Numerical analysis in a MOLB-type SOFC considering different operating conditions

J.J. Ramirez-Minguela, V.H. Rangel-Hernandez
Departamento de Ingeniería Mecánica, Universidad de Guanajuato, Carretera Salamanca–Valle de Santiago km. 3.5 + 1.8 km, Comunidad de Palo Blanco, Salamanca, Gto., MEXICO
Teléfono: 01 464 64 79940
minguela_rjj@hotmail.com, vrangel@ugto.mx

Abstract

The present work numerically investigate the behavior for a fuel cell MOLB-type (mono-block-layer built) SOFC (solid oxide fuel cells), with different thickness in the electrolyte and different operating conditions at the inlet of the fuel cell like mass fraction, temperature and velocities. The investigation is based on a three-dimensional CFD model using the finite volume method derived from a control-volume formulation that takes in account mass transfer, heat transfer, transport of species and electrochemical reactions. Different simulations are performed and detailed comparisons of fluid flow, concentration species, temperature and electric fields along of the fuel cell are made in the present study. The results indicate that numerical predictions of fuel cell behavior are strongly influenced by operating conditions adopted in the model.

1. Introduction

SOFC (Solid Oxide Fuel Cells) in the last years have been studied at large since they are considered as promising energy conversion devices due to their high performance to generate electricity with different type of fuels, and the possibility to build hybrid systems, taking advantage of their generation of heat. Thus, the SOFC is expected to reach commercialization in a few years and could be a promising alternative energy source for the residential and distributed power plants in the 21\textsuperscript{st} century [1-3]. However, the further development of the SOFC has some challenges that necessitate to be researched such as mechanical stress, electrode sintering, electrode and interconnect materials and fabrications, startup time, the maximization of the power density and the minimization of the non-uniform distribution of temperature, which contributes to thermal stress in the SOFC components, so that the goal of highly efficient and clean energy system can be reached with at least the same reliability, costs and lifetime of the “traditional” energy systems [4-5].

In the past are several investigations about modeling planar SOFC during steady operation to calculate the temperature and current density distribution [6-8]. However, only less work has been performed on the influence of variation in operating conditions in MOLB-type (mono-block layer built) geometry SOFC, which is composed of trapezoidal flow channels separated by a corrugate PEN (positive-electrolyte-negative) plate. Most of the authors are focused in the study of planar geometries instead of MOLB-type geometry due to the simplicity of its construction.

One of the objectives of this work is to demonstrate and develop a CFD-based model to solve the complex interaction between fluid dynamics and electrochemical kinetics in a MOLB-type SOFC. Therefore, this works is focused mainly on studied the behavior and effects in SOFC for different operating conditions, and predict the temperature distributions, species concentrations, current density and potential losses. Ten cases were considered; changing the electrolyte thickness, fuel inlet mass fraction, inlet temperature and fuel inlet velocity. In order to investigate how the operating conditions affect the performance of the SOFC.

2. SOFC materials and geometry

The electrolyte of SOFC is a solid, nonporous ceramic, usually Y$_2$O$_3$-stabilized ZrO$_2$ (YSZ). The SOFC operates at 600-1000°C where the ceramic electrolyte becomes conductive to oxygen ions, O$_2^-$, but nonconductive to electrons. Typically, the anode is made of nickel/yttria-stabilized zirconia (Ni/YSZ) cermet and the cathode is Sr-doped LaMnO$_3$ [9].
In this paper a single-cell module of the MOLB-type SOFC is investigated (Fig. 1). The fuel and air run in parallel flow in the trapezoidal channels that are separated by a corrugate PEN plate. In particular, fuel is considered as a mixture of hydrogen and water vapor.

