# SIMULATION OF A HYBRID SOLID OXIDE FUEL CELL CYCLE: A SUMMER UNDERGRADUATE RESEARCH PROJECT

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Abstract

This paper describes a research project conducted by a senior mechanical engineering student in the Summer Undergraduate Research Institute (SURI) at the Virginia Military Institute. The SURI teams undergraduate students with faculty mentors to conduct research in a wide variety of disciplines. The work reported here examines the simulation of hybrid solid oxide fuel cells (SOFC) for power production.

The use of solid oxide fuel cells for power production has some interesting future possibilities. Because SOFCs operate most efficiently at high pressure and high temperature there are some very real possibilities of developing hybrid cycles incorporating a SOFC and a gas turbine engine (SOFC-GT). There are several possible hybrid system arrangements that may be of interest. But in general, the fuel cell would act in place of the gas turbine combustor receiving high-pressure air from the compressor and delivering high-pressure high temperature gas to the turbine while producing direct electrical power. Operating the fuel cell at high temperature also allows for some internal reforming of hydrocarbon fuels. The hybrid cycle would allow for maximum efficiency from the fuel cell by operating it at high pressure and temperature as well as recovering a portion of the waste thermal energy in the high temperature exhaust stream from the fuel cell. Previous researchers have examined hybrid SOFC cycles and conducted parametric studies to determine optimum design cycle parameters.

The present work describes the development of a computer simulation model of a hybrid SOFC-GT cycle. The simulation includes the variation in performance of both the fuel cell and the gas turbine as operating parameters are changed. The model can then be used to predict the operating temperatures, pressures, air to fuel ratio, and efficiency, of the hybrid cycle when operating at off-design conditions.

## Introduction

In the spring of 2002 the Virginia Military Institute established the Summer Undergraduate Research Institute (SURI). The goals of the SURI are:

* *To create long-lasting professional relationships between students and faculty*



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** To enable students to explore and further develop their academic interests outside of regular course work*
** To help students clarify their career goals*
** To prepare students for graduate study and professional careers*
** To give students exposure to all parts of the research process*
** To sharpen critical thinking and creative problem solving skills*
** To expose students to research in a variety of disciplines*

In an effort to meet these goals the SURI funded research teams that were comprised of one VMI cadet and one VMI faculty mentor, with the cadet being the principal investigator. Cadets and mentors participating in the program each received a stipend. Each project concluded with the cadet writing a research paper that was presented by the cadet at the concluding symposium. In addition to funding the research teams the SURI sponsored, as part of the summer activities, an orientation program, guest speakers, workshops, social functions, and the concluding symposium. The present paper is the result of the research completed by one of eighteen research teams during the inaugural summer of the program.

Introduction to Research

The use of solid oxide fuel cells (SOFC) for power production has some interesting future possibilities. Because SOFCs operate most efficiently at high pressure and high temperature there are some very real possibilities of developing hybrid SOFC cycles incorporating a gas turbine cycle (SOFC-GT). There are several possible hybrid system arrangements that may be of interest. But in general, the fuel cell would act in place of the gas turbine combustor receiving high-pressure air from the compressor and delivering high-pressure high temperature gas to a smaller combustor that would burn the fuel, hydrogen and product gases not utilized by the fuel cell while producing direct electrical power. The resulting gas mixture would then be delivered to the turbine. Operating the fuel cell at high temperature also allows for internal reforming of hydrocarbon fuels. The hybrid cycle would allow for maximum efficiency from the fuel cell by operating it at high pressure and temperature as well as recovering the waste thermal energy in the high temperature exhaust stream from the fuel cell. Previous researchers have conducted parametric studies to determine optimum design cycle parameters.

The goal of the present work was to develop a computer simulation of a hybrid cycle composed of a compressor, a turbine, and a SOFC that delivered high-pressure high-temperature gases to the turbine while producing electric power. The hybrid cycle's efficiency could be maximized by these operating conditions and by recovering the waste thermal energy from the fuel cell. The hybrid cycle model was constructed by developing a model for each component of the fuel cell and gas turbine. The combustor element of the gas turbine model was initially replaced with the fuel cell and combined with the remaining gas turbine components, however it was found that a significant amount of the methane fuel used in the fuel cell was not totally consumed in the reforming process. A smaller combustor was introduced between the fuel cell and the turbine inlet to burn this excess fuel, as well as some hydrogen, $H_2$, not utilized in the fuel cell and some carbon monoxide, CO, produced in the reforming process in order to increase the efficiency of the system.

