A COMPUTATIONAL FLUID DYNAMICS MODEL OF A SOFC

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ABSTRACT

A three-dimensional model has been developed to simulate the steady state single cell performance of a planar solid oxide fuel cell (SOFC). The governing equations for heat and mass balances were solved numerically with a computational fluid dynamics code (CFD) based on the finite volume method. Numerical results from this simulation show that the concentration of fuel is reduced along the flow direction as the reactant is consumed, leading to a similar distribution for the current density. Temperature variation due to the conjugate heat transfer between fluid and solid also rise with the flow. The results are indicative of significant temperature gradients within the cell, and identify mechanical integrity as a significant issue for SOFCs.

INTRODUCTION

To date, much of the research into the emerging SOFC technology has been concerned with development of the electrochemical and materials issues necessary to produce a working fuel cell. However, as this technology is advancing from the prototype to the manufacture stage, issues affecting the reliability and durability of cells are becoming increasingly important. Several factors are known to introduce mechanical concerns into SOFCs (1) and these are directly related to the operating conditions and design of the cell. In particular, the temperature distributions caused by fluid flow and reactions impinge directly on stresses within ceramic components (2) and these stresses can be significant. For this reason, it is timely to develop models of flow and temperature to help quantify these effects in SOFCs. Furthermore, modelling is an essential stage in advancing design because it is relatively inexpensive compared to manufacturing.

Some simulations of SOFCs have been reported in the literature recently (3, 4), reporting CFD analyses, although this work tends to be on single channel models. In the current work, a co-flow planar SOFC has been modelled using a CFD code that includes a three-layer cell. Anode, electrolyte and cathode are enclosed by metallic interconnects which contain pillars functioning as contacts for current collectors above and below. The electrical performance of the SOFC is determined by measuring the current and voltage, and these are reported in this paper. The aim of this work is a parametric study due to changes of inlet gas temperatures and operating temperature levels to observe their effects on cell performance. The presented hydrogen concentration, current density, Nernst potential and cell voltage are self consistent and as anticipated and all are observed to decline as the fuel moves further into the cell.
Furthermore, cell current and voltage are also affected by several factors, such as operating temperature and pressure, making parametric studies on the cell performance important. The objective of this work is to conduct the first stage of a parametric study due to changes of inlet gas temperatures and operating temperature levels to observe their effects on cell performance. In addition, temperature distributions in the cell due to conjugate heat transfer between the hardware (solid cells) and gas streams (fluid cells) will also be investigated.

CELL DESCRIPTIONS AND ASSUMPTIONS

Direct current is generated by the flow of electrons through the component hardware and external loads. For any value of current, the voltage drop is composed of (i) overpotentials of the electrochemical reactions (ii) the ohmic drop across cell components, and (iii) the mass transport limitations of reactants and products (5).

Table I. Geometries of MEA components.

| Component       | Geometry                                      |
|-----------------|-----------------------------------------------|
| Electrolyte     | YSZ 200 µm thick                              |
| Anode coat      | Ni-YSZ 50 µm thick                            |
| Cathode coat    | LSM 50 µm thick                               |
| Interconnect    | 70 mm square, 1.9 mm thick, including pocket to take the coated electrolyte |

The geometry of the cell is shown in Table I and Figure 1. This particular geometry is chosen because it exists at Imperial College London as the result of a teaching project. One single cell consists of an electrolyte made of yttria stabilised zirconia (YSZ) in
contact between a nickel zirconia cermet anode (Ni/YSZ) and strontium doped lanthanum manganite (LSM) cathode. The cell is sandwiched by strontium doped lanthanum chromite interconnects with pillars functioning as the current collectors on top and bottom. The modelled fuel is 100% H₂, and is fed into the anode inlet and, likewise, 100% O₂ to the cathode. Because of symmetry only half of the cell has been modelled.

