Energy 107 (2016) 295–304

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Pore scale investigation of gaseous mixture flow in porous anode of solid oxide fuel cell

Zheng Dang, Han Xu*

Dept. of Building Environment and Energy Engineering, Xi'an Jiaotong University, Xi'an 710049, China

A R T I C L E I N F O

Article history:
Received 4 October 2015
Received in revised form
19 February 2016
Accepted 4 April 2016
Available online 29 April 2016

Keywords:
Solid oxide fuel cell
Porous anode
Lattice Boltzmann method
Pore scale
Microstructure
Mass transfer

A B S T R A C T

A two-fluid finite-difference LB (Lattice Boltzmann) model is developed for multi-component flow. Then, a pore scale LB model is further developed for multi-component flow in porous media with heterogeneous microstructure. Thus, the present LB model is independent on any structure statistical parameters of the porous media, which is contrary to the numerical methods assuming the porous media is homogeneous. Compared with existing LB models for multi-component flow in the SOFC (solid oxide fuel cell) anode, the present LB model is capable of simulating mixture flow with larger ratios of molecular weights, thus it is qualified to meet the fuel flexibility of the SOFC. By using this model, the mass transfer of gaseous mixture flow in a SOFC anode is studied and the local molar fraction distributions of gaseous mixture are obtained within the irregular porous anode directly. The influences of anode microstructure, dimensionless reaction flux and fuel composition on anode performance are investigated. The quantitative relationship between the porous microstructure and anode performance is obtained.

1. Introduction

SOFC (solid oxide fuel cell) has been considered as one of the most promising power generation devices [1] due to its high electrical efficiency [2] and fuel flexibility [3]. However, the design and manufacture of durable electrodes with high performance is a technological barrier to the commercialization of SOFC [4]. It is crucial to study various transport processes and reactions in electrodes to improve their performance and durability [5]. Notably, the momentum and heat transport in porous electrodes, electronic and ionic transport in electronic and ionic conductors and reaction characteristic at chemical/electrochemical active sites are all significantly affected by the multi-component mass transport existing in pore phase, since it determines the concentration distribution of each species in porous electrodes. Therefore, the multi-component mass transport within porous electrodes plays a key role in cell performance, especially at high current densities [6], and a detailed understanding of multi-component mass transport is the fundamental of establishing a comprehensive mathematical model of SOFC.

Concentration overpotential is often employed to describe mass transport-related losses of SOFC electrodes. The concentration overpotential of cathode is negligible compared to that of anode [7]. Moreover, when hydrocarbon fuel is adopted, the transport processes and reactions in the anode are much more complicated and important than that in the cathode [8,9]. Consequently, plenty of works have been devoted to the performance improvement of SOFC anodes [10,11].

SOFC anodes are usually porous microstructures with submicron-sized pores, the heterogeneity of which significantly affects the performance and durability of anodes. It is important to find the quantitative relationship between the anode microstructure and its performance [12]. Due to the limitation of expensive equipment and measuring techniques, it is difficult to obtain distributions of related physical quantities in the heterogeneous porous anodes by experiments under high temperature conditions. In contrast, numerical simulation is a competent alternative. The extended FM (extended Fick's model), SMM (Stefan–Maxwell model) and DGM (dusty-gas model) are extensively employed to simulate the mass transport in previous studies of SOFC [13–16]. However, they are not qualified to simulate the gas transport in the porous anode at micro/meso-scale. Moreover, in these models, the heterogeneity of the electrode microstructure is neglected and hence structure statistical parameters and flow empirical relations have to be employed, which extremely limits their applications.

---

* Corresponding author.
E-mail address: xuhanxh@mail.xjtu.edu.cn (H. Xu).

http://dx.doi.org/10.1016/j.energy.2016.04.015
0360-5442/

To fully understand the mass transport in porous anodes, modeling methods considering the micro/meso-scale effect and the microstructure heterogeneity are required, which are usually named as pore scale modeling methods. LB (Lattice Boltzmann) method is thought to be a qualified candidate, since it is deduced from kinetic theory and hence is capable of solving transport processes at micro/meso-scale. Besides, it is very competitive for modeling the mass transport in complex geometries, such as porous structures, because of the simple bounce-back rule for no-slip boundary condition. Several studies have adopted various pore scale LB models to investigate the mass transport in SOFC anodes [17–21]. However, all these models suffer the drawbacks of the existing multi-component LB models. Some of them have adopted single-fluid LB model employing single relaxation time which is restricted to unity Prandtl and Schmidt numbers for the multi-species flow [17,18]. Others have adopted a relatively more accurate two-fluid LB model [19–21], in which viscosity and diffusion coefficients can be varied independently by changing the cross- and self-collision relaxation times and hence variable Prandtl and Schmidt numbers can be considered. However, the maximum ratio of molecular weights that can be accurately simulated by this two-fluid LB model is limited to be below 9 [22], which undoubtedly limits the applicability of this model and cannot simulate the transport processes in SOFCs fed by other common fuels.