This paper describes the development of the computer simulation model of a hybrid SOFC-GT cycle. The simulation includes the variation in performance of both the fuel cell and the gas turbine as operating parameters are changed. The model can be used to predict operating temperatures, pressures, air to fuel ratios, and efficiency, of the hybrid cycle when operating at off-design conditions. This model could be used to show how performance varies as the hybrid SOFC-GT cycle is used to follow load changes.

The Fuel cell

A fuel cell, as shown in Fig. 1, is an electrochemical device that continuously changes the chemical energy of a fuel such as hydrogen and an oxidant directly into electrical energy (Hirschenhofer[1]). The basic structure of a fuel cell is similar to that of a battery, consisting of an electrolyte in contact with a porous anode and cathode on either side. However, the fuel cell and the battery differ in that the battery is an energy storage device, and the fuel cell is an energy conversion device. In fuel cells, the gaseous fuel is fed to the negative electrode (anode) and an oxidant is fed to the positive electrode (cathode). The electrochemical reactions occur at the electrodes to produce an electric current. The solid oxide fuel cell (SOFC) was used in the current model. In this fuel cell the electrolyte is a solid metal oxide. The SOFC is a high temperature fuel cell. These fuel cells are reported to be suitable for large power plants as well as small cogeneration units.

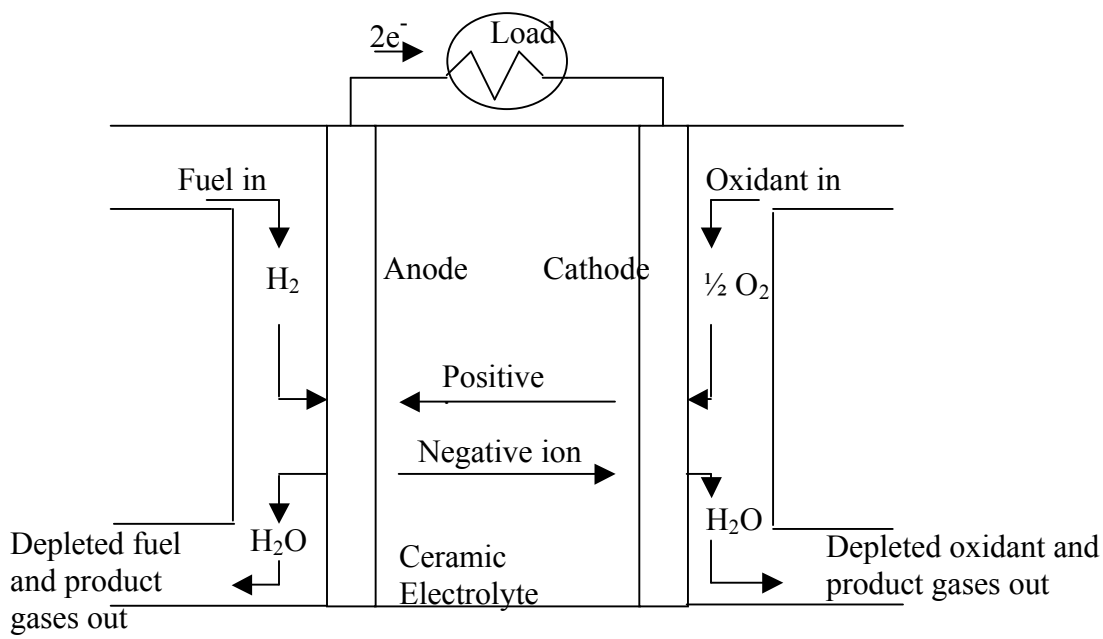


Fig. 1 Schematic of Individual Fuel Cell

Description of the fuel cell model

The model of the fuel cell cycle is based on three particular chemical reactions: The fuel reforming, the shifting, and the electrochemical processes. During the fuel reforming process, the

gaseous fuel (here methane was used) is combined with steam to produce carbon monoxide and hydrogen. The chemical reaction for the reforming process is:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

In the shifting process the carbon monoxide reacts with the steam in the mixture to produce more hydrogen and some carbon dioxide.

