Implementation of multi-component dusty-gas model for species transport in quasi-three-dimensional numerical analysis of solid oxide fuel cell. Part I: hydrogen fuel

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Abstract. Quasi-three-dimensional numerical model of solid oxide fuel cell, which assumes constant physicochemical properties within the cell components in the thickness direction, typically employs a simple gas diffusion model for species transport in the porous electrodes, such as the Fick’s model. In this study, a three-dimensional grid system is introduced in the anode layer and coupled with the quasi-three-dimensional solid oxide fuel cell model. The multi-component dusty-gas model is implemented to solve the conservation of species on this three-dimensional grid system. The results with the developed model are compared with experimental data obtained under hydrogen fuel. The obtained results show that the dusty-gas model can accurately predict the transport of gas species in the porous anode.

1. Introduction

Solid oxide fuel cell (SOFC) is one of the high-efficiency fuel cells that are operated at high temperatures. It can convert the chemical energy of fuel to electrical energy through electrochemical processes. The performance of an SOFC is strongly related with the transport of mass and species in the channels and porous electrodes, transport of charge carriers in the cell, and transport of thermal energy. A numerical analysis allows researchers to understand such transport phenomena in SOFCs. A quasi-3D numerical model was developed in the authors’ group to study the effect of cell aspect ratio on cell performance [1] and the effects of the air-flow configuration in a short stack [2]. The developed quasi-3D model can be used to analyze the transport of gas species in the streamwise and spanwise directions in the channels. It is also useful for analysis involving significant temperature gradient in the streamwise and spanwise direction and/or various flow configurations of a stack. The developed quasi-3D model applied Fick’s model (FM) for the transport of gas in the porous anode. The species transport in a porous medium can also be expressed by the Stefan–Maxwell model (SMM), dusty-gas model (DGM), or binary-friction model (BFM). The SMM considers the interactions of gas species in a gas mixture [3]. The DGM extends the SMM by considering the Knudsen diffusion, which is important when the pore size of the porous medium is comparable to or smaller than the mean free path of the gas species. The BFM also extends the SMM, which takes into account diffusive slip as well as viscous slip phenomena [4,5] on the porous wall. Vural et al. [6] reported that the BFM requires the most computation time compared to the SMM and DGM. Suwanwarangkul et al. [7] compared the FM, SMM, and DGM in predicting concentration
overpotential in electrodes and recommended the DGM for use in a multi-component system consisting of H2, H2O, CO, and CO2. The DGM can be simplified by assuming either constant pressure gradient [8,9] or linear pressure gradient [10] to reduce the computation cost. However, the simplified DGM with a constant pressure gradient is only applicable to thin porous electrodes. Pisani [11] proposed rewriting the DGM in terms of molar densities instead of molar fractions to express the non-uniform pressure within the porous medium. García-Camprubí and co-authors [12–14] adopted the suggestion by Pisani and rewrote the DGM equation to express the total molar flux of each species in the gas mixture. The advantages of the DGM include the ability to consider an unlimited number of gas species in the mixture, and to capture the non-uniform pressure gradient in the gas mixture.

In this work, we implement a gas diffusion model based on the DGM to the anode in a quasi-3D numerical model by newly introducing a 3D grid system to predict the species transport in the anode. The simulation results are compared to the experimental data from a hydrogen-fueled six-cell stack in reference [1].

2. Numerical modeling

A cell unit consists of top and bottom separators, fuel and air channels, and a positive-electrolyte-negative assembly (PEN) is considered in this study. Each component has only one mesh in the y-axis. Note that both fuel and air channels consist of solid- and fluid-phase meshes. Additionally, two layers of mesh located at the top and bottom of the cell unit are introduced as boundary layers. Hence, a cell unit with a dimension of 89.0 x 3.40 x 60.0 mm3 consists of 101 x 9 x 71 meshes in the quasi-3D model. The unique feature of this study is the introduction of the anode mesh, which is an additional 3D grid system for the anode in the PEN. This additional grid system is solely used in the gas diffusion analysis in the anode. The anode mesh consists of 16 layers with 18 grid points including two grid points for the coupled boundary, which are located at the anode surface and the anode-electrolyte interface. All the anode mesh layers have an equal thickness along the y-axis. The size of the anode mesh in the xz-plane is the same as that of the meshes used in the channels. Values at the coupled boundaries are determined by considering the following data: molar fraction of species \( x \) and total pressure \( P \) from the fuel channel, and molar flux of species \( N_i \) due to the electrochemical reaction at the anode-electrolyte interface. The molar flux of species at the anode surface is evaluated by the implemented DGM model and converted to mass flow rate, and feedbacked to the fuel channel as a mass sink or source term \( S_{yi} \). The electrochemical reaction is assumed to occur at the anode-electrolyte interface to provide the molar flux at the coupled boundary of the anode-electrolyte interface. Note that the FM is applied in the thin porous cathode to reduce the computation cost because no chemical reaction occurs in the cathode. Details of the quasi-3D numerical modeling have already been described in our previous reports [1,2], therefore only essential equations are summarized below.

