TECHNICAL DEVELOPMENT ISSUES AND DYNAMIC MODELING OF GAS TURBINE AND FUEL CELL HYBRID SYSTEMS

Eric A. Liese and Randall S. Gemman
Federal Energy Technology Center, Morgantown, WV

Faryar Jabbari and Jacob Brouwer
National Fuel Cell Research Center, Univ. of California, Irvine, CA

ABSTRACT
This paper describes safety issues important to the operation of combined fuel cell and gas turbine (hybrid) systems, and provides motivation for building dynamic modeling tools to support their development. It also describes two models—a steam reformer and a fuel cell—that will be used to investigate the dynamic performance of a hybrid system. The present goals are to develop dynamic models for these two components, ensure their reliability, and obtain a basic understanding of their performance prior to integration into a complete hybrid system model. Because of the large physical domain to be analyzed in the integrated hybrid system, both reformer and fuel cell models are simplified to a one-dimensional system of equations. Model results are presented for a tubular, counterflow steam reformer showing methane conversion and temperature behavior during initial startup, and following several step change perturbations. For the fuel cell model, a generic planar type is analyzed showing voltage and current behavior following step changes in load resistance and fuel input. The results provide confidence in each model's reliability, enabling them to be integrated for hybrid system simulation. Results from the integrated simulations will provide guidance on future hybrid technology development needs.

NOMENCLATURE

A Area at the inlet/outlet of the control volume [m²]
A₀ Inside surface area of reformer wall [m²]
C_i Molar concentration of species i [kg mole/m³]
C_a Average specific heat [kJ/kg mole/K]
C_p Average specific heat of material [kJ/kg/K]
C_u Courant number
dt Time step differential [sec]
dz Axial differential length [m]
D Diameter [m]
D₀ Energy diameter [m]
D_p Particle diameter [m]
E Energy storage [kJ/hr] for reformer and total energy within control volume [joule/kg] for fuel cell
F Faraday Constant
F_s Control volume surface frictional force [N]
G Gibbs free energy
h_a Style heat transfer coef. between hot side gas and hot side wall [kJ/m²/hr/K]
h_a,sw Heat transfer coef. between hot side gas and reformer wall [kJ/m²/hr/K]
h_r Heat transfer coef. between reformer gas and reformer wall [kJ/m²/hr/K]
ΔH_i Reforming heat of reaction [kJ/kg mole]
ΔH_3 Watershift heat of reaction [kJ/kg mole]
i i Exchange Current Density
i_s Diffusion Limiting Current Density
k Thermal conductivity [kJ/m/hr/K]
k_s Specific rate constant [kg mole/hr]
K_i Equilibrium constant reaction 1 [MPa]
K_2 Equilibrium constant reaction 2 [MPa]
K_3 Equilibrium constant reaction 3 [1]
L Reform length [m]
M Average molar mass of mixture
M' Momentum within control volume [kg/m/sec]
N_i Molar flow rate of specie i (in/out of control volume) [kg mole/sec]
n Number of participating electrons

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This paper begins with a description of some basic operational characteristics of a given recuperated hybrid system. The paper continues with a presentation of the reformer and fuel cell submodels necessary for eventual integration into a complete hybrid model. A commercial transient analysis software package, ProTRAX, which is widely employed for power generation applications, will be used for model development and integration. ProTRAX is prepackaged with many process elements required for typical power generation applications; however, at this time the user is required to supply the reformer and fuel cell models separately.

**OPERATIONAL CHARACTERISTICS**

**Background**

This paper will present a description of the operational issues for a recuperated gas turbine hybrid system as given in Figure 1. Such hybrid systems, can provide exceptionally high thermal efficiencies. The conversion efficiency of fossil fuel (such as natural gas) to electricity can approach levels greater than 70%; which is considerably higher than what is achievable by either system alone.

The selection of a recuperated gas turbine rather than simple cycle machine is largely driven by the design and construction of the solid oxide fuel cell (SOFC). If it is possible to recirculate part of the anode exhaust flow (slightly fuel rich to avoid any oxygen content) to the fuel reformer, then no steam need be raised in the exhaust stream eliminating the need for a boiler. When anode flows are used to provide steam, the reformer is often integrated into the SOFC proper. With these SOFC systems it is advantageous to use a recuperated gas turbine to increase fuel cell efficiency, since both inlet air temperature and air pressure is increased. The pressure ratio for recuperated engines (3:1 to 8:1) is reasonable for use with a SOFC. The high inlet air temperatures also minimize temperature gradients through the fuel cell thereby prolonging its life.

While the excellent efficiencies noted for these systems provide great motivation for their development, there are a number of control and safety issues (particularly starting and emergency shut-down) that will have to be resolved before hybrid systems can become commercially successful. Some of these issues are introduced in the following sections.

**System Start Operation**

Initial system start (black-start) will follow a sequence similar to the one given below.