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The equilibrium amount of the various species present in these reactions is a function of mixture temperature and pressure. The electrochemical process occurs at the cathode. The hydrogen fuel resulting from the shifting and reforming process is oxidized in the air as shown in the following reaction:

$$H_2 + 1/2O_2 \rightarrow H_2O$$

These shifting and reforming processes occur at the anode and combined with the electrochemical process they account for a transfer of 8 electrons as shown in the following reaction:

$$CH_4 + 4\,O^- \rightarrow 2H_2O + CO_2 + 8e^-$$

Equilibrium constant equations, Eq. (1) and (2), were developed for both the shifting and fuel reforming processes based on the partial pressure of products and reactants as described in Jones and Dugan[2].

$$Kp_R = e^{\frac{\left(f_{CH4}(To3)+f_{H2O}(To3)\right)-\left(f_{CO}(To3)+3\cdot f_{H2}(To3)\right)}{R_u\cdot To3}} \quad (1)$$

$$Kp_S = e^{\frac{\left(f_{CO}(To3)+f_{H2O}(To3)\right)-\left(f_{CO2}(To3)+f_{H2}(To3)\right)}{R_u\cdot To3}} \quad (2)$$

In addition, knowing the fuel consumption coefficients in terms of moles of both hydrogen and oxygen, mass flow equations Eqs. (3) through (8) were developed for the other gases present in the mixture as described by Massardo and Lubelli[3].

$$m_{H2out} = m_{H2in} + 3\cdot X + Y - Z \quad (3)$$

$$m_{COout} = m_{COin} + X - Y \quad (4)$$

$$m_{CO2out} = m_{CO2in} + Y \quad (5)$$

$$m_{H2Oout} = m_{H2Oin} - X - Y + Z \quad (6)$$

$$m_{CH4out} = m_{CH4in} - X \quad (7)$$

$$m_{O2out} = m_{O2in} - 0.5 \cdot Z \quad (8)$$

Two additional equilibrium constant equations, Eq. (9) and (10), were modeled as a function of the mass flows of the products and reactants for the shifting and reforming processes following the example of Massardo and Lubelli[3]:

$$Kp_R = \frac{\left(\frac{m_{COin} + X - Y}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right) \cdot \left(\frac{m_{H2in} + Y + 3 \cdot X}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right)^3}{\left(\frac{m_{CH4in} - X}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right) \cdot \left(\frac{m_{H2Oin} - X - Y}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right)} \quad (9)$$

$$Kp_S = \frac{\left(\frac{m_{CO2in} + Y}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right) \cdot \left(\frac{m_{H2in} + Y + 3 \cdot X - Z}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right)}{\left(\frac{m_{COin} + X - Y}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right) \cdot \left(\frac{m_{H2Oin} - X - Y + Z}{NM_{in} + 2 \cdot X} \cdot \frac{Po2}{P_o}\right)} \quad (10)$$

The actual cell voltage was obtained by subtracting the electrode and electrolyte losses from the ideal voltage, Eq (11). These losses were mainly due to Ohmic polarization or resistance losses, the cell resistance was assumed to remain constant. The current through the cell was determined from the electron transfer occurring during the electrochemical process. The voltage losses were calculated using Ohm's law, Eq. (12).

$$E_{act} = E_{ideal} - V_{losses} \quad (11)$$

$$V_{losses} = IR \quad (12)$$

The electrical power produced by the fuel cell was the product of the actual cell voltage and the current through the fuel cell. This calculated electric power was used in the energy balance equation of the fuel cell model to determine the overall fuel cell properties.

Description of the Gas Turbine model

The open cycle gas turbine engine simulation model, as shown in Fig. 2, was developed after a model described by Sexton[4]. The simulation modeled the performance of each component in the engine using energy and mass balances along with the performance characteristics for each component. This model by Sexton[4] was modified to allow the integration of the fuel cell. The present model was improved by using polynomials, as given by Çengel and Boles[5], to describe the temperature dependent specific heats for gases rather than constant properties as assumed by Sexton[4]. The system simulation was accomplished by matching speeds, mass flow rates, pressure

ratios, and work for each of the components in the engine. The component models included a compressor and a turbine model. A combustor model was added after the fuel cell to burn the remaining methane not reformed by the SOFC as well as hydrogen and carbon monoxide not consumed in the fuel cell. The development of these models is described below.

