1 Introduction

1.1 Fuel Cell Operation. Solid oxide fuel cells (SOFCs), like all other fuel cells, produce electrical power through an electrochemical reaction. Working at a high operating temperature (600–1000 °C), a SOFC is a clean, quiet, and highly efficient power generation device [1,2]. Due to the high working temperature, a SOFC can be combined with other power generation systems (e.g., gas turbines) to achieve high overall electrical power generation efficiency. Another attractive feature of a SOFC over other fuel cells is its ability to directly utilize hydrocarbon fuels, since other types of fuel cells have to rely on a clean supply of hydrogen for their operation. Because SOFCs operate at high temperatures, there is an opportunity to reform hydrocarbons within the system either indirectly in a discrete reformer or directly in the anode of the cell. SOFC technology is now considered to be one of the most promising power generating methods for the future. Studies of heat/mass transfer and electrochemical performance on SOFCs currently are focused on tubular and planar structured models [3–7]. However, with the development of a configuration for a SOFC, the high power density (HPD)–SOFC, a modeling study for this type is very necessary.

A solid oxide fuel cell basically consists of three major parts, a porous air electrode (cathode), a porous fuel electrode (anode), and an electrolyte, which is gas tight but conductive to oxide ions. Oxygen at the cathode accepts the electrons from the external circuit to form oxide ions. The oxide ions conduct through the electrolyte to the interface of the anode and the electrolyte, and combine with the hydrogen to form water. The electrons released in this process flow through the external circuit back to the cathode. The reactions in a hydrogen-consuming solid oxide fuel cell are

\[
\text{Anode: } \text{H}_2 + \text{O}^- \rightarrow \text{H}_2\text{O} + 2e^- \tag{2}
\]

\[
\text{Overall: } \text{H}_2 + 1/2\text{O}_2 \rightarrow \text{H}_2\text{O} \tag{3}
\]

The free energy of the chemical reaction given by Eqs. (1)–(3) is converted to electrical energy via an electrical current. The electrical potential or the electromotive force (EMF) between the cathode and the anode is related to the Gibbs free energy change of the chemical reaction, the temperature \( T \) at the reaction site, and the partial pressures of the participating species

\[
\text{EMF} = -\frac{\Delta G^0_{\text{H}_2\text{O},\text{H}_2}}{2F} + \frac{RT}{2F}\ln\left(\frac{p_{\text{H}_2}p_{\text{O}_2}^{1/2}}{p_{\text{H}_2\text{O}}^{0}}\right) \tag{4}
\]

where \( p_{\text{H}_2\text{O}}^{0} \) and \( p_{\text{H}_2} \) are the partial pressures of water vapor and hydrogen at the interface of the anode and the electrolyte, \( p_{\text{O}_2}^{1/2} \) is the partial pressure of oxygen at the interface of the cathode and the electrolyte. \( T \) is the temperature at the interface of the anode and the electrolyte, and \( \Delta G^0_{\text{H}_2\text{O}} \) is the standard Gibbs free energy change of the electrochemical reaction (for a hydrogen fuel case), which is a function of temperature at the interface of the anode and the electrolyte.

1.2 SOFC Configurations. There are currently two major types of SOFCs, planar and tubular. In a planar SOFC, the cathode, anode, electrolyte, and interconnection (see Fig. 1) are all aligned in a plate-type structure. The major advantages of a planar SOFC are manufacturing ease and high current density. The tubular SOFC design is a concept developed by Westinghouse (currently Siemens Westinghouse) in the 1980s. It consists of same components as a planar SOFC, namely, a cathode, an anode, an electrolyte, and an interconnection, but in a different structure, as seen in Fig. 2. Air and fuel are provided in the arrangement as shown in Fig. 3. Due to the geometry, tubular designs have a self-sealing structure, which improves thermal stability and eliminates the need for the highly thermal-resistant sealants that are required in the planar configuration [8].