**Gas Turbine Start.** The first step in starting the hybrid system from cold is to start the gas turbine. This can be done by spinning the gas turbine to 20% design speed by using the direct drive generator as a motor. Electrical power from batteries or the electrical grid can be used to power the generator. Once up to speed, fuel (natural gas) can be supplied to the start combustor and light-off initiated. After successful light-off, the fuel can be ramped slowly to maximum power. The air from the recuperator during startup, and at all other times, flows through the fuel cell before entering the start combustor.
SOFC Light-Off. The hot air from the recuperator heats the SOFC. When the fuel cell temperature approaches 800 K, the electric air heater in series and downstream of the recuperator can be started to increase the air temperature further —electric power for the heater comes from the gas turbine generator. When the air temperature reaches a level that is slightly above the cell light-off temperature, between 900 and 1000 K, the power to the heater is modulated to keep the air temperature constant. The SOFC during this time will slowly increase in temperature until it reaches the light-off temperature. The heater can be turned off when the air/gas mixture temperature leaving the SOFC is at the light-off temperature. Before the heater is turned off, fuel will be diverted progressively from the start combustor to the fuel reformer. It should be noted that the fuel flow to the start combustor will have to be reduced as the air temperature increases to ensure that the maximum firing temperature (1300 K) is not exceeded. At some point, the fuel flow to the start combustor will be sufficiently reduced such that extinction will occur. When combustion ceases, the fuel flow to the combustor can be stopped. At this point the fuel flow to the reformer can be increased. There is likely to be a drop in speed and power output from the gas turbine when the fuel flow is stopped. Gas turbine speed and power will then gradually increase as the SOFC temperatures increase to the typical operating levels of approximately 1300 K. Once the SOFC reaches this condition, the gas turbine will be at full power.

Load-Following

Load-following, which will be required of certain installations, is a complex issue that will probably require different solutions for the different load-following regimes. The SOFC follows load transients very quickly by changing the efficiency of the cells. During load drops, less fuel is reacted and during load increases more fuel is reacted. The two effects tend to balance out during small, or short lived, transients so that there is little or no residual unburned hydrogen or carbon monoxide retained in the system (one of the primary safety concerns for load-following applications). Thus, short term (<10^6 sec) load excitations that are no greater than 10 to 15% of the base-load condition will probably be handled by the fuel cell alone. The inertia of the rotating machinery will probably keep the gas turbine at a near constant output during these short-lived transients.

Short term decreases in current load that are in excess of 15% will probably cause the power output and speed of the gas turbine section to drop. This will lengthen the time needed to recover to the base-load condition. Thus large excursions in load will probably be dominated by the response time of the gas turbine, while smaller excursions will be handled almost instantaneously by the fuel cell.

If the load excursions are not short transient but are of long duration, a standard fuel control system may be able to respond sufficiently quickly to reduce the fuel flows to the SOFC. This will prevent any large accumulation of hydrogen and carbon monoxide in the SOFC. Long lived load drops in excess of the base-load level will cause the temperature of the fuel cell to drop until a new equilibrium point is reached. The fuel controller would measure the power output (kW) and speed (AC frequency) of the gas turbine and the power output of the fuel cell. The control system would decrease or increase fuel flow rate when a demand signal is received. The total power produced would be compared to the demand level and if a match is made within preset gas turbine speed limits the fuel flow would be maintained at the matching level.

Turn-down of the system, however, may not be handled well by the simple fuel flow reductions of a standard fuel control system. Power reduction is hampered by the efficiency increase of the fuel cell as the fuel cell is unloaded. To turn-down successfully the system air flow may have to be reduced in conjunction with reductions in fuel flow. This would probably involve bleeding air (using a controllable blow-off valve) from the compressor exit and dumping it overboard probably into the system exhaust. Alternatively air could be by-passed around the recuperator which reduces the inlet temperature at the fuel cell and lowers fuel cell efficiency. This in combination with reduced fuel flows may be sufficient to predictably reduce the fuel cell power output. Combinations of all three actions may be required to effectively turn-down to a desired power level within a reasonable time period.

Load Loss

A sudden loss of load will be very difficult to handle in a hybrid gas turbine SOFC system. When a load loss occurs the SOFC immediately stops reacting fuel which will then accumulate in the system and at some point possibly reach an explosive mixture ratio. Fuel will continue to enter the SOFC and accumulate after the load loss because the response time of the fuel control system (fractions of a second) is much slower than that of the reaction rate drop (milliseconds). In addition there will be fuel in the lines and the reformer that will also contribute to the hazard. Air will also continue to be pumped through the system by the gas turbine because the large thermal load of the SOFC will maintain adequate turbine inlet temperature for some considerable time (minutes). These relatively large time differences make load loss a major safety issue.