![Figure 1. Schematic view mesh layers in the y-direction for the quasi-3D model with an anode mesh.](image-url)
2.1. Governing equations

The numerical analysis was based on conservation equations of the mass, momentum, species, and energy.

**Mass conservation:**
\[
\frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho w)}{\partial z} = \sum S_Y
\]  
(1)

**Momentum conservation:**
\[
\begin{aligned}
&\frac{\partial}{\partial x} \left( \frac{\rho u^2}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\rho w^2}{\varepsilon} \right) = -\varepsilon \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{\mu}{\varepsilon} \frac{\partial u}{\partial z} \right) \\
&+ \frac{1}{3} \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial u}{\partial x} \right) - 2 \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial z} \right) - \varepsilon \frac{\mu}{K} \frac{\partial u}{\partial x} - \varepsilon \frac{\mu}{K} \frac{\partial w}{\partial z} + |U| u \\
&+ \frac{\partial}{\partial x} \left( \frac{\rho u w}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\rho w w}{\varepsilon} \right) = -\varepsilon \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial z} \right) \\
&+ \frac{1}{3} \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial x} \right) - 2 \frac{\partial}{\partial x} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\mu}{\varepsilon} \frac{\partial w}{\partial z} \right) - \varepsilon \frac{\mu}{K} \frac{\partial w}{\partial x} - \varepsilon \frac{\mu}{K} \frac{\partial w}{\partial z} + |U| w
\end{aligned}
\]  
(2)

**Energy conservation:**
(Fluid phase in the channels filled with metal foam)
\[
\frac{\partial}{\partial x} \left( \frac{\rho C_{p,m} T_f}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\rho C_{p,m} T_f}{\varepsilon} \right) = \frac{\partial}{\partial x} \left( \frac{\lambda_{f}^e \frac{\partial T_f}{\partial x}}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\lambda_{f}^e \frac{\partial T_f}{\partial z}}{\varepsilon} \right) + h_{nf} a_{nf} (T_s - T_f)
\]  
(4)

(Solid phase in the channels filled with metal foam)
\[
0 = \frac{\partial}{\partial x} \left( \frac{\lambda_{s}^e \frac{\partial T_s}{\partial x}}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\lambda_{s}^e \frac{\partial T_s}{\partial z}}{\varepsilon} \right) + h_{ns} a_{ns} (T_f - T_s)
\]  
(5)

(Solid phases in the separator and the cell)
\[
0 = \frac{\partial}{\partial x} \left( \frac{\lambda_{s}^e \frac{\partial T_s}{\partial x}}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\lambda_{s}^e \frac{\partial T_s}{\partial z}}{\varepsilon} \right) + Q
\]  
(6)

**Species conservation:**
\[
\frac{\partial}{\partial x} \left( \frac{\rho Y_i}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\rho Y_i}{\varepsilon} \right) = \frac{\partial}{\partial x} \left( \frac{\rho D_{i,m} \frac{\partial Y_i}{\partial x}}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\rho D_{i,m} \frac{\partial Y_i}{\partial z}}{\varepsilon} \right) + S_Y
\]  
(7)

**Charge conservation:**
\[
\frac{\partial}{\partial x} \left( \frac{\sigma^e_r \frac{\partial \Phi}{\partial x}}{\varepsilon} \right) + \frac{\partial}{\partial y} \left( \frac{\sigma^e_r \frac{\partial \Phi}{\partial y}}{\varepsilon} \right) + \frac{\partial}{\partial z} \left( \frac{\sigma^e_r \frac{\partial \Phi}{\partial z}}{\varepsilon} \right) = S_\Phi
\]  
(8)

Both fuel and gas channels are filled with the metal foam, which acts as a current collector in the equivalent circuit model [15]. The developed model adopts the geometric parameters representing the porous metal foam in the channels from Bhattacharya et al. [16] and Calmidi and Mahajan [17]. An in-house code is developed and used for the calculations. The grid independence in the quasi-3D model was confirmed by conducting preliminary calculations in our previous works [1,2].

