Numerical Simulation of Solid Oxide Fuel Cell: 
Mesh Sensitivity Analysis

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Abstract

Due to environmental problem from using energy and the fuel fossil is dramatic decreasing from human usage. The alternative renewal energy is maybe the solution. Solid oxide fuel cell is a fuel cell normally using yttrium stabilized zirconia (YSZ). The cost for this fuel cell is now very expensive. Therefore, the mathematical simulation is crucial. Governing equations consist of Maxwell - Stefan equations for chemical transport, current balance equations, and Brinkman equations for flow in porous media. The numerical simulation is then solved with appropriate boundary conditions. However, the verification of the solution is very important. In this research, the mesh sensitivity analysis is performed. The results show that the solutions from three different mesh are closed to each others. It is indicated that the solutions corresponding to mesh sensitivity analysis.

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Keywords: Mathematical Simulation, Mesh Sensitivity Analysis, Solid Oxide Fuel Cell

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1 Introduction

Due to global warming and limitation of fossil fuel, alternative energy is crucial. Fuel cell maybe a solution of this problem because it is produces almost no pollution. A fuel cell is a device that can convert fuel directly into electricity using chemical energy. The fuel cell will produce electricity as long as fuel is supplied. Solid oxide fuel cells (SOFCs) offer great flexibility in the choice of fuels; not only pure hydrogen, but also many reformate composition consisting of multi-component species maybe used as fuel, such as water ($H_2O$), carbon-monoxide ($CO$), carbondioxide ($CO_2$), including biofuel. The planar design of SOFCs has the higher power density and simplicity in manufacturing than the tubular design [3, 4, 5]. Therefore, the planar SOFCs are widely used in both small and large scale applications.

Over the last decade, the number of research in solid oxide fuel has been carried out with various investigation [2, 6, 7] . In 2006, Bove and Ubertini [1] investigated the phenomena in each component of solid oxide fuel cell using a three-dimensional, time-dependent numerical model. The results show that the boundary conditions affect the accuracy of the model and represent a significant part of the computation. In 2011, Meng Ni [5] developed a two dimension thermo-electrochemical model to studied the performance of planar solid oxide fuel cells fed ammonia by using a two dimensional computational fluid dynamics model with an electrochemical model and a chemical model. The result indicates that ammonia in the solid oxide fuel cell impacts the electric output and temperature field. Recently, numerical simulation of porous solid oxide fuel cell was carried out to solve the carbon deposition problem of solid oxide fuel cells using comsol multiphysics commercial software. The modeling result are valid with experiments [8]. However, the studied in mathematical modeling for the solid oxide fuel cell is still crucial due to demand of developing the performance of solid oxide fuel cell because of the cost of experiments. Thus, in this work, the mathematical modeling of planar solid oxide fuel cell is investigated. Moreover, the mesh analysis is performed to show the effect of mesh quality on numerical results of the model.

2 Mathematical Model

Solid oxide fuel cells normally produced electrical power by added cells into the stack. To model the solid oxide fuel cell, a single cell solid oxide fuel as shown in figure 1 is assumed to produce a unit of electrical power to save time and computational resources. The computational domain is created as shown in the figure 2.
Figure 1: Three dimensional of a single cell planar solid oxide fuel cell.

Figure 2: Configuration of a unit cell solid oxide fuel cell; anode flow channel ($\Omega_1$), anode electrode ($\Omega_2$), electrolyte ($\Omega_3$), cathode electrode ($\Omega_4$), and cathode flow channel ($\Omega_5$).
2.1 Governing Equations

The governing equations consist of Maxwell-Stefan equations for chemical transport as shown in equation (1)

$$\frac{\partial}{\partial t} (\rho c_i) + \nabla \cdot (\rho c_i u) = -\nabla \cdot j_i + R_i$$

where, $\rho$ (kg/m$^3$) is the mixture density, $u$ (m/s) is the mass average velocity of the mixture, $c_i$ is the mass fraction, $j_i$ (kg/(m$^2$s)) is the mass flux relative to the mass average velocity, and $R_i$ (kg/(m$^3$s)) is the rate expression describing its production or consumption.