A methodology considered for solving the safety issue of load loss takes a two-prong approach involving a rapid shut-down of the gas turbine and the flooding of the SOFC with inert gases. The latter approach has been the choice of fuel cell manufacturers for those non-hybrid systems operating at near ambient pressures. Typically, in the small fuel cell systems operated to date, a bank of high pressure nitrogen bottles is located close to the SOFC and in case of emergencies is used to flood and purge the system with nitrogen. In large installations this will probably be neither economically feasible nor practical.

In the hybrid system, the gas turbine section can be stopped rapidly by using a blow-off valve that vents the high pressure air leaving the compressor to atmosphere before it can enter the SOFC. This minimizes the entry of oxygen into the SOFC and also stops the gas turbine. At the same time that the blow-off valve is being operated, the gas flow to the reformer can be diverted to an inert gas generator. This generator, which consists of a catalytic combustor and a cool-down heat exchanger, employs a blower to mix air with the fuel before it enters the catalytic combustor. In the catalytic combustor, the
fuel burns completely to carbon dioxide and water. The products of combustion are then cooled by a combination of direct injection of water and by an air or water cool-down heat exchanger. The cooled products would then be used to purge the fuel cell. However, the various delay times inherent in this approach create cause for concern. If the blow-off valve acts sufficiently quickly to cut-off the air flow to the SOFC, the gas mixture inside the system will be sufficiently fuel rich that it probably will not burn or explode. Also, if the inert gas generator can be brought on-line quickly, perhaps augmented by some bottled nitrogen, the hydrogen and carbon monoxide can be diluted and purged from the system before a dangerous accumulation of fuel occurs. With both of these conditions met, a flammable mixture is avoided, and the hybrid system can be safely shut-down after a load loss.

**Modeling Needs**

It is clear that the operational complexity for hybrid systems is relatively high, which indicates that to reduce technical development risks, new engineering tools will be needed. Fortunately, as evidenced in the following sections, our basic understanding of the dynamic characteristics of major hybrid components (reformer and fuel cell) is also fairly high. When fully integrated into models representing hybrid systems, these modeling tools will enable greater insight into the operational characteristics for hybrid systems, and provide opportunities for resolving any identified problems.

**REFORMER MODEL**

A one-dimensional transient model of a steam-methane reformer is presented. A tube containing the catalyst and steam-methane gas is surrounded by another concentric tube containing a counterflow gas supplying thermal energy to the endothermic reforming reaction. Heat transfer is by convection and radiation (wall-to-wall) and includes thermal inertia effects due to the tube walls and catalyst. Modeled transients include changes to flow, composition and inlet temperatures. In this paper, “reformer gas” will refer to the gas flowing through the catalyst and “hot-side gas” will refer to the gas that is used to provide heat to the endothermic reforming reaction.

**Assumptions**

1. A heat transfer coefficient for the reformer, $h_{R,w}$, accounts for two-dimensional effects as will be described.
2. Heat transfer is by convection and wall-to-wall radiation.
3. There is no carbon deposition.
4. The CO$_2$ concentration is proportional to the methane conversion.
5. A rigorous kinetic model is proportional to the methane conversion.
6. The effects of diffusion in the catalyst pellet can be accounted for by the activation energy.

**Stoichiometry**

Reforming: $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$  \hspace{1cm} (1)

Overall reaction: $\text{CH}_4 + 2\text{H}_2\text{O} \rightarrow \text{CO}_2 + 4\text{H}_2$ \hspace{1cm} (2)

Watershift: $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$ \hspace{1cm} (3)

**Conservation Equations**

The conservation of mass for the reformer is:

$$\frac{dx}{dt} = -\frac{r_{CH_4,\text{in}}}{[nCH_4]_{\text{init}}} \frac{dx}{dz}$$  \hspace{1cm} (4)

where, $x$ is the molar methane conversion (a number from zero to one) and, $[nCH_4]_{\text{init}}$ is the moles of methane per hour at the inlet.

A prescription for the mass balance also needs CO$_2$ conversion. Hyman (1968) modeled the CO$_2$ concentration as a function of methane conversion and distance from the reformer inlet:

$$\frac{d(CO_2)}{dz} = (0.666 - 0.10\frac{x}{L})(\frac{dx}{dz}) - (0.10)x$$  \hspace{1cm} (5)

where, $z$, is the axial position and $L$, the reformer length.

Given these two molar changes, the molar mass of all components in the mixture may be calculated by a molar balance. The conversion process affects the number of moles in the mixture (per mole of inlet methane) and is simply the inlet value plus 2 times the conversion, $x$.

