient load fluctuations. Further integration of developed SOFC-GT system with other components of the power generation system will provide complete understanding of the system’s behavior with the other components.
APPENDIX A: MATLAB/SIMULINK MODEL FILES

To make this mathematical model user-friendly, the number of files needed to run simulations was minimized. All model parameters are stored in one Microsoft Excel file known as “Model Paramerts.xls”. Each component to the model has its own Excel sheet full of parameters. A MATLAB script file was written to read in every parameter from the Excel file using MATLAB’s “xlsread” command. In doing this, if a user needed to make a parameter change and re-run a simulation, all they would need to do would be update the Excel workbook and save. This file organization relieves a lot of complexities that can be involved in computer aided numerical modeling. The Matlab model that reads all the SOFC-GT’s parameters is known as “OpenModel.mat”. The published version of the file us shown below:

Contents

- Sets the required path variables
- Initialize Model
- DATA FILES

```matlab
clear all;
close all;
```

Sets the required path variables

```matlab
modelBaseDir = pwd;

addpath( modelBaseDir, genpath([modelBaseDir,'\','Tools']),... -0 );  % the -0 option forces directories to top of the path stack
```

Initialize Model
sampletime=1;

  %MODEL INPUTS From EXCEL Files
  %---------------------------------------------
  %Model Variables
  %General Parameters
  [Variable_Text]=xlsread('Model_Parameters','General','B3:g12');
  Parameter2Structure;
  %Engine Parameters
  [Variable_Text]=xlsread('Model_Parameters','Engine','B3:I40');
  Parameter2Structure;
  %   Engine.Compressor.SurgeLine=xlsread('Model_Parameters','Engine Maps','b67:C129');
  %SOFC Parameters
  % [Variable_Text]=xlsread('Model_Parameters','SOFC','B5:I13');
  % Parameter2Structure;
  %GENERAL PARAMETERS
  [Variable_Text]=xlsread('Model_Parameters','SOFC','B3:G100');
  Parameter2Structure;
  %FLUID PROPERTIES
  Leonard_Jones=xlsread('Model_Parameters','Fluid Proper
  ties','D4:E10');
  ColsInt_Dif=xlsread('Model_Parameters','Fluid Properties','H4:I85');
  ColsInt_Vis=xlsread('Model_Parameters','Fluid Properties','K4:L84');
  
  MW=[16 28.01055 44.00995 2.0158 18.01528 28.0134 32]; % Molecular weight vector
  %---------------------------------------------
  % Activation Polarization Anode
  %---------------------------------------------
  %Constants in SOFC_Parameters.xls/Variables FILE
  Kanode=SOFC.ANODE.CEJO.Value*SOFC.ANODE.GRAIN2NECK.Value*72*...
  (SOFC.ANODE.PORE.Value-
  (SOFC.ANODE.GRAIN.Value+SOFC.ANODE.PORE.Value)*SOFC.ANODE.POROSITY.Value)*...
  SOFC.ANODE.POROSITY.Value/SOFC.ANODE.PORE.Value^2/SOFC.ANODE.GRAIN.Value^2/(1-
  sqrt(1-SOFC.ANODE.GRAIN2NECK.Value^2)); %anode activation constant

  %---------------------------------------------
  Activation polarization Cathode
  %---------------------------------------------
%Constants in SOFC_Parameters.xls/Variables FILE

Kcathode=SOFC.CATHODE.CEJO.Value*SOFC.CATHODE.GRAIN2NECK.Value*72*...
(SOFC.CATHODE.PORE.Value-
(SOFC.CATHODE.GRAIN.Value+SOFC.CATHODE.PORE.Value)*SOFC.CATHODE.PORISITY.Value)*...

SOFC.CATHODE.PORISITY.Value/SOFC.CATHODE.PORE.Value^2/SOFC.CATHODE.GRAIN.Value^2/(1-sqrt(1-
SOFC.CATHODE.GRAIN2NECK.Value^2)); %cathode activation constant

%------------------------------------------------------------------------------------------------------------------------------
%- Reaction Vectors
%------------------------------------------------------------------------------------------------------------------------------
%- ANODE
R_anode=[0 0 0 -1/(2*F.Value) 1/(2*F.Value) 0 0]/1000/SOFC.NODES.Value; %[kmol/s]

%- CATHODE
R_cathode=[0 0 0 0 0 0 -1/(4*F.Value)]/1000/SOFC.NODES.Value; %[kmol/s]

disp('Excel Variables LOADED')

%-END-------------

Excel Variables LOADED

DATA FILES

%load ENGINE_Parameters
load IPP_LP_Map

%load param_NIST2

%clear all
disp('Model Ready to run')

Model Ready to run
APPENDIX B: EFFECTIVE DIFFUSIVITY: LEONARD-JONES POTENTIALS

The effective diffusivity has been calculated using the Chapman-Enskog Theory which has been proven to be accurate to approximately eight percent. In kinetic gas theory, diffusivity is dependent on both the properties of the particle doing the diffusing and the particles that are being diffused. Typically $i$ denotes the diffusing party and $j$ denotes the party being diffused. To calculate the binary gas diffusion coefficient, a weighted average of all seven gas species has been taken. The interaction between the particles has been accounted for using Leonard-Jones potential parameters such as collision diameter and collision integrals.

**Binary Diffusion Coefficient:**

$$D_{ij} = 0.0018583 \left[ \frac{T^{3/2} \left( \frac{1}{M_i} + \frac{1}{M_j} \right)^{1/2}}{P_t \sigma_{ij}^2 \Omega_{ij}} \right]$$

**Leonard-Jones Collision Diameter:**

$$\sigma_{ij} = \frac{1}{2} (\sigma_a + \sigma_b)$$
### Table 9. Leonard-Jones Potential Parameters found from Viscosities.

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<thead>
<tr>
<th>Substance</th>
<th>(\sigma (\text{Å}))</th>
<th>(\varepsilon /k (K))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{CH}_4)</td>
<td>3.758</td>
<td>148.6</td>
</tr>
<tr>
<td>(\text{CO})</td>
<td>3.69</td>
<td>91.7</td>
</tr>
<tr>
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<td>(\text{H}_2\text{O})</td>
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<tr>
<td>(\text{O}_2)</td>
<td>3.467</td>
<td>106.7</td>
</tr>
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</table>

### Table 10. Collision Integral Tabulated Data from (Klein, Hanley, Smith, & Holland, 1974)

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<tr>
<th>(kT/e)</th>
<th>(\Omega)</th>
<th>(kT/e)</th>
<th>(\Omega)</th>
<th>(kT/e)</th>
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