However, the fuel cell is a complicated system involving the microstructures of materials, fluid dynamics, heat and mass transfer processes and other issues. In order to simplify the calculations in the model, following assumptions and simplifications are made:

- The fuel cell is in a steady state of operation
- The gas reactants are assumed to be incompressible ideal gases and contain 100% concentration of H₂ for fuel and O₂ for oxidant so that there is no internal reforming required in the fuel flow channel
- Theoretically, the electrochemical reactions occur at the three-phase-boundary where electrode, electrolyte and reactants meet. However, in this model, the active areas are modelled as thin layers evenly covering the electrolyte. In actuality this is not over-restrictive since electrodes are composed of mixed conducting materials, which are small in thickness; porosity calculations are a level of detail not required at this stage;
- Some solid cells on each cathode and anode are occluded by the current collector pillars, and therefore do not contribute to the reactions. These regions are termed 'dead' areas;
- Heat is generated in the electrolyte layer (6).
- Heat transfer by thermal radiation is not included.

**MATHEMATICAL MODEL**

At the electrolyte-cathode interface, O₂ reduces to O²⁻ and these ions are then conducted ionically through the electrolyte to the electrolyte-anode interface, where in the simplest consideration, they combine with H₂ to produced H₂O and electrons, equations [1] and [2] respectively. The system as a whole is represented by [3].

\[
\begin{align*}
\frac{1}{2}O_2 + 2e^- & \rightarrow O^{2-} [1] \\
H_2 + O^{2-} & \rightarrow H_2O + 2e^- [2] \\
H_2 + \frac{1}{2}O_2 + 2e^- & \rightarrow H_2O + \text{Electricity} + \text{Heat} [3]
\end{align*}
\]

The conservation laws of mass, energy and momentum as shown below are the basis of the CFD analysis. Each of the solid and fluid domains are divided into small discrete regions, each called a 'cell', where the governing differential equations of conservation laws are applied and then solved iteratively. All the source terms used in these equations correspond to the amount of reactant consumed and product generated according to the electrochemistry.

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Conservation of mass:

\[ \rho \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) = S_m \]  

where \( S_{\text{m,anode}} = S_{H_2} + S_{H_2O} \) and \( S_{\text{m,cathode}} = S_{O_2} \)

Each of these terms can be written in terms of the local current density, \( i \), molecular mass and Faraday's constant, \( F \):

\[ S_{H_2} = -\frac{M_{H_2}}{2F} i, \quad S_{H_2O} = \frac{M_{H_2O}}{2F} i \quad \text{and} \quad S_{O_2} = -\frac{M_{O_2}}{4F} i \]

Conservation of momentum (Navier-Stokes) in each of the \( x \), \( y \) and \( z \) directions:

\[ u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = \frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \]

\[ u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = \frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \]

\[ u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = \frac{1}{\rho} \frac{\partial P}{\partial z} + \nu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \]

Conservation of a chemical species:

\[ u \frac{\partial (\rho M_A)}{\partial x} + v \frac{\partial (\rho M_A)}{\partial y} + w \frac{\partial (\rho M_A)}{\partial z} = -\rho \left( D_x A \frac{\partial^2 M_A}{\partial x^2} + D_y A \frac{\partial^2 M_A}{\partial y^2} + D_z A \frac{\partial^2 M_A}{\partial z^2} \right) + S_{M_A} \]

where \( A \) takes each value of \( H_2, O_2 \) and \( H_2O \) as in [6].

Conservation of energy (convection and conduction):

\[ u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{k}{\rho C_p} \left( u \frac{\partial^2 T}{\partial x^2} + v \frac{\partial^2 T}{\partial y^2} + w \frac{\partial^2 T}{\partial z^2} \right) + Q \]

**Heat Generation and the Relation Between Electrical Power and Thermal Energy**

The heat released from the electrolyte layer can be calculated from the following (7):

\[ Q_{\text{cell}} (W/m^3) = (-\Delta H_f H_2O) r_{H_2} - i V_{\text{cell}} \]
In equation [10], $V_{\text{cell}}$ is assumed to be 0.7 V. The rate of hydrogen consumption $r_{H_2}$ is calculated from Faraday's law:

$$r_{H_2} (\text{mol}/\text{sm}^3) = \frac{i}{2F}$$ \[11\]

and the enthalpy change is a function of temperature:

$$\Delta H_{f, H_2O} (\text{J}/\text{mol}) = -(240506 + 7.3835T)$$ \[12\]

The current density, $i$, can be defined by

$$V_{\text{cell}} = E_{\text{Nernst}} - iR_{\text{cell}}$$ \[13\]