The energy balance for the reformer gas is:

$$\frac{\partial T_R}{\partial t} = \frac{1}{\rho_R} \left[ \sum \Delta H_f \tau_{1,1} \frac{A_{R,m}}{C_p \rho_R} \right] + \frac{\pi D_{R_e} h_{R,w}}{C_p \rho_R} \left( T_{R_{\text{wall}}} - T_R \right) \frac{\partial T_R}{\partial z}$$  \hspace{1cm} (6)

The energy balance for the hot-side is:

$$\frac{\partial T_H}{\partial t} = \frac{1}{\rho_H} \left[ \sum \Delta H_f h_{H,w} \left( T_{H_{\text{wall}}} - T_H \right) \right] + \frac{\pi D_{R_e} h_{H,\text{RW}}}{C_p \rho_H} \left( T_{R_{\text{wall}}} - T_H \right) \frac{\partial T_H}{\partial z}$$  \hspace{1cm} (7)

Heat added to a system is positive.

**Reaction Rates**

The rate of methane conversion used is the one given by Hyman (1968), which is based on the overall reaction:

$$r_{CH_4} = k_1 \left( K_2 P_{CH_4} P_{H_2}^2 P_{H_2O} - P^4 P_{CO_2}^4 \right)$$  \hspace{1cm} (8)

Alatiqi, Meziou and Gasmelseed (1989) give the following
expressions for the reaction rate constant and equilibrium constants (converted from English to SI units):

\[ k_2 = \frac{1}{2.205} \exp \left[ \frac{17622}{T} - 7.912 \right] \]  

\[ K_1 = (0.101330)^2 \exp \left[ -\frac{27464}{T} + 37.707 \right] \]  

\[ K_2 = \exp \left[ \frac{4578}{T} - 4.33 \right] \text{ for } T < 867^\circ K \]  

\[ K_3 = \exp \left[ \frac{4082.02}{T} - 3.765 \right] \text{ for } T = 867^\circ K \]  

\[ K_2 = K_1 K_3 \]  

Heat Transfer with Thermal Inertia

As formulated in the conservation equations, the heat transfer terms for the reformer and hot-side gas require a wall temperature. (This is how the thermal inertia of the catalyst and tube walls are incorporated into the model.) The heat balance may be thought of in the following manner. The hot-side gas either loses heat to or gains heat from both the hot-side tube and the reformer. The reformer gas loses thermal energy to the endothermic reaction, and loses or adds heat to the reformer catalyst and reformer tube. The thermal inertia of the materials at each axial position is modeled as a lumped system. The governing differential equation for either solid is:

\[ \frac{\partial \varepsilon}{\partial t} = \rho C_{pw} \frac{\partial T_m}{\partial t} \]  

The reformer's energy storage includes the catalyst and reformer tube. The energy absorbed or lost by the hot-side tube and reformer material is:

\[ E_{Hab} = \pi dx D_{Hab} \left[ h_{H-Hab} (T_h - T_{Hab}) \right] \]  

\[ = \pi dx D_{Rad} \left[ h_{Rad} (T_{Hrad} - T_{Rad}) \right] \]  

\[ E_{Rm} = \pi dx D_{Rm} \left[ h_{Rm} (T_h - T_{Rm}) \right] \]  

\[ = \pi dx D_{Rad} \left[ h_{Rad} (T_{Hrad} - T_{Rad}) \right] \]  

\[ \text{where } D_{Rad} \text{ is the inner diameter of the hot-side tube if the hot side tube temperature is greater than the external reformer tube.} \]

From the above equations a new hot-side wall temperature, and reformer wall temperature are calculated at every timestep. The energy storage governing equation is solved explicitly, since the bulk temperatures are expected to change slowly compared to the gas temperatures. The update of the external wall temperature assumes a uniform change to the implied radial temperature profile in the reformer, and that the difference in the radial profile is small enough so as not to affect calculations in the material specific heat or thermal conductivity all that greatly. The variable, \( h_{H-W} \), is an average heat transfer coefficient between the gas and material from the inside of the reformer to the external wall of the reformer tube. The formula (Xu and Froment, 1989) is used to help predict the cross-sectional averaged conversions and temperatures that would be calculated by a two-dimensional model:

\[ \frac{1}{h_{H-W} \cdot \ln \left( \frac{D_{Hab}}{D_{Hab}} \right)} + \frac{1}{\alpha_{pb}} \]  

\[ \alpha_{pb} = \frac{8k_{er} \alpha_w}{8k_{er} \alpha_{D_{Rin}}} \]  

\[ \alpha_w = \frac{8.694 k_{er}^3}{D_{Rin}^4} \]  

\[ k_{er} = k_{er}^0 + 0.14k_{er} Re Pr \]  

The value for \( k_{er}^0 \) shown here is an estimate for this problem based on a formulation for packed beds by Kunii & Smith (1960).