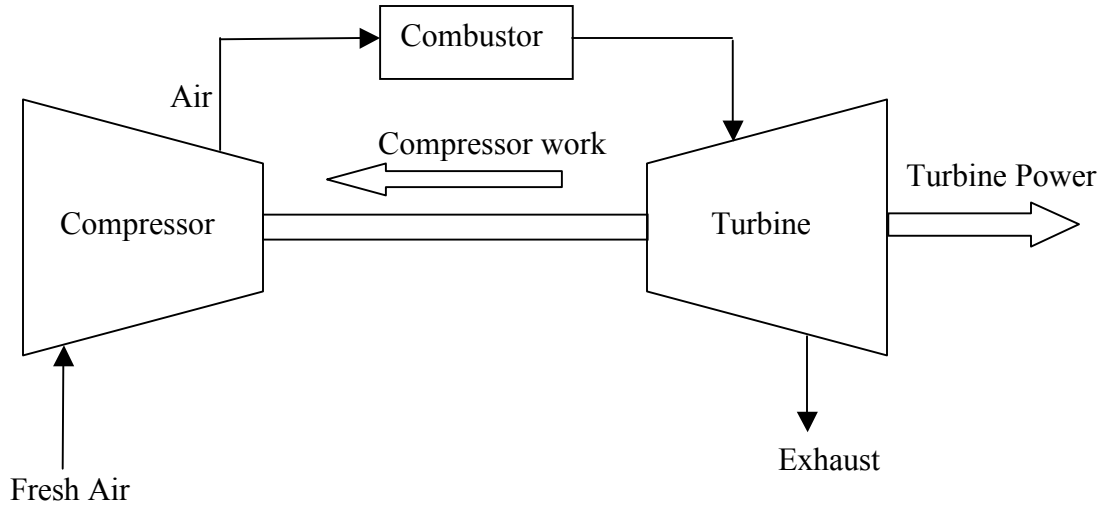


Fig. 2 Open Cycle Gas Turbine Engine

Compressor Model

The compressor model was developed using the thermodynamic relationships for the compressor work, Eq (13); the isentropic temperature rise, Eq. (14); and the definition of compressor isentropic efficiency, Eq. (15). The operating characteristics of the compressor were modeled by developing multiple regression curve fits for the compressor pressure ratio and efficiency as functions of non-dimensional speed and flow. Equations (16) and (17) define the non-dimensional mass flow and speed parameters. Equation (18) describes the compressor pressure ratio and equation (19) describes the compressor efficiency. For the current model the variable specific heat of the gases was incorporated using the polynomial curve fits from Çengel and Boles[5].

Engine Compressor Model

$$\mathrm{CompPwr} = \int_{To1}^{To2} m_c \cdot Cp(To)\, dTo \qquad (13)$$

$$0 = \int_{To1}^{To2s} \frac{Cp(To)}{To}\, dTo - \int_{Po1}^{Po2} \frac{Rg}{Po}\, dPo \qquad (14)$$

$$\eta c = \frac{\int_{To1}^{To2s} m_c \cdot Cp_{air}(T)\, dT}{\int_{To1}^{To2} m_c \cdot Cp_{air}(T)\, dT} \quad (15)$$

$$mc = \frac{\dfrac{m_c \cdot \sqrt{To1}}{Po1}}{\dfrac{md \cdot \sqrt{To1d}}{Po1d}} \quad (16) \qquad Nc = \frac{\dfrac{N}{\sqrt{To1}}}{\left(\dfrac{Nd}{\sqrt{To1d}}\right)} \quad (17)$$

$$Pr = -0.090124 - 7.32282881 mc + 8.99802494 Nc - 36.8122668 mc^2 - 33.4803159 Nc^2 + 72.7075081 mc \cdot Nc \quad (18)$$

$$\eta c = 0.139072009 - 3.05135506 mc + 5.00200918 Nc - 10.3933081 mc^2 - 13.7719419 Nc^2 + 22.9155228 mc \cdot Nc \quad (19)$$

Combustor model

The combustor model was added to burn the remaining methane not transformed into hydrogen by the fuel cell as well as hydrogen and carbon monoxide not completely utilized in the fuel cell. An adiabatic energy balance, Eq (20), on the combustion chamber was used to calculate the temperature of the products leaving the chamber. Equation (21) provided the mass flow from the combustor.

