A detailed model is presented for the analysis of temperature, species concentration, and current density profiles as well as the efficiency and power density of a planar solid oxide fuel cell at direct internal reforming condition. The model describes the interactions of mass transport, heat transport, heterogeneous chemistry, and electrochemistry. The heterogeneous chemistry model for the catalytic reactions in the anode structure uses a multi-step reaction mechanism for the steam reforming of methane on Ni based catalysts. The porous media transport is modeled using the Dusty Gas Model, and electrochemistry is modeled using a modified Butler-Volmer setting assuming hydrogen as the only electrochemically active species. The impact of flow rate, anode thickness, and catalyst loading on power density and efficiency is discussed for isothermal and adiabatic operating conditions.

Introduction

In the recent past solid oxide fuel cells (SOFC) have attracted considerable attention due to its potential to convert chemical energy into electrical energy at high efficiencies. The potential of the direct use of hydrocarbons and alcohols as fuels in SOFC is of great interest. In particular strategies are currently explored for direct internal reforming of those fuels and partially pre-reformed fuels. Since SOFCs offer a wide range of operating possibilities, identifying the effect of operating conditions such as air flow rate, inlet fuel composition, catalyst loading, and anode thickness on the efficiency and power density is critical for optimal operation of SOFCs. This paper reports on the efficiency and power density analysis for a variety of parameters. However, the analysis presented here is quite different from the maximum efficiency analysis. Here we analyze the influence of various parameters for a given cell dimensions. A schematic representation of the model of the planar single cell geometry studied is shown in Fig 1.

Figure 1. Schematic representation of planar cell under consideration.
Approach

In the approach adopted here a detailed numerical model is developed to describe the interaction of various chemical and physical processes that occur in the cell. This model is described in our previous publications (1,2). In short, the model assumes plug flow equations in the flow channels and the transport within the porous electrodes is described by Dusty Gas Model (DGM). The heterogeneous chemistry within the anode is represented by an elementary-step reaction mechanism for the steam reforming of methane on Ni based catalysts (3). The electrochemistry is modeled by a modified Butler-Volmer equation assuming H$_2$ as the only electrochemically active species. A detailed description of the derivation of these equations is described in (1).

The parameters analyzed here cover air flow rate, anode thickness, and catalyst loading. In the analysis made it is assumed that the extremes of the stack behavior are represented by isothermal and adiabatic operations. Although these are only idealizations, such an analysis can throw meaningful insight into the influence of temperature distribution on the resulting cell performance.

Results and Discussion

To demonstrate the capability of the model in describing the details of the physico-chemical processes, Fig. 2 represents the species profiles within the fuel channel and within the anode. For the example discussed here, the partially pre-reformed inlet fuel is

Figure 2. Species profiles within the fuel channel and within the anode. The inlet fuel is assumed to consist of 14% CH$_4$, 63% H$_2$, 2% H$_2$O, 20% CO, and traces of CO$_2$. The drop down panels shows the profiles across the thickness of anode at selected axial positions.
assumed to consist of 14% CH₄, 63% H₂, 2% H₂O, 20% CO, and traces of CO₂ entering at 800°C (volumetric rates). Air is assumed to enter the cathode channel at 650°C. The drop-down panels show the profiles across the thickness of anode at selected axial positions. It is quite obvious from the figure that H₂ and H₂O have opposite fluxes within the anode, because the former is being consumed and the latter is being produced as a result of electrochemical reactions at the three-phase interface.

The influence of the air flow rate on the resulting efficiency and power density are shown in Figs. 3a and 3b. The inlet fuel is assumed to consist of 40% CH₄ and 60% H₂O. In the case of isothermal operation, an increase in air flow rate results in increased efficiency and power density. However, in the case of adiabatic operation the efficiency and power density decreases with increase in air flow rate.

In the case considered here air is assumed to enter the cathode at 650°C. Hence, an increase in flow rate results in an overall decrease in cell temperature, and this further results in decreased average current density and hence decreased performance. However, in the case of isothermal operation increasing air flow rate results in increased fuel utilization due to the low air depletion on the cathode side.

The influence of anode thickness on efficiency and power density for an isothermal operation is shown in Fig. 4a. The efficiency and power density in this case increases with increasing anode thickness. In the case of an isothermal operation the greater extent
of reforming reaction with increasing anode thickness results in increased performance. However, in the case of adiabatic operation the anode thickness has an optimal value which results in the best performance.

Figure 4a. Influence of anode thickness in the case of isothermal operation.

Figure 4b. Influence of anode thickness in case of adiabatic operation.

In the case of adiabatic operation, Fig. 4b, thicker anodes lead to greater extent of reforming and hence higher temperature drop near the cell inlet. This temperature drop basically leads to a decreased average current density and therefore the efficiency and power density drops for thicker anode. In the case of thin anode, the lower extent of reforming reactions results in lower average current density and therefore lower performance.

The influence of catalyst loading for isothermal as well as for adiabatic cases is shown in Figs. 5a and 5b, respectively. However, the results presented here are in terms of specific active area. The specific area is a direct measure of catalyst loading in the pore networks. The specific area can be calculated by analyzing the catalyst sample by techniques such as BET measurements. Like in the case of anode thickness, an increasing specific area results in increased extent of reforming and hence higher fuel utilization in the case of isothermal operation (Fig. 5a). This results in a higher cell performance in the case of isothermal operation. However, in the case of adiabatic operation, the increased catalyst loading results in higher temperature drop near the inlet boundary and the temperature drop leads to lower average current density, which further leads lower cell performance.
Conclusions

Based on a detailed numerical model we have analyzed the influence of various parameters on the resulting cell efficiency for a given geometry. The critical factor for optimal cell performance has been found to be the resulting temperature distribution within the cell. In all cases, isothermal conditions lead to the better cell performance compared to adiabatic operations. Therefore within a cell stack, a uniform temperature distribution will be highly desirable to achieve the best cell performance. Furthermore, a uniform temperature distribution can also eliminate the thermal stresses within the cell and hence longer cell life.

Acknowledgments

We gratefully acknowledge many fruitful discussions with Professor R. J. Kee and Dr. H. Zhu, both at Colorado School of Mines.

References