In the last 15 years, Siemens Westinghouse has made significant progress in tubular SOFC development. Up to November 2001,
the demonstration unit of a tubular SOFC and micro gas turbine system had worked continually for more than 18,000 h, and achieved an efficiency of 52%. By varying the working pressure of the SOFC, the performance of this system can still improve. It is expected that the efficiency of a SOFC and gas turbine hybrid system can approach up to 70% [9,10].

In the near future, a goal for the tubular SOFC is to be developed as an economically acceptable system. It is expected that the capital costs can be lowered through advancement in cell manufacturing and cell design. An increase in power density is a major technical contribution to further cut costs. So far, research into increasing the power density has produced the cell design of a flat-tube HPD–SOFC. This an innovation that enhances the power density and yet retains the feature of secure sealing [9–11]. The current modeling work described in this paper is aimed at simulating the flow, heat and mass transfer, and the electrochemical performance throughout the structure of the HPD–SOFC.

1.3 Flat-Tube HPD–SOFC Configuration. A flat-tube solid oxide fuel cell has the same components and working principles as that of a tubular solid oxide fuel cell. It is comprised of a cathode, an anode, an electrolyte, and an interconnection in a flat-tube structure (Fig. 4). The air and fuel delivery method is also similar to that of a tubular SOFC (Fig. 5).

The difference between a tubular solid oxide fuel cell and a flat-tube type solid oxide fuel cell is the geometry and the structure of the cell stack. The cross section of the flat-tube type SOFC looks like a flattened tube. Multiple ribs may be built into the cathode (air electrode) side, and the airflow area is divided into several chambers. Each chamber has its own air introducing tube. The number of chambers is decided by how many ribs are constructed. The ribs are ion conductive and can serve as a short cut for the inner ion conducting circuit, which will reduce the cell resistance and hence increase the cell power density [9]. The flat-tube shape makes it possible to keep the secure sealing feature of a tubular SOFC.

For a one-rib case, the left half of a flat-tube type solid oxide fuel cell has same structures for fluid flow and heat transfer as that of right half due to the symmetry. For simplicity, the left chamber behavior is considered as generally typical for all of the chambers. In this simulation, the three dimensional (3D) heat transfer and fluid flow inside and outside such a typical chamber (as shown in Figs. 6 and 7) are investigated. In our future work, currently in progress, the chambers' temperature and flow fields in a multirib case will be studied based on the present numerical modeling and computational programming.

2 Heat Transfer and Fluid Flow Model

The fuel and air stream flow patterns of a whole cell and of a left channel are schematically illustrated in Figs. 5 and 7, respectively. The cross section of the left chamber is shown in Fig. 6.

The fluid in this problem has multiple components. The heat transfer and fluid flow are coupled with each other. The governing equations for flow and temperature for this three dimensional case are

\[ \nabla \cdot (\rho u) = 0 \]  

(5)
Since the arrangement of cells is symmetric in a cell bundle, the domain borders for heat transfer are considered to be adiabatic. For the sake of simplicity, the velocities at the border are assumed to be zero. In the heat transfer calculation, the radiative heat transfer is not considered in this research. The inlet velocity of the fuel and the air are determined based on the power output

\[ U_{\text{fuel}} = \frac{I}{2F\eta_{H_2}c_{H_2}A_{\text{fuel}}} R T_{\text{if}} P_{\text{if}} \]

where \( U \) is the inlet velocity, \( F \) is Faraday’s constant, \( \eta_{H_2} \) and \( \eta_{O_2} \) are the oxygen and hydrogen utilization factors, respectively, \( A_{\text{fuel}} \) and \( A_{\text{air}} \) are the fuel and air inlet cross-sectional areas, \( c_{H_2} \) and \( c_{O_2} \) are the fuel and air inlet molar fractions of the fuel and air, \( P_{\text{if}} \) and \( T_{\text{if}} \) are the pressure and the temperature of the fuel at the inlet, and \( P_{\text{ia}} \) and \( T_{\text{ia}} \) are the pressure and the temperature of the air at the inlet.