$E_{\text{Nernst}}$ in equation [13] is defined as

$$E_{\text{Nernst}} = E^0 + \frac{RT}{2F} \ln \left( \frac{P_{H_2}P_{O_2}}{P_{H_2O}} \right)^{1/2}$$ \[14\]

$$E^0 = 1.2723 - 2.7645 \times 10^{-4}T$$ \[15\]

$R_{\text{cell}}$ is the resistance, which was estimated from the experimentally measured I-V data for a single cell (4).

$$R_{\text{cell}} (\Omega/\text{m}^2) = \left( \frac{T}{-34 + 1.25 \times 10^6 \exp(-7185/T)} + 0.04 \right) \times 10^{-4}$$ \[16\]

IMPLEMENTATION

At the inlet, the fluid velocities are fixed, and clearly the symmetry plane boundary is also assigned. Sink and source terms are assigned in the users' subroutine according to the stoichiometry from electrochemical reactions occurred on each electrode. On other boundaries, adiabatic walls are assumed which approximates to the cell being modelled being located in the middle of the fuel cell stack.

Heat is assumed generated from the electrolyte layer according to equation [10] where the majority comes from the enthalpy of the reactions. Current density is calculated simply from Ohm's law since the activation polarisation is very small and approximately constant over the whole plate so that the temperature is the only factor affecting current density.

RESULTS

The consequences of the geometry of the design can be seen more clearly in the figures below- in each case the symmetry plane is across the top of the figure; the fuel inlet is
through the smaller cells top right, and the outlet is top left. The blank areas within the figures correspond to pillars which exist to ensure the gas channel does not collapse but also provide electrical connexion to the interconnect.

Figure 2 shows the hydrogen concentration within the fuel flow. The fuel modelled here is 100% hydrogen at the inlet, and it can be seen that in the nether regions, the hydrogen is severely depleted at the velocities considered here. Figure 3 shows the current density in the electrolyte from which it is clear that in this model the reaction is much more pronounced near the inlet rather than the outlet. This might be expected to cause thermal stress distributions across the cell. Figures. 4 & 5 show respectively, the Nerst potential and cell voltages. Both of these also tail off away from the entry point as might be expected because of the decrease in cell activity.

These results are consistent, but the very high rate of reaction at the entry is a cause for further investigation. At present there is no limit on reaction rates, although presumably there is a limit in diffusion of oxygen through the electrolyte and hence a restriction on the current density and hence reaction rates.

Figure 2. $H_2$ concentration contour plot in the flow channel.

Figure 3. Current density distribution plot at the anode.
At the outset, it was stated that SOFCs are complicated situations, and therefore a sensible approach is to develop a parametric analysis of the cell – allowing input variables and boundary conditions to be varied and determining their effect on the behaviour of the cell. This work is underway and will be reported in due course. In addition to this, further consideration of the input fuel is required, and is being studied.

**CONCLUSIONS**

The initial stages of a CFD model for a SOFC has been created and demonstrated. The model incorporates mass, momentum and energy conservation within the electrochemical environment of the SOFC. The presented hydrogen concentration, current density, Nernst potential and cell voltage are in good agreement, and all are observed to decline as the fuel moves further into the cell. The work is currently progressing to consider parametric studies of the behaviour of the cell.
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REFERENCES

1. S. T. Hagos and R. P. Travis, in these Proceedings.
2. H. B. M. Lau, A. J. Marquis, and R. P. Travis, International Journal of Numerical Heat Transfer Part A: Applications, 41, 2, 149 (2002).
3. E. Achenbach, Journal of Power Sources, 49, 333 (1995).
4. H. Yakabe, T. Ogiwara, M. Hishinuma, and I. Yasuda, Journal of Power Sources, 102, 144 (2001).
5. S. Um, C.-Y. Wang, and K. S. Chen, Journal of the Electrochemical Society, 147(12), 4485 (2000).
6. N. Q. Minh and T. Takahashi, Science and Technology of Ceramic Fuel Cells: Elsevier, (1995).
7. J.-H. Koh, H.-K. Seo, Y. S. Yoo, and H. C. Lim, Chemical Engineering Journal, 87, 367 (2002).