Electrochemical performance study of solid oxide fuel cell using lattice Boltzmann method

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A B S T R A C T

A comprehensive numerical model was developed to predict the electrochemical performance of solid oxide fuel cell (SOFC). The multi-component Lattice Boltzmann (LB) model based on kinetic theory for gas mixtures combined with a representative elementary volume (REV) scale LB algorithm based on the Brinkman equation for flows in porous media, the Butler–Volmer equation and Ohm's law were adopted to deal with the concentration, activation and ohmic overpotentials, respectively. The volt–ampere characteristics were calculated and compared with those obtained by the existing electrochemical model, as well as the experimental data. It was shown that the electrochemical model given by this paper was capable of describing the electrochemical performance much more accurately because of the kinetic nature of the LB method which was based on microscopic models and mesoscopic kinetic equations for fluids, and the accurate prediction of multi-component mass transfer in SOFC porous electrodes affected the simulation of the cell electrochemical performance significantly. Moreover, the effects of different electrode geometrical and operating parameters on the cell performance were investigated. The developed electrochemical model based on LB algorithm at REV scale is useful for the design and optimization of SOFC.

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1. Introduction

Solid oxide fuel cell (SOFC), with advantages of high electric efficiency, low pollutant emission, and high operating temperature which allows a variety of cogeneration possibilities and fuel flexibility, is identified as one of the most promising energy conversion devices in future. However, several pressing technological barriers related to energy conversion efficiency, fuel reforming techniques, the use of novel materials, architecture design, and techniques for improved fuel utilization, etc., which may result in high production costs and reduced reliability of SOFC [1,2], still exist to its commercialization. Because the problems concerning single cells have not been totally eradicated, the design and optimization of SOFC stack and relevant thermodynamic systems are caught in a dilemma [3]. The electrochemical characteristics of the single cell are very important for the SOFC design, which directly affect the cell power generation performance, temperature management, etc. and are influenced significantly by the three polarizations

(activation, ohmic and concentration polarization) within electrolyte and electrodes. Statistics show that the vast majority of the published articles about SOFC are devoted to the research about anode, cathode and electrolyte [3].

Numerical simulation is thought to be an important approach to the research of SOFC. The accuracy of overpotential models directly affects the precise simulation of the SOFC electrochemical performance. Generally speaking, Butler–Volmer equation (or Achenbach model) and Ohm's law are usually used to determine the activation and ohmic overpotentials, respectively. However, the research about concentration overpotential is relatively rare, and it is unspecified and not fully resolved in the literature concerning to what degree the mass transfer affects the electrochemical performance of the SOFC [3]. There are three frequently used modeling approaches: (1) concentration overpotential is usually ignored because the gas transport in the electrode is believed to be an efficient process [4–6]; (2) the mass transfer in the porous electrodes is not calculated, and the concentration overpotential is predicted using limiting current density which is usually assumed to be an estimated constant [7,8] or a function with respect to gas concentration, pressure at the gas channel of fuel cell, effective diffusion coefficient, temperature and geometrical structure of

electrodes [9–12]; (3) the mass transfer in the porous electrodes is described by simplified macroscopic models [2,13,14] (extended Fick's model (extended FM), Dusty Gas model (DGM), and Stefan Maxwell model (SMM)), and the concentration overpotential is expressed in terms of the gas concentration difference between the electrodes surface and three phase boundary (TPB) regions. It is clear from our previous research that the concentration over-potential reaches the same order of magnitude as the other two overpotentials for low porosity, low reactant concentrations, and high average current densities [15]. Therefore, the neglect of concentration loss is unreasonable for the fact that the reactant concentration and current density vary sharply along the flow channel of fuel cell, and they achieve the minimum and the maximum at where the electrochemical reaction occurs dramatically, respectively. Meanwhile, the employed limiting current density and aforementioned simplified macroscopic models (extended FM, DGM, and SMM) for concentration overpotential may result in imprecise prediction of the polarization loss of fuel cell because they are not competent to study the gas transport accurately in the porous electrodes at micro- or meso-scale.