The inlet temperatures of the fuel and air are set as 800° and 600 °C, respectively. The heat source is calculated based on the electrochemical reaction heat through the thermodynamic relationship

\[ T\Delta S = \Delta H - \Delta G \]

where \( \Delta H \) is the enthalpy change and \( \Delta G \) is the Gibbs free energy change, which is, ideally, converted to electrical power. The entropy change \( T\Delta S \) is released at the interface of the anode and electrolyte as thermal energy. The Joule heat and irreversible heat are in the range of 50%–100% of the reaction heat based on the current density [12]. The heat source in the Eq. (7) is then calculated by the addition of the entropy change, Joule heat, and irreversible heat. At this stage, the Joule heat and irreversible heat are estimated according to the current density. In future research, this numerical step will incorporate the calculated value from the electrical simulation. The inlet fuel composition is 90% hydrogen and 10% water vapor. The inlet air stream composition is 21% oxygen and 79% nitrogen. The properties of the gases are from Perry’s Chemical Engineers’ Handbook [13]. The thermal properties of the solid materials of the cell components are from the literature [5,14].

The major dimensions used in the computation are given in Table 1.

In our future work, the cell dimensions and rib numbers will be optimized and then compared to the actual products under development.

### 3 Results and Discussions

In this study, the finite volume method is adopted. In the simulation, it is found that using a 50 × 50 × 490 grid system for the domain in the simulation can attain grid independency.

Simulations have been conducted to investigate the temperature, velocity, and pressure field. Some typical results are shown and discussed in this section.

#### 3.1 Temperature Profiles

The 3D temperature field of the computation domain is obtained through numerical analysis of the
For the case of a current density of 400 A/cm², the temperature profile of the cross-section A-A (shown in Figs. 6 and 7) is given in Fig. 8. For a single cell stack, the temperatures of the cell stack ends are slightly higher than the middle part. This overall feature of the temperature field, shown in Figs. 8–10, matches the temperature distribution presented in Vora’s report [15]. The air in the air introducing tube is heated gradually by the air flowing toward the outlet of the air channel, which also obtains heat from the heat generating cell components. The fuel stream in the fuel channel is heated quickly due to the larger thermal conductivity and relatively small velocity, and does not change much near the reaction site. The air temperature in the air channel near the rib is slightly lower than the air temperature in the other places in the channel. This is because the electrochemical reaction does not occur in the rib. The largest temperature gradients occur at the inlet tube wall of the air introducing tube and the inlet of the fuel stream. The air heating effect inside the air introducing tube changes with variation in the dimensions of the air introducing tube, because this will change the velocity ratio of the air inside and outside the introducing tube.

The current density determines the power output and the fuel and air consumption, which in turn affect the inlet fuel and air velocity. The inlet fuel and air velocity and the temperature field therefore vary with the current density. Figures 9 and 10 show the two temperature fields for two different current densities of 300 and 500 A/cm². From Figs. 8–10, it can be seen that the temperatures of the air and fuel stream increase with the current density, while the temperature distributions in the air and fuel channels do not change significantly.

For the solid region, the temperature gradients are not large except at the entrances and exits. Figure 11 is the temperature field of the typical cell stack surface 1 shown in Fig. 6. The largest temperature gradient happens at the entrance and exit areas where the largest thermal tensions in the cell stack occur. Figure 12 shows the temperature field of the typical air tube surface 2 shown in Fig. 6. This temperature field has similar features to that of the cell stack surface, except it exhibits a lower overall temperature.

### 3.2 Velocity Profiles

The 3D velocity field of the computation domain is also obtained as described in the previous subsection.