$$\begin{aligned} & m_{CH4out} \cdot h_{CH4}(To3) + m_{H2out} \cdot h_{H2}(To3) \ldots \\ & + m_{O2out} \cdot h_{O2}(To3) + m_{COout} \cdot h_{CO}(To3) \ldots \\ & + m_{H2Oout} \cdot h_{H2O}(To3) + m_{CO2out} \cdot h_{CO2}(To3) \ldots \\ & + m_{N2} \cdot h_{N2}(To3) \end{aligned} = \begin{aligned} & \left(m_{O2out} - 0.5 \cdot m_{COout} - 0.5 \cdot m_{H2out} - 2 \cdot m_{CH4out}\right) \cdot h_{O2}(To3n) \ldots \\ & + \left(m_{H2Oout} + m_{H2out} + 2 \cdot m_{CH4out}\right) \cdot h_{H2O}(To3n) \ldots \\ & + \left(m_{CO2out} + m_{COout} + m_{CH4out}\right) \cdot h_{CO2}(To3n) \ldots \\ & + m_{N2} \cdot h_{N2}(To3n) \end{aligned} \quad (20)$$

$$m_t = m_c + m_f + m_{steam} \quad (21)$$

Turbine Model

The turbine model was developed using the thermodynamic relationships for the turbine work, Eq. (22), the isentropic temperature change Eq. (23) and the definition of turbine isentropic efficiency, Eq. (24). The operating characteristics of the turbine were modeled by developing a multiple regression curve fit for the turbine efficiency as a function of non-dimensional speed and pressure ratio. Equation (25) defined the non-dimensional speed parameter and Eq. (26) described the turbine efficiency as a multiple regression curve fit. For this model the turbine flow was assumed choked, as is common with gas turbines, and the non-dimensional mass flow rate was held constant as shown in Eq. (27).

$$
\begin{aligned}
TurbPwr = {} & \left[\left(m_{CO2out} + m_{COout} + m_{CH4out}\right)\cdot M_{CO2}\right]\cdot\int_{To4}^{To3n} Cp_{co2}(T)\,dT \ldots \\
& + \left[\left(m_{H2Oout} + m_{H2out} + 2\cdot m_{CH4out}\right)\cdot M_{H2O}\right]\cdot\left(\int_{To4}^{To3n} Cp_{h2o}(T)\,dT\right)\ldots \\
& + \left[\left(m_{O2out} - 0.5\cdot m_{COout} - 0.5\cdot m_{H2out} - 2\cdot m_{CH4out}\right)\cdot M_{O2}\right]\cdot\int_{To4}^{To3n} Cp_{o2}(T)\,dT \ldots \\
& + m_{n2}\cdot\int_{To4}^{To3n} Cp_{n2}(T)\,dT
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
0 = {} & \left[\left(m_{CO2out} + m_{COout} + m_{CH4out}\right)\cdot M_{CO2}\right]\cdot\left(\int_{To3n}^{To4s}\frac{Cp_{co2}(T)}{T}\,dT - \int_{Po3}^{Po1}\frac{Rg_{CO2}}{Po}\,dPo\right)\ldots \\
& + \left[\left(m_{H2Oout} + m_{H2out} + 2\cdot m_{CH4out}\right)\cdot M_{H2O}\right]\cdot\left(\int_{To3n}^{To4s}\frac{Cp_{h2o}(T)}{T}\,dT - \int_{Po3}^{Po1}\frac{Rg_{H2O}}{Po}\,dPo\right)\ldots \\
& + \left[\left(m_{O2out} - 0.5\cdot m_{COout} - 0.5\cdot m_{H2out} - 2\cdot m_{CH4out}\right)\cdot M_{O2}\right]\cdot\left(\int_{To3n}^{To4s}\frac{Cp_{o2}(T)}{T}\,dT - \int_{Po3}^{Po1}\frac{Rg_{O2}}{Po}\,dPo\right)\ldots \\
& + m_{n2}\cdot\left(\int_{To3n}^{To4s}\frac{Cp_{n2}(T)}{T}\,dT - \int_{Po3}^{Po1}\frac{Rg_{N2}}{Po}\,dPo\right)
\end{aligned}
\tag{23}
$$