For the hot-side gas heat transfer there are two coefficients. The coefficient, \( h_{Hab} \), is used for heat transfer to the reformer, and \( h_{H-W} \) is used for heat transfer to the hot-gas tube wall since it must include the pipe resistance. Both use a Nusselt relation taken from Cebeci & Bradshaw (1988).

\[ h_{H-W} = \frac{Nu \cdot k_{er}^0}{D_{Rin}} \]  

\[ \frac{1}{h_{H-W} \cdot \ln \left( \frac{D_{Hab}}{D_{Hab}} \right)} + \frac{1}{h_{H-W}} \]  

where \( D_{Hab} \) is the inner diameter of the hot-side tube if the hot side tube temperature is greater than the external reformer tube.
if the wall temperatures used in the reformer gas calculations do not match those used for the hot-side gas calculations, the calculations are repeated.

Flow Calculations

In order to accommodate integration with ProTRAX, an inlet and outlet pressure to both the reformer and hot-side gas is used to calculate the mass flow rate and velocity.

Mean fluid properties are calculated based on the average reformer and hot-side temperatures and average pressure. The mass flow is calculated as:

\[
\dot{m} = A \sqrt{\frac{D_{fL}}{fL}} \sqrt{\rho \Delta P}
\]

where \( A \) is the Loss Factor. For the reformer, \( D \) is the catalyst particle diameter, and for the hot-side it is the hydraulic diameter. The friction factor for the heater is taken from an equation similar to that used in ProTRAX (Churchill, 1977) and for the reformer an expression given by Froment and Bischoff is used (1990). Both friction factors are functions of Reynolds Number. Since a velocity is necessary to calculate the Reynolds number, the friction factor, which determines the mass flow and velocity, is determined by an iterative process. As expected the pressure drop in the reformer depends significantly on the particle diameter, and for a given flow the reformer's pressure drop is a great deal more than the hot-side. Since conversion will depend on the partial pressure, and since the pressure drop in a packed bed can be significant, the pressure is calculated at each axial position. This is calculated simply as a linear variation over distance.

Since the flow rate and velocities will change the heat transfer coefficients and transport time, if the values calculated change from those originally used in the conservation equations, the conservation equations are recalculated using the new mass flows and velocities.

Numeric Representation and Solution Technique

A trapezoidal implicit algorithm with upwind differencing was used for solving the conservation equations. The method is first-order accurate in time and space. Convergence for the cases shown in this paper in general required a timestep of 0.1 seconds. Some changes to inlet conditions required a timestep an order of magnitude smaller during the initial response period. The reformer was divided into 60 sections. When analyzed for 120 sections, the exit conversion was generally only 0.3% higher.

FUEL CELL MODEL

A generic bi-polar, co-flow, planar fuel cell is considered for the present analysis as shown in Figure 8. The analysis considers the behavior of a single unit cell located within an infinite series of cells undergoing the same dynamics; hence, the overall thickness of the unit cell (separator plate to separator plate) is a symmetry length, and for computational efficiency, the only length that needs to be resolved. Finally, because the present analysis considers the electrochemistry as quasi-steady and assumes a low Biot number for the solid/gas heat transfer, only the bulk (transverse-lumped) behavior of the separator plate and cell components need to be modeled. Here, the term cell is used to describe the lumped anode and cathode electrodes together with the electrolyte material.

Fuel cell parameters and operating conditions employed for the present analysis are shown in Table 1. The operating conditions are those at the initial steady-state condition. The values of the cell parameters and operating conditions do not represent any particular cell currently under development—as known by the authors. As is apparent from Table 1 and Figure 8, cooling of the fuel cell is achieved by a relatively large and cool cathode gas flow.

<table>
<thead>
<tr>
<th>Table 1. Unit Cell Data and Operating Conditions</th>
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<tbody>
<tr>
<td>Parameter</td>
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<tr>
<td>Load Resistance</td>
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<tr>
<td>Anode Specification</td>
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<tr>
<td>Inlet Temperature</td>
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<td>Inlet Pressure</td>
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<tr>
<td>Exit Pressure</td>
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<tr>
<td>Inlet ( \text{H}_2 ) Mole Fraction</td>
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<tr>
<td>Inlet ( \text{H}_2\text{O} ) Mole Fraction</td>
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<tr>
<td>Cathode Specification</td>
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<td>Inlet Temperature</td>
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<td>Density</td>
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Assumptions

1. One-dimensional behavior along the streamwise direction.
2. Lumped temperature for the cell.
3. Heat transfer by convection. Radiation is ignored at this time, but in general can be important.
4. There is no carbon deposition.
5. Although in reality some rates in the overall electrochemical process can occur on the order of \( 10^3 \) s, Andrew (1966), the electrochemistry is assumed quasi-
steady as described by the Butler-Volmer equation.

6. No gas phase reactions occur.
7. Diffusional losses are based on a constant transport coefficient and diffusion layer—i.e., fully developed flow exists.
8. Cell ohmic resistance is fixed, but in general is a function of temperature.
10. The fuel cell has 100 percent current efficiency—all reactants generate their ideal number of electrons. This is characteristic of a hydrogen fuel cell that avoids such side reactions as reduction of metal oxides, Liebhafsky and Cairns (1968).