As hydrogen is used as fuel, the electrochemical reactions are at the cathode side:
\[ \frac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \] (1)

At the anode side:
\[ H_2 + O^{2-} \rightarrow H_2O + 2e^- \] (2)

The overall cell reaction is:
\[ H_2 + \frac{1}{2}O_2 \rightarrow H_2O \] (3)

3.2 Dynamics of electrochemical reactions

The activation polarization of electrolyte-supported SOFC occurs in both electrodes. The activation polarization can be determined from the Butler–Volmer equation [11] which is used to relate the surface overpotential and the rate of reaction (3) as the following:
\[ i = i_0 \left[ \exp \left( \frac{\alpha n F V_{act}}{RT} \right) - \exp \left( -\frac{(1-\alpha) n F V_{act}}{RT} \right) \right] \] (4)

Where \( i \) is the net current density, \( i_0 \) is the exchange current density or the current densities for the forward and reverse reaction at equilibrium, and \( \alpha \) is the charge transfer coefficient [12]. This equation was solved by Newton-Raphson multivariable method. The exchange current density is defined for the cathode as 2300 and for the anode as 5300 A/m².

The ohmic polarization caused by the electrical resistances of the electrodes and resistance of ion transport in the electrolyte was considered as:
\[ V_{ohm} = \bar{\epsilon} R_{ohm} \] (5)

The ionic conductivity in the cathode, electrolyte and anode are considered as reference [13]. The open-circuit voltage is given by:
\[ V = V_N - V_{act} - V_{ohm} \] (6)

Where \( V_N \) is the Nernst voltage considering the concentration polarization losses, obtained by:
Where $K$ is the chemical equilibrium constant, $Y_{H_2}$, $Y_{O_2}$ and $Y_{H_2O}$ are the local molar concentrations at the electrodes respectively.

### 3.3 Thermo-fluid model

In the simulation, the solid and fluid domains were divided into some discrete meshes, and in each computational mesh, the conservation equation of species, mass, momentum and energy were solved using the finite volume method.

The continuity conservation equation is model as:

$$\nabla (\rho \vec{v}) = 0$$  \hspace{1cm} (8)

In general, gas species transfer mainly by convection in the flow channels and diffusion in the porous electrodes. The mass conservation can be analytically described by the following transportation equation:

$$\nabla (\rho \vec{v} X_j) = -\nabla J_j + S_j$$  \hspace{1cm} (9)

where $J_j$ is the diffusion flux of species $j$, $X_j$ the mass fraction of the $j$th specie, and $U$ is the gas velocity. For full multicomponent diffusion the diffusive mass flux $J_j$ is described by the Fick’s law:

$$J_j = -\rho D_{i,eff} \nabla X_j$$  \hspace{1cm} (10)

Binary diffusivity $D_{ij}$ required to compute $D_{i,eff}$ are obtained through the Fuller-Schettler-Gidding correlation. The volumetric diffusion coefficients are obtained from [14]. In the fuel and air channels $D_{i,eff}$ coincides with $D_{ij}$ while in the porous media the effective binary diffusivity is computed as:

$$D_{i,eff} = \frac{\varepsilon}{\tau} D_{ij}$$  \hspace{1cm} (11)

The rate of production or consumption of species is given according to the Fadaray Law, by:

$$S_j = \frac{i}{\eta F} M_j$$  \hspace{1cm} (12)

where $M_j$ is the molar mass of species $j$.

Both the air and fuel flows were considered as ideal gas mixtures. The momentum conservation equation:

$$\rho \varepsilon \left(u \frac{\partial u}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial w}{\partial z}\right) = -\varepsilon \nabla P + \varepsilon \mu_{eff} \left(\frac{\partial u^2}{\partial x^2} + \frac{\partial v^2}{\partial y^2} + \frac{\partial w^2}{\partial z^2}\right) + S_M$$  \hspace{1cm} (13)

where $S_M$ is momentum source, and $S_M = 0$ in the flow channels. However, in the porous electrodes, Darcy law with constant porosity and permeability is applied to model the momentum source as follow [7]:

$$S_M = -\frac{\mu_{eff}}{K} \varepsilon U$$  \hspace{1cm} (14)

where $\mu_{eff}$ is the effective viscosity of the mixture gas and is given as reference [7]. The energy conservation equation:

$$\nabla \left(\rho \vec{v} E\right) = \nabla \left(k_{eff} VT - \sum h_j J_j\right) + S_E$$  \hspace{1cm} (15)