For the case of a current density of 400 A/cm² and fuel and air utilization percentages of 85% and 15%, respectively, the velocity profile of the cross-section A-A (shown in Figs. 6 and 7) is given in Fig. 9. From Fig. 9, it can be seen that air flows in the introducing tube through the entrance, and turns back at the closed end of the air channel, from where it then flows along the air channel and gives its oxygen to the cathode when it is near the exit of the air channel. Figure 10 is an enlargement of the airflow in the returning area. The fuel enters the fuel channel from the closed end of the cell stack and flows toward the open end of the cell stack along the fuel channel. At the inlet of air introducing tube, the mean velocity of the air increases due to the increasing temperature. The mean velocities in the other parts of the air introducing tube and the air channel outside the air introducing tube are quite stable due to the stable temperature fields. Compared to the fuel stream velocity, the mean velocity of the air stream is much larger. (The Reynolds numbers at the air stream inlet and fuel stream inlet, in this particular case, are 617 and 2.2, respectively.) This is because the quantity of the air is much greater than the fuel’s due to the smaller oxygen utilization and its concentration in the air. The velocity distribution of the fuel stream is shown separately in Fig. 11. The dimensions of the cell stack and air introducing tube affect the fuel velocity and the velocity of the air inside and outside the air introducing tube, and hence, the temperature distribution. The optimization of these dimensions will be discussed together with the overall performance simulation in our future work.

The power output affects the velocity and temperature fields significantly due to the different heat generation in the fuel cell. The pressure drops of the air and fuel streams depend on their inlet velocities and the dimensions of the cell stack and air introducing tube. For an air introducing tube dimension of 0.9 cm × 0.9 cm × 45 cm, a current density of 400 A/cm², and fuel and air utilization percentages of 85% and 15%, the airflow and fuel flow pressure drop is 66 and 5 Pa, respectively. The pressure drops of the fuel and air stream for different current densities is shown...
in Fig. 16.

In the case of one rib built in the air chamber, only the left side stack is studied due to the symmetry. When multiple ribs are built in the air chamber, the left side stack has several channels, and the temperature and flow fields will vary in the different channels. However, to avoid untenably large computational time, some simplifications can be made for the other channels based on the typical left channel. These simplifications will be discussed in more detail in the authors’ future work.

4 Conclusions

Modeling and simulation for the three dimensional heat and fluid flow in a flat-tube HPD–SOFC has been performed, and the resultant computer code has been developed and operated. The heat transfer and fluid flow behaviors of the fuel and air streams in a representative channel are obtained as expected. This work provides an important basis for an overall simulation and optimization of the flat-tube HPD–SOFC in the future.

Nomenclature

\[ A_{\text{fuel}} = \text{cross section area for fuel stream, m}^2 \]
\[ A_{\text{air}} = \text{cross section area for air stream, m}^2 \]
\[ c = \text{mole fraction} \]
\[ c_p = \text{heat capacity, J/kg °C} \]
\[ e^- = \text{electron} \]
\[ \text{EMF} = \text{electromotive force, V} \]
\[ F = \text{Faraday’s constant 96,486.7, C/mol} \]
\[ \Delta G = \text{Gibbs free energy change, J/mol} \]
\[ \Delta G^0 = \text{standard Gibbs free energy change, J/mol} \]
\[ \Delta H = \text{enthalpy change of the reaction, J/mol} \]
\[ H_2 = \text{hydrogen} \]
\[ H_2O = \text{water} \]
\[ I = \text{current, A} \]
\[ k = \text{thermal conductivity, W/(m °C)} \]
\[ O_2 = \text{oxygen} \]
\[ O^{2-} = \text{oxide ion} \]
\[ P = \text{pressure, Pa} \]
\[ q = \text{volumetric heat source, W/m}^3 \]
\[ R = \text{universal gas constant 8.314,34 J/mol K} \]
\[ \Delta S = \text{entropy change of the reaction, J/(mol K)} \]
\[ T = \text{temperature} \]
\[ U = \text{velocity} \]
\[ \eta = \text{utilization percentage} \]
\[ \mu = \text{dynamic viscosity, kg/(m s)} \]
\[ \rho = \text{density, kg/m}^3 \]

References