Gas Phase Equations

For both the anode and cathode gases, the following conservation equations are employed at each finite control volume, Lucas et al. (1999). For species conservation:

\[ \frac{dC_i}{dt} = N_{i_{\text{inlet}}} - N_{i_{\text{outlet}}} + R_i \]  

(27)

For momentum conservation:

\[ \frac{dM^e}{dt} = P_{i_{\text{inlet}}} A_{i_{\text{inlet}}} - P_{i_{\text{outlet}}} A_{i_{\text{outlet}}} - F_s \]  

(28)

For energy conservation:

\[ \frac{dE}{dt} = \sum_{i} w_{i_{\text{inlet}}} F_{i_{\text{inlet}}} - \sum_{i} w_{i_{\text{outlet}}} F_{i_{\text{outlet}}} + Q_s + P' \]  

(29)

The molar source of species \( i \), \( R_i \), arises from the electrochemistry occurring at the surface of the gas phase control volume. These sources are directly related to the current flow according to the number of electrons carried by the ions created in the electrochemical process. For the present analysis, two electrons are carried by each oxygen ion which consumes two hydrogen atoms at the anode surface.

For all control volumes but at the exit, \( E \) is the sum of internal energy and kinetic energy. For the exit control volume we assume pressure fluctuations are zero (constant pressure boundary condition), and the enthalpy is used in place of the internal energy. In Equation (29), a summation over all inlet and outlet energy flows arises due to species transport by bulk convection, and diffusion at the electrode surfaces.

Solid Phase Energy Equation

For both the cell and separator plate, an energy equation similar to Equation (29) arises, but the flow energy terms for the separator plate will be zero. For the cell, an additional term due to internal heat generation is required, which is discussed more fully in the following section.

Cell Voltage and Loss Mechanisms

The quasi-steady electrochemistry is modeled by assuming ideal behavior and then accounting for various loss mechanisms. The ideal voltage from the fuel cell is given by:

\[ E = \frac{\Delta G}{nF} \]  

(30)

The main losses (i.e., referred to as overpotentials by electrochemists) are due to electrical resistance, concentration, and activation, Hirschenhofer et al. (1994). For the present work, they are given here as, respectively:

\[ L_R = R_i \]  

(31)

\[ L_C = - \frac{R_T}{nF} \ln(1 - \frac{i}{i_l}) \]  

(32)

\[ L_A = \frac{R_T}{aF} \ln(i/i_l) \]  

(33)

where \( i \) is the local current density through the control volume. \( i_l \) is the diffusion limiting current density, which for the present work is limited by the cathode oxygen transport at near 4000 amp/m².

So the corrected cell voltage becomes:

\[ E_{corr} = E - L_R - L_C - L_A - L_{unach} \]  

(34)

which must equal the voltage across the load resistance.

Note, because the fuel and oxidant are consumed as they pass through the cell, the ideal cell voltage at the exit will be lower than that at the inlet. The actual overall cell voltage achieved will approach the lowest achievable voltage due to the high conductivity of the electrode surfaces, Hirschenhofer et al. (1994). As for all loss mechanisms, it is assumed that the unachieved voltage over the surface is dissipated as heat directly into the cell material. Finally, an additional heat generation term in the energy equation for the cell results from the fundamental irreversibility of the process:

\[ Q_{gen} = \frac{4.187 A S_i}{nF} \]  

(35)

Numeric Representation and Solution Technique

The one-dimensional problem outlined above was modeled using 10 finite difference control volumes along the streamwise direction for each of the four major components: anode gas, cathode gas, cell, and separator plate. It was assumed, however, that the inlet and exit nodes could not support heat transfer nor any electrochemistry. The equations were solved following the techniques outlined by Patankar (1980), wherein the pressure and velocity nodes are staggered. To determine the current density profile, an iterative approach at each time step is
required to ensure that the actual cell voltage matches the voltage achieved across the load. Finally, the present objective is to examine the short time scale (10^2 s) behavior of the fuel cell, and an explicit time marching technique was employed. Future work will model the fuel cell’s long time scales as needed when integrated into hybrid system models.

RESULTS

Reformer Model

The reformer physical data and some of the initial conditions are shown in Table 2. The reformer geometry is similar to that in Murray (1985), and is generic in design. All start-up cases presented begin with the reformer at 300 K and inlet reformer and hot-side gas temperatures of 1000 K and 1475 K respectively.