The first two terms on right-hand side represent energy transfer due to conduction and diffusive species transport. Heat transfer between the fluid and solid materials was limited to conduction and convection, radiation was neglected because it is very small relative to the other kinds of heat transfer. The effective thermal conductivities of porous electrodes are calculated as reference [15]. Additionally $S_E$ is the energy source term that represents the heat generated due to:
1. Joule effect, due to the ohmic resistance $S_{\text{ohm}}$.
2. Reversible heat, associated to chemical reaction $S_C$.
3. Activation loss $S_{\text{act}}$.

While the Joule effect takes place in the entire electrode domain the last two sources are localized in the TPB (triple-phase-boundary) [16].

$$S_E = \begin{cases} S_{\text{ohm}} + S_C + S_{\text{act}} & \text{in the TPB} \\ S_{\text{ohm}} & \text{elsewhere} \end{cases} \quad (16)$$

Where:

$$S_C = \frac{T \Delta S_{H_2O}}{M_{H_2O}}$$ \quad (17)$$

$$S_{\text{ohm}} = \frac{i^2}{\sigma_{\text{eff}}} \quad (18)$$

$$S_{\text{act}} = \dot{\epsilon} V_{ac} \quad (19)$$

Where $\Delta S$ is the entropy change, the ionic conductivity in the cathode, electrolyte and anode equations are given in reference [13], and the generation of water is calculated by (18) equation, $V_{ac}$ is calculated from Butler–Volmer equation (5).

### 4. Cases studied and boundary conditions

In this study ten cases have been considered; as illustrated later in the paper, such cases are used to investigate the sensitivity of the performance of the fuel cell on different operating conditions. The cases are characterized by different electrolyte thicknesses, fuel inlet mass fractions, inlet temperatures and fuel inlet velocities. Table 1 summarizes the cases studied.

Furthermore ambient pressure is imposed on the outlet cross-sections. Fuel cell is considered to be adiabatic and symmetry boundary conditions are imposed on left and right planes depicted in Fig. 2. Finally fuel cell voltage is imposed.

The transport properties and thermal properties of the SOFC used for the simulation are listed in Table 2 and 3.

| Table 2. The electrochemical and transport properties of the solid oxide fuel cell components [12] |
| Description | Values |
| Anode transfer coefficient | 2 |
| Cathode transfer coefficient | 0.6 |
| Faraday constant (F) | C/mol 96487 |
| Anode electrode porosity | 0.5 |
| Cathode electrode porosity | 0.5 |
| Permeability of anode electrode | m² $1.7 \times 10^{-10}$ |
| Permeability of cathode electrode | m² $1.7 \times 10^{-10}$ |

### Table 1. Analyzed cases in this work

<table>
<thead>
<tr>
<th>CASE NUMBER</th>
<th>DYNAMIC PART</th>
<th>SOLID PART</th>
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<tbody>
<tr>
<td>VELOCITIES (m/s)</td>
<td>TEMPERATURES (K)</td>
<td>COMPOSITION FUEL</td>
</tr>
<tr>
<td>V_AIR_IN</td>
<td>V_FUEL_IN</td>
<td>T_FUEL_IN</td>
</tr>
<tr>
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<td>3</td>
<td>973</td>
</tr>
<tr>
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<td>973</td>
</tr>
<tr>
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<tr>
<td>4</td>
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<td>5</td>
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<td>973</td>
</tr>
<tr>
<td>6</td>
<td>1.5</td>
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</table>