$$
\eta t = \frac{\left[\begin{aligned}
& \left[\left(m_{CO2out} + m_{COout} + m_{CH4out}\right)\cdot M_{CO2}\right]\cdot\int_{To4}^{To3n} Cp_{co2}(T)\,dT \ldots \\
& + \left[\left(m_{H2Oout} + m_{H2out} + 2\cdot m_{CH4out}\right)\cdot M_{H2O}\right]\cdot\left(\int_{To4}^{To3n} Cp_{h2o}(T)\,dT\right)\ldots \\
& + \left[\left(m_{O2out} - 0.5\cdot m_{COout} - 0.5\cdot m_{H2out} - 2\cdot m_{CH4out}\right)\cdot M_{O2}\right]\cdot\int_{To4}^{To3n} Cp_{o2}(T)\,dT \ldots \\
& + m_{n2}\cdot\int_{To4}^{To3n} Cp_{n2}(T)\,dT
\end{aligned}\right]}{\left[\begin{aligned}
& \left[\left(m_{CO2out} + m_{COout} + m_{CH4out}\right)\cdot M_{CO2}\right]\cdot\int_{To4s}^{To3n} Cp_{co2}(T)\,dT \ldots \\
& + \left[\left(m_{H2Oout} + m_{H2out} + 2\cdot m_{CH4out}\right)\cdot M_{H2O}\right]\cdot\left(\int_{To4s}^{To3n} Cp_{h2o}(T)\,dT\right)\ldots \\
& + \left[\left(m_{O2out} - 0.5\cdot m_{COout} - 0.5\cdot m_{H2out} - 2\cdot m_{CH4out}\right)\cdot M_{O2}\right]\cdot\int_{To4s}^{To3n} Cp_{o2}(T)\,dT \ldots \\
& + m_{n2}\cdot\int_{To4s}^{To3n} Cp_{n2}(T)\,dT
\end{aligned}\right]}
\tag{24}
$$

$$Nt = \frac{\frac{N}{\sqrt{To3n}}}{\left(\frac{Nd}{\sqrt{To3nd}}\right)} \quad (25)$$

$$\eta t = (0.4828332 - 0.0155\,Pr + 1.15 \cdot Nt) - 0.01625\,Pr^2 - 1.0208333\,Nt^2 + 0.1525\,Pr \cdot Nt \quad (26)$$

$$\frac{m_t \cdot \sqrt{To3n}}{Po3} = \frac{md_t \cdot \sqrt{To3nd}}{Po3d} \quad (27)$$

Engine energy balance

The final relationship necessary to complete the engine model was an energy balance on the engine cycle; that is, the difference between the turbine's power output and the work input to the compressor, Eq. (28).

$$SHP = TurbPwr - CompPwr \quad (28)$$

Summary of the Hybrid SOFC-GT Cycle Model

In the development of the Hybrid SOFC-GT Cycle simulation model the fuel cell and the gas turbine models, described above, were combined as shown in Fig. 3.