The Lattice Boltzmann (LB) method is thought to be an efficient tool for the simulation of multi-component mass transfer in porous anode and cathode. It is deduced from the kinetic theory which makes it capable of solving transport process at micro- or meso-scale. Meanwhile, this algorithm is parallel in nature due to the fact that all the information transfer is local in time and space, so that it is relatively easier to implement and more suitable for the massively parallel computation. Based upon the above mentioned advantages of LB method, several references employed pore scale LB method for the investigation of multi-component gas transport in SOFC porous anode [16–23]. Compared with the pore scale LB model in which detailed geometric information is needed and the computation domain cannot be too large due to limited computer resources, representative elementary volume (REV) scale LB model can be used for systems of larger size and is much more competitive for parametric study. In the researches using REV scale LB method for the multi-component gas transport in porous media [24–29], the majority have adopted single-fluid model employing single-relaxation-time approximation which is restricted to unity Prandtl and Schmidt numbers for the multi-species flow [24–28] or taken the species concentration field as a passive scalar [29]. Nevertheless, the relatively more accurate two-fluid model, which treats mutual collisions and self-collisions independently so that the viscosity and diffusion coefficients can be varied independently by a proper choice of mutual- and self-collision relaxation-time scales, has not been adopted. Furthermore, the REV scale LB model has rarely been applied to the simulation of mass transfer of SOFC electrodes [15].

In our previous research, a two-dimensional (2D) multi-species LB model based on the two-fluid theory coupled with a porous model at REV scale was developed to study the multi-component reactant gases transport in the porous anode and cathode of SOFC, and the prediction of concentration overpotential agree much better with the experimental data compared with those obtained by extended FM, DGM, and SMM, which proves that LB method is a much more accurate method for the simulation of mass transfer within fuel cell electrodes [15]. This paper presents a subsequent investigation of our previous work, in which a comprehensive electrochemical model is established based on the existing LB model developed by our group in Ref. [15] to study the electrochemical characteristics of a planar anode-supported SOFC. The influence of multi-component reactant gas mass transfer on the electrochemical performance of SOFC is investigated. Furthermore, the established model is also applied to discuss the impacts of geometrical and operating parameters on the cell electrochemical performance, which is very useful for the design, optimization and fabrication of SOFC.

2. Mathematical models

Fig. 1 illustrates the schematic of the representative element volume of a planar SOFC which consists of a dense ceramic electrolyte sandwiched between porous anode and cathode. At the cathode, oxygen from the air channel diffuses to the TPB, and receives electrons to be reduced to oxygen ions which pass through the solid oxide electrolyte to the anode. At the anode, hydrogen from the fuel channel diffuses to the TPB, and reacts with the oxygen ions to generate steam and electrons. Finally, the electrons formed in the hydrogen oxidation reaction migrate to the cathode by external circuit to meet the electrical load.

2.1. Conservation equations

Conservation equations for multi-species gas in porous anode and cathode are given as follows.

Continuity equation:

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

Momentum equation:

$$\nabla p = -\frac{\mu}{K}\vec{u} + \mu_e \nabla^2 \vec{u} \tag{2}$$

Species equations:

$$\nabla \cdot J_A = 0 \tag{3}$$

where A represents H_2 or H_2O in the anode, and O_2 or N_2 in the cathode.

In the LB method, Eqs. (1)–(3) are satisfied with calculations of distribution functions by solving the LB equation, which has been introduced in detail in Section 3.

2.2. Electrochemical model

Fig. 2 shows the equivalent circuit model for the calculation of SOFC electrochemical characteristics, from which we have obtained some important equations as summarized in Table 1.
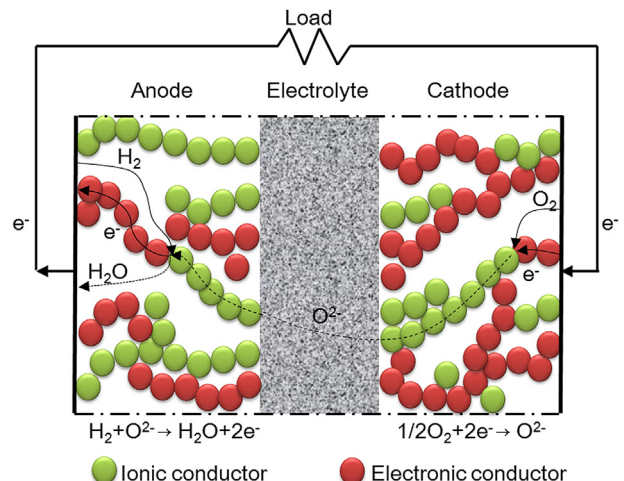

Fig. 1. Schematic of an SOFC representative element volume.