<table>
<thead>
<tr>
<th>Cell component</th>
<th>Density (kg/m³)</th>
<th>Effective thermal conductivity (W/mK)</th>
<th>Specific heat (J/kgK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode</td>
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<td>650</td>
</tr>
<tr>
<td>Cathode</td>
<td>6000.0</td>
<td>9.6</td>
<td>900</td>
</tr>
<tr>
<td>Electrolyte</td>
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<td>2.7</td>
<td>300</td>
</tr>
<tr>
<td>Interconnect</td>
<td>7700.0</td>
<td>13</td>
<td>800</td>
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</table>

5. Numerical approach

As mentioned earlier, the MOLB unit is symmetric about the mid-planes of the air and fuel channels. So the present computational domain takes into account the region between these two planes for memory and time saving. In the simulation governing equations were numerically solved by using the finite volume method using ®FLUENT. The finite-volume Navier-Stokes and transport equations are solved to obtain the gas species concentrations and temperatures at each position in the cell. The information is passed to an iterative algorithm implemented through user define functions (UDFs) in order to deal with the coupled multi-physics equations previously illustrated in the electrochemical model. Then the local current density is calculated and applied to obtain the hydrogen reaction rate, heat source and species sources. Gas species concentrations and temperature distributions are then calculated for the next iteration, and so on, until convergence of solution is achieved.

Fig. 3. Distributions along the cell of: a) current density, b) temperature, c) activation loss, d) ohmic loss and e) concentration loss. Cases 1 to 3 (different thickness).
SIMPLE algorithm has been employed to deal with pressure-velocity coupling while convective terms have been approximated by means of a second-order upwind scheme. Central difference second-order scheme has been used to computed diffusive terms. The numerical procedures are described in [17]. Scaled residuals are monitored for all the variables and solution is considered to be converged when residuals are lower than $10^{-6}$. The computational grid has been subsequently refined and a structured mesh of 290000 cells has been found to be sufficient to achieve grid-independent solutions.

Finally the model validation has been done applying the previous equations described considering the parameters and operating conditions available in [18] obtaining similar behavior and numerical values in the current, species and temperature distributions into the fuel cell.

### 6. Results

This section shows the results of the behavior of the current density, temperature, activation loss, ohmic loss and concentration loss distributions along of the cell obtained from the analysis previously described.

#### 6.1 Comparing different electrolyte thicknesses

Fig. 3 compares the behavior of the fuel cell according to the cases 1 to 3, where different thicknesses in the electrolyte are considered. The results show higher current density for the case 3 (thicker electrolyte), therefore, temperature, activation loss, ohmic loss and concentration loss distributions are higher than the cases 1 and 2 (thinner thicknesses) for obtain the same output power (5800 W/m²). These results are related to the ionic resistivity of the electrolyte; while the electrolyte is thicker the ionic resistivity is higher, thus, it is necessary to increases the current density throughout the fuel cell for obtain the same output power that used thinner thicknesses of the electrolyte. The reduction in the z direction (larger than 0.06 m) is due to the higher concentration losses in the TPB as can be seen in Fig. 3 e) or in a local distribution for the case 2 and 3 in Fig. 4. According to the above, the case 2 has the lower current density, temperature, ohmic
loss and concentration loss distributions due to its thinner electrolyte and whereby correspond to the case with the lower temperature gradient.

Fig. 4 depicted the $\text{H}_2$ and $\text{O}_2$ mass fractions distribution on anode-electrolyte and cathode-electrolyte interfaces for the cases 2 and 3 which correspond to the lower and higher current density distributions. Each reactant has a large drop in the mass fraction from the entrance of the channel towards the end, due to the rates of consumption and production of each chemical species involved in the electrochemical reactions, this phenomenon increases the concentration losses (Fig. 3 e)). A local minimum in the hydrogen and oxygen mass fraction are observed on the bottom and upper plane respectively. Along these edges, forced convection is weak due to corner effect and the porous material represents an obstacle to the fuel and air flow and for that reason the diffusivity is predominant in these areas.