The current balance in the electrolyte is governed by

$$\nabla \cdot J = Q, \quad \text{in } \Omega_2, \Omega_3, \Omega_4$$

where $J$ denotes the current density vector in the electrolyte, $Q$ can be any source or sink. Navier-Stokes equations for describing the flow in open regions, and the Brinkman equations for the flow in porous regions are shown in equations (3)-(6).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u_c) = 0,$$  

$$\rho \frac{\partial u_c}{\partial t} + \rho (u_c \cdot \nabla) u_c = \nabla \cdot \left[ -p_c I + \mu \left( \nabla u_c + (\nabla u_c)^T \right) - \frac{2}{3} \mu (\nabla \cdot u_c) I \right] + F,$$  

$$\frac{\partial (\epsilon_p \rho)}{\partial t} + \nabla \cdot (\rho u_c) = Q_{br}$$  

$$\rho \left( \frac{\partial u_c}{\partial t} + (u_c \cdot \nabla) \frac{u_c}{\epsilon_p} \right) = \nabla \cdot \left[ -p_c I + \frac{\mu}{\epsilon_p} \left( \nabla u_c + (\nabla u_c)^T \right) - \frac{2\mu}{3\epsilon_p} (\nabla \cdot u_c) I \right]$$

$$- \left( \frac{\mu}{\kappa_{br}} + \beta_F |u_c| + \frac{Q_{br}}{\epsilon_p^2} \right) u_c + F$$

where $\mu$ (kg/(m·s)) is the dynamic viscosity, $u_c$ (m/s) is the velocity vector, $\rho$ (kg/m$^3$) is the density, $p_c$ (Pa) is the pressure, $\epsilon_p$ is the porosity, $\kappa_p$ (m$^2$) is the permeability of the porous medium, and $Q_{br}$ (kg/(m$^3$·s)) is a mass source or sink. $\beta_F |u_c| u_c$ is viscous force proportional to the square of the fluid velocity where $\beta_F$ is the Forchheimer drag option (kg/m$^4$).
2.2 Boundary Conditions

The fuel feed in the cathode and anode is counterflow, with hydrogen-rich anode gas entering from the left. For the ionic charge balance equations in cathode electrode, electrolyte, and anode electrode, the insulating boundary condition is applied on all external boundaries as shown below.

\[-n \cdot J = 0.\]  \hspace{1cm} (7)

For the transport of species in anode, initial mass fraction \((\omega_{h_2}) 0.4\) is used at the left of the anode flow channel. The outflow is at the right of the anode flow channel. No flux boundary condition is applied to all external boundaries of the anode electrode and the anode flow channel as given below.

\[-n \cdot (j_i + \rho u \omega_i) = 0.\]  \hspace{1cm} (8)

3 Numerical Results

There are 3 different mesh as shown in Figure 3. The numerical solutions of the fully couple equations (1) - (6) and all boundary conditions are obtained by Comsol Multiphysics.

![Figure 3: Computational mesh for a unit cell solid oxide fuel cell (a) 2,328 hexahedral elements (b) 144,943 tetrahedral elements (c) 707,828 tetrahedral elements.](image)

Numerical simulation of the hexahedral elements are shown in Figure 4. The results when use different mesh are the same patterns. The values of maximum average current density and maximum average cell power are calculated as shown in Table 1. It is easy to see that time depends on number of elements. Due to the exact solution of the model still undiscovered. The average relative error \(E_a\) is computed using formula as shown in equation
Table 1: Values of average current density, average cell power, and computational time of the different elements mesh.

<table>
<thead>
<tr>
<th>Elements</th>
<th>Average Current Density (A/m²)</th>
<th>Average Cell Power (W/m²)</th>
<th>Computational Time (Minute)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexahedral</td>
<td>2,328</td>
<td>4,567.54257</td>
<td>1,359.39648</td>
</tr>
<tr>
<td>Tetrahedral</td>
<td>144,943</td>
<td>4,869.31055</td>
<td>1,454.31055</td>
</tr>
<tr>
<td>Tetrahedral</td>
<td>707,828</td>
<td>5,411.87402</td>
<td>1,627.57703</td>
</tr>
</tbody>
</table>

(9). The average relative errors of average current density are 7.72%, 1.62%, and 9.34%, respectively. Due to the computational time and average relative errors, the governing equations with hexahedral elements as shown in figure 2 (a) should be used in further investigation of the solid oxide fuel cell.

![Figure 4: Surface plot of the numerical results using 2,328 hexahedral elements (a) oxygen mole fraction (b) hydrogen mole fraction.](image)

\[ E_a = \left| \frac{\text{approximate solution} - \text{average solution}}{\text{average solution}} \right| \]  

(9)

4 Conclusion

From the number of research in alternative renewal energy, solid oxide fuel cell is a kind of clean energy for the future. To investigate the new design or physical property in the cell, mathematical simulation is crucial. The mesh sensitivity analysis is used to make sure that the simulation result is stable. In this paper, three different mesh sizes are investigated with average relative error and computational times. The result show that the hexahedral elements suit for solving the governing equations of the single cell solid oxide fuel cell.
References


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