2.2. Species transport in the anode mesh

The anode mesh as shown in Figure 1 is introduced to determine the transport of species in the anode of the SOFC. The multi-component DGM can be expressed in terms of the total flux of species \( i \) as a function of molar densities as follows [14]:
\[
N_i = -I_i^{\text{DGM}} \nabla X_i + v_i^{\text{DGM}} X_i + v_i^{\text{DGM}} X_i,
\]  
(9)

\[
I_i^{\text{DGM}} = \frac{1}{P} \sum_{j=m} \left( \frac{X_i}{D_{i,j}^{\text{eff}}} + \frac{1}{D_{K_i}^{\text{eff}}} \right),
\]  
(10)
where $D_{i,j}^{\text{eff}}$ and $D_{K,i}^{\text{eff}}$ are the effective binary diffusion and the effective Knudsen diffusion coefficient of gas species. The molar flux of species $i$ in the porous medium depends on the three contributors as described in Equation (9). These are, from the left to right, global molecular diffusion, flux due to the pressure gradient, and flux induced by the flux of other species. The species conservation within the anode mesh can be expressed as follows:

\[ \nabla \cdot N_i = S_{x_i}, \]  

where $N_i$ is the molar flux of species $i$ in the porous medium. Equations (13) to (12) are solved implicitly by using Equations. (9) to (12). First, the molar densities of species at the anode surface are calculated from the partial pressure of species in the fuel channel. At the same time, the molar flux of species at the anode-electrolyte interface is determined from the local current density. Then, the pressure gradient, molar densities gradient, and molar densities are used to compute $I_i^{\text{DGM}}, \nu_i^{\text{DGM}},$ and $v_i^{\text{Neff}}$. The species molar source/sink term in Equation (13), within each mesh volume $V$, is associated with the chemical reaction in the anode.

2.3. Calculation conditions

The boundary conditions are given in Table 1. Note that the electric potential difference between the top and bottom separators is the terminal voltage of the stack and is iteratively tuned to achieve a predetermined average current density. Grid independence analysis was conducted for the anode mesh. The results suggest that the 16 layers with 18 grid points for the anode mesh are sufficient.

3. Results and discussion

The numerical results from the developed quasi-3D model implemented with the DGM in this work are compared with the numerical results from our previous work using the FM [1]. Both numerical results are compared with a six-cell short stack experiment conducted under diluted hydrogen fuel at temperatures of 973, 1023, and 1073 K. The details of the short-stack experiment can be found elsewhere [18,19]. The developed model adopts the real microstructure properties of the electrodes quantified by Brus et al. [20,21]. Figure 2 shows the comparison of the current-voltage characteristics.
The prediction of present SOFC numerical model with the implementation of the DGM in the anode is shown by the solid lines while that of the FM is expressed by the dashed lines. No significant difference in the results between the DGM and FM is found. Therefore, the FM appears to be sufficient in the case of hydrogen fuel, as no chemical reaction occurs in the anode.

Figure 2. Comparison of current-voltage characteristics.

4. Conclusions
The multi-component dusty-gas model (DGM) was introduced in the quasi-three-dimensional (quasi-3D) numerical model of solid oxide fuel cell (SOFC) with the aids of anode mesh to predict species transport in the anode. The SOFC numerical model with the DGM was successfully validated with experimental results from a six-cell stack fueled with hydrogen. The developed model with the DGM was able to qualitatively capture the trends observed in the experiment.

Acknowledgments
This work was partially supported under “Fundamental study on rapid evaluation method of SOFC durability” by the New Energy and Industrial Technology Organization (NEDO, Japan), and by the Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Energy Carrier” (Funding agency: JST).

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