### 6.2 Comparing different inlet compositions of the fuel

Fig. 5 depicts the results of cases 1, 4 and 5 with fuel inlet mass fraction variable. The cases 4 and 5 show practically the same distributions of the phenomena under study. This means, if the inlet mass fraction of hydrogen is higher than 0.5, is not possible to obtain a meaningful improvement in the performance of the fuel cell.
However, considering 0.1 the inlet mass fraction of hydrogen, the average current density increases due to the concentration loss growth throughout the fuel cell. Therefore, temperature and activation loss distributions follow a similar behavior. The reduction in the current density in cases 4 and 5 is due principally to the Nernst potential because depend directly of the composition of the fuel (eq. 7). It should be noted that the case 1 has a lower ohmic loss distribution contrary to the case analyzed previously; this is due to the increment of temperature related to the electrochemical reactions.

Considering the results obtained, the performance of the fuel cell is highly affected by the geometrical parameter than changing the inlet mass fraction of fuel.

6.3 Comparing different inlet temperatures

Fig. 6 depicts the results of cases 1, 6, 7 and 8 with different effects along of the fuel cell changing the inlet temperature of fuel and air respectively. The case 8 with 873 K in the air and fuel entrance has the higher temperature gradient because is the lower temperature entrance condition of the cases analyzed.
and correspond to the higher current density average necessary to obtain the desired output power. This increases the temperature throughout the fuel cell achieving 1400 K at the outside due mainly to the electrochemical reactions. Furthermore, the case 6 with 973 K in the air and fuel entrance has the lower temperature gradient and more homogeneous current density distribution and has the lower ohmic loss, this is mainly due to the variability of the ion conductivity of the electrolyte with respect to the temperature (Fig. 6 d)).

Besides to the variability of the current density, temperature, activation loss and ohmic loss distributions, the concentration losses has no significant variations (Fig. 6 e)).

### 6.4 Comparing different inlet velocities

Fig. 7 compares the behavior of the fuel cell according to the cases 1, 9 and 10, with different inlet velocities of the fuel. The results show in cases 9 and 10 the current density, temperature, activation loss, ohmic loss and concentration loss distributions similar, while the mean difference with respect to the case 1 is that the concentration losses are predominant, but the contributions of ohmic losses are lower. This particular behavior, is because the velocities of 1 and 1.5 m/s reduces the temperature along of the cell and this results in high ohmic loss, which are predominant in the cell.

![Fig. 7. Distributions along the cell of: a) current, b) temperature, c) activation loss, d) ohmic loss and e) concentration loss. Cases 1, 9 and 10 (different inlet velocities).](image-url)
7. Conclusions

In this paper the numerical analysis of a solid oxide fuel cell has been performed. The effects on the performance of different operating conditions used have been computed by means of a CFD three dimensional model that takes in account the major transport phenomena occurring in the fuel cell. In particular the influence of thickness of the electrolyte, inlet mass fraction and velocities of fuel, such as the inlet temperature of the fuel and air have been studied. The analysis indicates that:

- Numerical predictions of fuel cell behavior are strongly influenced by the change of the electrolyte thickness and inlet temperatures adopted in the model. These variations are directly related to the ohmic losses: if a thinner thickness of the electrolyte and higher inlet temperatures are adopted, the model predicts lower ohmic losses due to the ion conductivity reduction.

- Considering the results obtained changing the inlet mass fraction and inlet velocities of fuel, it could be expected that the concentration of the fuel was a determinant factor, however is almost negligible. Therefore, in comparison with the variability of the thickness of the electrolyte and inlet temperatures, no significant results were obtained in the performance of the fuel cell.

- As a result, from this analysis it can be stated that the decisions on the design improvement are significantly affected by the inlet temperature and the electrolyte thickness, which must be carefully selected.

References