In our previous study [6,23], a coupled LB model was developed to simulate the mass transport in porous anode, which employed the LB model proposed by McCracken and Abraham [22] for multi-component flow and a REV (representative elementary volume) scale LB algorithm based on the Brinkman equation for flows in porous media, and this model is proved to be more accurate than extended FM, SMM and DGM. In present study, a new multi-component LB model extending the applicability of model developed by McCracken and Abraham [22] to mixture flow with ratio of molecular weights above 9 is established, which is not only based on two-fluid theory, but also capable of meeting the fuel flexibility of the SOFC. Moreover, a pore scale LB model is further developed based on the heterogeneous microstructure of a porous anode to investigate the multi-component mass transport in an SOFC anode, so as to investigate the quantitative relationship between the porous microstructure and anode performance. Furthermore, the influences of anode microstructure, dimensionless reaction flux and fuel composition on anode performance are discussed in terms of local concentration distributions, molar fraction of reactive gas along the primary mass transport direction and concentration overpotential.

2. Lattice Boltzmann model

2.1. General description

The transport processes and electrochemical reactions in the SOFC anode are illustrated thoroughly in Ref. [23]. As shown in Fig. 1(a), hydrogen from the fuel channel diffuses to the TPB (three phase boundary), i.e., the interface among electronic conductor, ionic conductor and gas species, then reacts with the oxygen ion diffusing from the electrolyte to generate steam and electrons (Eq. (1)). Finally, the electrons formed in the hydrogen oxidation reaction are collected by the current collector and migrate to the cathode via external circuit to meet the electrical load.

$$H_{2(TPB)} + O^{2-}{}_{(TPB)} \rightarrow H_2O_{(TPB)} + 2e^- \tag{1}$$

The anode is usually a porous cermet composed of electronic conductor and ionic conductor. An SEM (scanning electron microscope) image of the microstructure of an SOFC anode made up of Ni and SSZ (scandium stabilized zirconia) is presented in Fig. 1(b). By binarization processing, a binary image of the anode microstructure is then obtained (Fig. 1(c)). Higher contrast between the solid and pore phases is obtained in Fig. 1(c) compared with Fig. 1(b), which is used as the geometric input condition of the pore scale simulation. The imaging and description of the porous anode microstructure will be introduced in Sec.2.3 in detail.

Since the present study is mainly focused on the multi-component mass transport in the anode, the anode/electrolyte interface is assumed to be the TPB for simplicity, which is commonly employed in relevant literatures [24–26]. The relevant physical model and boundary conditions are presented in Fig. 2. At the fuel channel/anode interface (i.e., $x = 0$), the mixture total concentration and molar fraction of each species are specified by Eq. (2),

$$c_{\mathrm{m,bulk}} = c_{\mathrm{T}} \cdot y_{\mathrm{m,bulk}} \tag{2}$$

where m represents the m$^{\mathrm{th}}$ species, c is the molar concentration, c_{T} is the total molar concentration of mixture and y is the molar fraction. At the anode/electrolyte interface (i.e., $x = \mathrm{L}$), the molar flux of each species is specified by Eq. (3) based on the current drawn by the SOFC,

$$J_{H_2} = \frac{i}{2F}, \; J_{H_2O} = -J_{H_2} \tag{3}$$

where J and i are molar flux and average current density at TPB, respectively. Since the thickness of the anode is far less than the length of the cell and this paper primarily focuses on the mass transport along the thickness of electrodes (x direction), periodic boundaries in Eq. (4) are employed at both top and bottom of the computational domain and a reasonable height H is adopted to provide a realistic representation of the porous anode,

$$\psi_{\mathrm{m}}|_{z=0} = \psi_{\mathrm{m}}|_{z=\mathrm{H}} \tag{4}$$

where ψ represents the relevant physical quantity. The solid obstacles are impermeable and no-slip boundary conditions are applied at the obstacle surfaces, thus,

$$\frac{\partial c_{\mathrm{m}}}{\partial \boldsymbol{n}} = 0 \tag{5}$$

where $\boldsymbol{n}$ is the unit normal perpendicular to obstacle surfaces.

The concentration overpotential of the anode is described as

$$\eta_{\mathrm{con}} = -\frac{RT}{2F} \ln\left(\frac{y_{H_2,\mathrm{A/E}}\, y_{H_2O,\mathrm{bulk}}}{y_{H_2,\mathrm{bulk}}\, y_{H_2O,\mathrm{A/E}}}\right) \tag{6}$$

2.2. LB model for multi-component flow

LB methods describe the fluid flow at each lattice point of a numerical grid by two steps: streaming and collision. In the streaming step, particles move along specified lattice directions; in the collision step, particles of the same or of different species interact with each other as they arrive at the lattice point from neighboring points. The Boltzmann equation for a binary system based on the two-fluid theory is as follows (taking the σ^{th} species as an example)