An overview of 5 cases studied is now given. Tables 3 through 6 list some of the flow conditions for each case. A change in flow is accomplished by changing the pressure drop as seen in cases 4 and 5 when the hot-side outlet pressure is increased at time 250 minutes. Note that the symbols "-" and "+" in the time row of each table represent the conditions just prior to and just after a condition change. The set boundary conditions, y_{in, reformer} and y_{out, reformer}, is the mole fraction of methane at the hot-side inlet (the balance is steam), and in cases 4 and 5 is changed from 0.001 to 0.15 mol/mol at 82 minutes. Finally, in Case 6 the hot-side inlet pressure, P_{in, reformer}, is increased at 164 minutes to simulate conditions where a fuel cell requires a reduction in fuel flow.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
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<tr>
<td>Length</td>
<td>m</td>
<td>2 and 4</td>
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<td>D_{in, reformer}</td>
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<td>D_{out, reformer}</td>
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<tr>
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<td>K</td>
<td>300</td>
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<tr>
<td>T_{in, initial} (inlet)</td>
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<tr>
<td>T_{in, initial} (inlet)</td>
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Figures 2 and 3 show heatup histories from start to steady state for the conditions given in Table 3. For Case 2 the hot-side gas pressure drop is 10% of the inlet pressure, and for Case 3 the pressure drop is 1% of the inlet pressure. As a result, the conditions of Figure 3 have less than half the hot-side flow and result in a noticeably longer time to reach steady state conditions. In spite of the large change in hot-side flow, there is only a 5% difference in conversion between the cases at steady state. Since the reformer flowrate and length (i.e., residence time) are nearly the same for the two cases, the higher conversion is due to a slightly higher overall reformer gas temperature for case 2.

Figure 4 (Case 4) shows results for reformer gas flow through a 2 meter long reformer. Methane flow is increased at 82 minutes, followed by a decrease in the hot-side gas pressure drop at 250 minutes. The noticeable reduction in the reformer gas temperature at 82+ minutes signifies the effect of the endothermic reaction. The response in conversion, x, is relatively rapid for the methane flow perturbation at 82 minutes compared to the flow perturbation at time 250 minutes, indicating the fast response due to short residence time and slow response due to a large thermal capacity.

The effect of reformer length was studied by increasing its length to 4 meters and imposing the same perturbations as described in Figure 4. These results are shown in Figure 5 (Case 5). The conversion is seen to increase significantly, but the heatup time is also increased. It is also seen in Figure 5 that following the increase in fuel flow, there is a sudden decrease in conversion followed by a gradual increase. The gradual increase results from a slow increase in reformer temperatures near the inlet. This clearly indicates that the conditions within the reformer are at least partially limited by the reaction rates.

Figure 6 shows the effect of a decrease in reformer flow which is intended to show the performance of the reformer during sudden load changes. The conversion response is fast initially due to the short residence time, and subsequently slows due to the thermal response. Table 6 shows that the reformer gas was lowered by 26 percent. However, Figure 6 indicates increased methane conversion leading to a net decrease in H2 mole flow of only 10 percent.

Finally, Figure 7 shows a profile of temperature and conversion vs. length (dimensionless) at the steady state conditions for Figure 5. The position, z/L=0, is the reformer inlet and hot-side outlet, and visa-versa for z/L=1. The conversion profile is similar to others (Murray, 1985), which provides added confidence in the current work.

Fuel Cell Model

Two perturbation mechanisms typical of power generation applications were selected: a load change and a fuel input change. These two perturbations are normally associated with each other for systems designed to supply a fixed voltage for varying current load, while maintaining good fuel efficiency. For the load perturbation, the load resistance is raised by 20 percent to simulate the effect of a drop in fuel cell current demand. The fuel stream perturbation results from a 20 percent drop in H2 mole fraction (associated with a 20% rise in H2O). The decrease in fuel input is accomplished in the present analysis simply by decreasing the H2 concentration in the anode supply stream—as opposed to simply decreasing the anode gas flow rate.
**Increase in Load Resistance.** The effect of increased resistance on the cell output voltage is shown in Figure 9a. The output voltage transient exhibits a relatively fast and large increase (time constant of order 10^4 s), followed by a slower and smaller increase (time constant of order 10^5 s). The first transient is due to the fast readjustment of the electrochemistry, and the second is due to the combined effects of material residence and thermal response times. The initial voltage increase is from 0.812 to 0.839 volts, or about a 3.4 percent increase. The final steady-state voltage is approximately 0.847 volts, for an overall voltage increase of about 4.4 percent.

Figure 9b shows the distribution in current density across the fuel cell, while Figure 9c shows the overall electrochemical efficiency for the cell. Here, the efficiency is defined as the ratio of actual and ideal amounts of electric energy produced from the fuel and oxidant employed. Also shown in Figure 9c is the distribution of losses across the different loss mechanisms (each normalized by the total loss). As Figure 9b shows, the increased load resistance results in a 14 percent decrease in total current flow. As is clearly evident in the model equations, a decrease in current decreases the losses for the fuel cell. This behavior is evident in Figure 9c, which shows that the cell efficiency increases by about 9.5 percent following the increase in load resistance. The results in Figure 9c also show a redistribution of the total losses between the various loss mechanisms. In particular, the electrode activation provides a relatively higher proportion of the total loss, while the ohmic losses have been decreased. Finally, as for the load voltage behavior, all the parameters shown in the latter two figures exhibit an initially fast transient followed by a slower second transient.