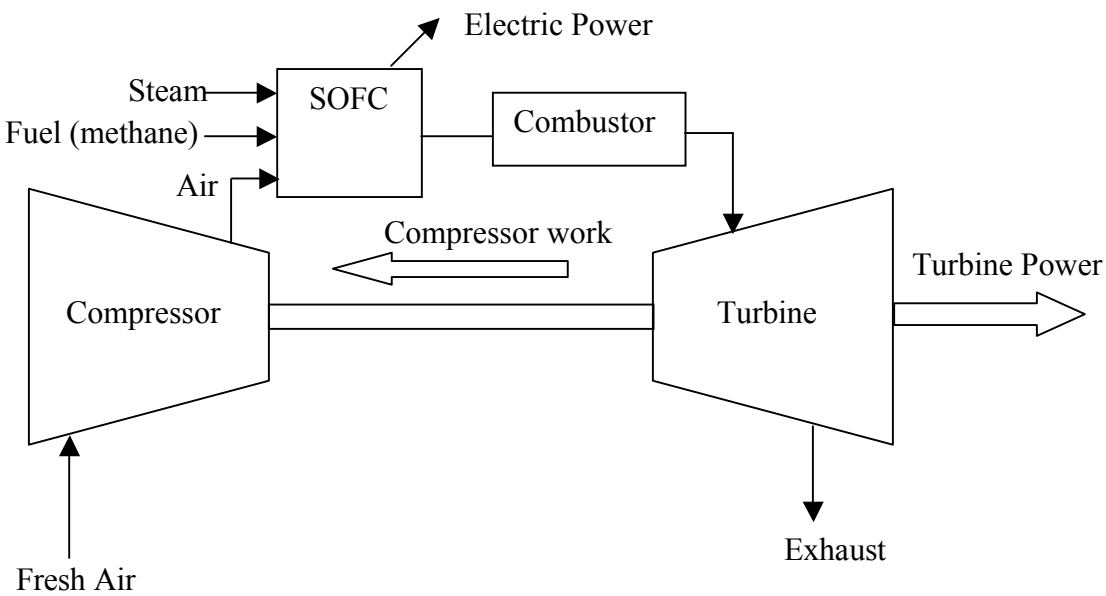


Fig. 3 Schematic of the Hybrid SOFC-Gas Turbine Cycle

In this hybrid configuration the compressed air was introduced to the SOFC at high-pressure high-temperature where it was used to oxidize the hydrogen generated by the internal reforming of the hydrocarbon fuel. Then the remaining fuel, hydrogen, and carbon monoxide from the SOFC was burned in the combustor and delivered with the carbon dioxide, water vapor and excess air at a higher temperature to the turbine. While the waste thermal energy generated by the fuel cell was recovered by the cycle and used to increase its overall efficiency, the fuel burned in the combustor also helped increase the hybrid cycle efficiency. The characteristics of the hybrid SOFC-GT cycle were determined by solving the system of equations developed in both models simultaneously. Preliminary simulations, using the model developed, predict that the SOFC-GT cycle could obtain cycle efficiencies as high as 63%. Appendix A shows the output of the model for a typical simulation.

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P.S. Lankeu Ngankeu completed the requirements for the B.S. degree in Mechanical Engineering at the Virginia Military Institute in December 0f 2002. He plans to attend graduate school in the fall of 2003 and pursue an M.S. degree in Mechanical Engineering.

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Michael R. Sexton is a Professor of Mechanical Engineering at the Virginia Military Institute. His current research and teaching interests include turbomachinery and energy system design and optimization. Dr. Sexton holds B.S., M.S., and Ph.D. degrees in Mechanical Engineering from Virginia Tech.

# APPENDIX A

## SOFC-GT Simulation Output

### Cycle Inputs

**Fuel Flow In**

$m_{CH4in} = 42.201 \frac{lbmole}{hr}$

**Steam Flow In**

$m_{H2Oin} = 83.264 \frac{lbmole}{hr}$

### Fuel Cell Operating Parameters

**Actual Cell Voltage**

$E = 1.095 volt$

**Cell Current**

$I = 1.932 \times 10^{6} amp$

**Electric Power produced by Cell**

$Pwr_{FC} = 2.115 \times 10^{3} kW$

**Air Flow into Cell**

$m_{O2in} = 140.364 \frac{lbmole}{hr}$

$m_{N2} = 527.767 \frac{lbmole}{hr}$

**Cell Temperature**

$To3 = 1.123 \times 10^{3} K$

**Gas Flows out of Cell**

$m_{H2Oout} = 161.356 \frac{lbmole}{hr}$

$m_{CO2out} = 39.991 \frac{lbmole}{hr}$

$m_{O2out} = 60.864 \frac{lbmole}{hr}$

$m_{N2} = 527.767 \frac{lbmole}{hr}$

$m_{CH4out} = 1.284 \frac{lbmole}{hr}$

$m_{H2out} = 3.742 \frac{lbmole}{hr}$

$m_{COout} = 0.926 \frac{lbmole}{hr}$

### Gas Turbine Operating Parameters

**Power produced by GT**

$SHP = 579.811 kW$

**Compressor Discharge Temperature**

$To2 = 460.644 K$

**Compressor Power**

$CompPwr = 408.115 kW$

**Compressor Efficiency**

$\eta c = 0.81$

**CompressorPressure Ratio**

$Pr = 3.767$

**Turbine Inlet Temperature**

$To3n = 1.199 \times 10^{3} K$

**Turbine Power**

$TurbPwr = 987.926 kW$

**Turbine Efficiency**

$\eta t = 0.866$

### Cycle Outputs

**Cycle Power Output**

$Output = 2.695 \times 10^{3} kW$

**Cycle Efficiency**

$\eta_{cycle} = 63.163\%$