Thermo-fluidic characteristics of open cell metal foam for use as anodes in DCFCs, part II: Triple phase boundary generation of metal foam

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ABSTRACT

In the present study, metal foam is used as the anode of a direct coal fuel cell (DCFC) system. A discrete element method-computational fluid dynamics (DEM-CFD) approach is used to assess the effects of the porous metal and particle diameter on the development of a triple phase boundary (TPB) between the coal, electrolyte, and anode. DEM-CFD analyses are conducted with various diameters of particles ranging from 10 to 350 μm. It is found that the number of contacts between the particles and metal ligaments decreases with increases in the particle size; however, the contact number increases after it passes a minimum number. The minimum number of contacts appears to increase as the pore size increases. Based on these results, an operable region map is developed that demonstrates the relationship between the particle size and pore size of porous metals.
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Introduction

A direct coal fuel cell (DCFC) produces electricity based on the electrochemical reaction at the triple phase boundary (TPB) of the coal, electrolyte, and anode. The electricity is directly produced from the chemical energy in the carbon fuel without gasification [1–3]. In addition, the DCFC system has good compactness because it has a high energy density of solid carbon [4]. Metal foam and porous metal are good candidates for the anode of the DCFC system because they aid in the development of a large TPB. Metal foam is able to provide good performance with enhanced flow mixing due to the tortuous path of the porous geometry and the high surface area [5]. Because metallic materials have good electrical conductivity and thermal conductivity, metal foam is acceptable as the anode of a DCFC [6–8]. In order to use metal foam as the anode material in a DCFC system, information about the transport characteristics of the carbon fuel-electrolyte mixture in the metal foam are necessary in terms of the pressure drop, heat transfer, and TPB generation [9–11]. Hence, these studies consist of three main components: (i) head loss coefficient of fluids in the porous metal in a low Reynolds number condition, which was investigated previously using experimental methods [12], (ii) convective heat transfer coefficient in the porous metal and fin performance, and (iii) triple phase boundary generation in the porous metal anode. The second component is currently under investigation and the third component is discussed in this paper.

A number of previous studies have proposed the use of porous metal anodes for fuel cell applications in order to increase the contact area between the fuel and the anode [13–16]. Ye et al. [13] demonstrated that the microstructure of porous metal anodes in solid oxide fuel cells could affect the TPB development through surface modifications. Yakabe et al. [14] examined the changes in the gas concentration in porous metal anodes of solid oxide fuel cells (SOFCs). In this study, the gas flow characteristics in porous metal anodes are estimated using Darcy's law, and it is demonstrated that the concentration polarization increases considerably along the fuel flow path at high fuel utilization. Joshi et al. [15] proposed a two-dimensional Lattice Boltzmann method (LBM) model for simulating the gas diffusion properties in complex structures and they evaluated the effect of porosity on TPB development. Izzo et al. [16] proposed a numerical model to understand the gas flow phenomena in SOFCs and to investigate the relationship between the gas concentration and TPB development. Most previous studies concerning TPB development in porous metal anodes have focused on the diffusion of the gaseous fuel in the anode.

There were also studies on transport of particles and their deposition on surface [17–20]. Fan and Ahmadi [17] and Li and Ahmadi [18] used classical turbulence concepts to investigate deposition of solid particles in ducts. Lakghomi et al. [19] investigated the dependence of capture efficiencies on droplet size and gas velocity using CFD. Sauret and Hooman [20] investigated the particle transport and deposition in metal foam heat exchanger using one-way coupling in CFD and particles. It was noted that the particle tend to deposit near both front and rear stagnation points. They explained the former is caused by the higher momentum and direct exposure of the particles on the foam while the latter is caused by the recirculation region behind the foam-wrapped tubes. Previous studies of particle transport and deposition considered the influence of the fluid phase on the particles' motion but did not considered the particle's effect on fluid phase.

A DCFC system generates electric power using the chemical reaction between the electrode and coal particles within an electrolyte at approximately 600 °C. The coal particle size was approximately 75 μm in diameter, which is the commonly used size in thermoelectric power plants. The complicated operation conditions make it difficult to observe the movement of coal particles in the DCFC system. However, it is necessary to determine the behavior of the particles around the electrode in order to optimize the DCFC system and electrode. Considering the abovementioned issues, the present study used CFD incorporated with the discrete element method (DEM) in order to determine the movement of the coal particles in the metal foam electrode. The TPB developed when a static structure of the porous metal anode, continuum fluid of molten carbonate (MC), and discrete object of coal particles simultaneously came into contact with each other. Therefore, the proposed DEM-CFD used a two-way coupled method [21,22] in order to consider the interactions among the porous metal anode, molten carbonate, and carbon particles. More specifically, the proposed model consists of two components: the fluid behavior is described using the Navier–Stokes equation and the movement of solid particles in the system is determined considering the influence of the MC on

the particles' motion, which includes interactions between the particles and working fluid, particle and particle, and particle and wall. The proposed DEM-CFD approach was applied to the assessment of the TPB development in a porous metal anode of a DCFC system. The DEM-CFD was used to analyze the MC flow containing carbon particles in a porous metal and the number of contacts between the porous metal and particles were counted. This number of contacts was assumed to be proportional to the TPB developments.

Computational models

Governing equations for the fluid phase

The Reynolds-averaged Navier–Stokes (RANS) equations were numerically solved for the fluid flow at the computational grid scale level with consideration of the particle phase. Equations (1) and (2) are the mass conservation and momentum conservation equations, respectively, of the RANS formulation in the Cartesian coordinates used in this study, for an unsteady incompressible flow with particle phase terms. The energy equation is not solved in the analysis in this paper.

$$\frac{\partial\left(\alpha\rho_f\right)}{\partial t} + \frac{\partial\left(\alpha\rho_f U_i\right)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial\left(\alpha\rho_f U_i\right)}{\partial t} + \alpha\rho_f U_j\frac{\partial\left(U_j\right)}{\partial x_j} = -\alpha\frac{\partial P}{\partial x_i} - S_p + \alpha\rho_f g + \frac{\partial}{\partial x_i}\left[\alpha\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \alpha\rho_f\overline{u_i u_j}\right], \tag{2}$$

where $\alpha = 1 - ((\sum_{i=1}^{n} V_{pi})/\Delta V)$ is the voidage of the working fluid. U_i, u_i, g, and $\alpha\rho_f\overline{u_i u_j}$ represent the mean velocity, fluctuating velocity component, gravitational acceleration, and Reynolds stress of the fluid phase, respectively. In order to compute the turbulent flows using the RANS equation, it is necessary to use the turbulence models to predict the Reynolds stresses. The Reynolds averaged values and the turbulence effects are represented by the Reynolds stress, which is the last term in equation (2), and they are approximated using the Boussinesq hypothesis:

$$-\rho\overline{u_i u_j} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{2}{3}k\delta_{ij}, \tag{3}$$

where μ_t is the turbulence viscosity, which is modeled using the standard $k - \varepsilon$ that defines the function of turbulence kinetic energy and turbulence dissipation rate as follows:

$$\mu_t = C_\mu\rho_f\frac{k^2}{\varepsilon}, \tag{4}$$

where C_μ is a constant, $C_\mu = 0.09$. The turbulence kinetic energy (k) and turbulence dissipation rate (ε) are represented as follows:

$$\frac{\partial\left(\alpha\rho_f k\right)}{\partial t} + \nabla\cdot\left\{\alpha\rho_f U k\right\} = \nabla\cdot\left[\alpha\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + P_k + P_{kb} - \alpha\rho_f\varepsilon + S_k, \tag{5}$$