Figures 9d and 9e show the results for the H₂ mole fraction in the anode gas stream and the anode gas temperature, respectively. In contrast to the electrochemical behavior, these two figures show only one relatively long transient, which is on the same order as the second transient noted previously for the electrochemistry (10^5 s). As is seen in Figure 9d, the upstream nodes have a relatively small H₂ response, while the downstream nodes show a relatively large H₂ response (~20% change in fuel utilized). As the consumption of H₂ is directly related to the current flow, the results shown in Figure 9d can be viewed as a time-wise cumulative representation of the perturbation in current density shown in Figure 9b. Regarding future hybrid developments, such large changes in fuel utilization need to be carefully considered in the design of any downstream combustor which may release this energy as thermal energy prior to entering a heat engine. Finally, since less fuel is being converted, and since conversion occurs at a higher efficiency, there should be less heat generated within the system resulting in a decrease in temperature. This is confirmed in the temperature results shown in Figure 9c.

**Decrease in H₂ Concentration.** The perturbation in H₂ concentration was imposed following the steady-state condition reached after the aforementioned load perturbation. The H₂ concentration was decreased by adding more H₂O to the fuel gas stream. The effect of decreased H₂ concentration on the cell output voltage is shown in Figure 10a. This time the output voltage transient contains a single slow transient with a time constant of order 10^5 s. The voltage decreases back down to about 0.817 volts, which is about 0.7 percent off from its voltage prior to the load perturbation. Further examination showed that over the course of this transient, the cell efficiency was not significantly changed.

To show the complexity that can result for even this somewhat simple fuel cell design, Figure 10b shows the anode gas temperature transient following the decrease in H₂ concentration. The first effect on nodes 1 and 2 is mainly a decrease in temperature from 868 K to 677 K. This initial transient is then followed by a gradual increase to about 680 K. All other nodes, however, see an initial rise in temperature. For nodes 3, 4, and 5, this is then followed by a decrease, which is then followed by another increase. The increasing temperature results at the downstream nodes arises from the increased current density that these nodes can initially achieve when the inlet nodes reduce their current densities as a lower fuel concentration passes by. Other features of the cell behavior are equally complex (e.g., initially decreasing inlet velocity concurrent with increasing exit velocity).

Finally, as seen in the change from initial condition to final steady-state, there is a decrease in anode gas temperature at all nodes. This overall change in temperature can be anticipated from the fact that the anode gas now has a greater mixture heat capacity due to the increased water vapor, and from the fact that slightly less fuel can be converted when diluted, which reduces the heat generated.

**SUMMARY**

Models have been generated and studied for two elements of a hybrid system, a steam reformer and a fuel cell. Each model shows anticipated behavior following the perturbations studied, which engenders confidence in their future application to hybrid system studies. In addition, the present results begin to highlight some of the features that need to be considered in the future design of hybrid systems; e.g., combustor design and necessary response times for control elements. The results also demonstrate the complexity of some of the transient behavior, which emphasizes the need for such simulation capability.

**REFERENCES**


Figure 1 - Recouperated Gas Turbine with Topping Solid Oxide Fuel Cell
### Table 3 - Flow and Velocity Results at 250 minutes for Figures 2 and 3

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>$Y_{CH4,inlet}$</th>
<th>$P_{H,inlet}$ (Pa)</th>
<th>$P_{H,outlet}$ (Pa)</th>
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<td>444,300.0</td>
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### Table 5 - Flow and Velocity Results for Figures 5 and 7

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<th>$P_{H,inlet}$ (Pa)</th>
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### Table 7 - Flow and Velocity Results for Figures 5 and 7

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<th>$P_{H,inlet}$ (Pa)</th>
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Figure 2 - Case 2 History; High $\Delta P_H$

Figure 3 - Case 3 History; Low $\Delta P_H$

Figure 4 - Case 4 History; 2m Reformer

Figure 5 - Case 5 History; 4m Reformer

Figure 6 - Case 6 History; Reformer Flow Reduction

Figure 7 - Case 5 Profiles at 249 minutes
Figure 8. A Generic Fuel Cell Model (ten streamwise nodes, 0-9).

Figure 9a. Voltage vs. Time following Load Resistance Increase.

Figure 9b. Current Density vs. Time following Load Resistance Increase. Nodes 1-8.

Figure 9c. Efficiency & Losses vs. Time following Load Resistance Increase.

Figure 9d. Hydrogen Mole Fraction vs. Time following Load Resistance Increase. Nodes 0-9.

Figure 9e. Anode Gas Temperature vs. Time following Load Resistance Increase. Nodes 0-9.
Figure 10a. Voltage vs. Time following Hydrogen Input Decrease

Figure 10b. Anode Gas Temperature vs. Time following Hydrogen Input Decrease. Nodes 0-9.