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Hydrophilicity effect on micro-scale flow of μDMFC

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ABSTRACT

The effective removal of carbon dioxide (CO_2) in the anode micro channels is critical to the performance of the micro direct methanol fuel cell (μDMFC). A Lattice-Boltzmann model coupled with liquid–gas surface tension, fluid–solid interaction and buoyancy force is adopted in this work to simulate the two-component flow with different hydrophilicity channels. The simulation results show that the emission speed of CO_2 gas in the cell patterned with the hydrophilic channel wall is faster than that with the hydrophobic wall. In order to mutually validate the simulation results, a μDMFC with an active area of 1.0 cm^2 is designed, fabricated, and tested. Data results show that with improved gas expelling and fuel supplying, the novel μDMFC with the hydrophilic flow field gets an increase of 15.7% in peak power density and a dramatically lowered polarization at high current density output.

1. Introduction

μDMFC is an ideal candidate for portable applications due to its high efficiency, simplicity and environmentally friendly [1,2]. But when its size comes to micro scale level, CO_2 bubbles will take up more than half of the anode flow field area when operated at high current density, which brings a strong concentration polarization and thus decreases the cell performance. Therefore, the removal of CO_2 in the anode micro channels is critical due to the fact that bubbles hinder the methanol mass transport from flow field to catalyst/diffusion layer [3].

The fluid motion in the channel is a three dimensional complex phenomenon coupled with time variation and nonlinear characteristics. The common continuous models which used to resolve two-phase transport of micro flows has to make many assumptions and simplifications. The novel mesoscopic kinetic models focus on the speed distribution function of the fluid molecules, and characteristics of microscopic flow can be resolved by researching time-space evolution and the relationship between microscopic physical quantities and distribution functions. So this method can solve the micro flow transport accurately [4–6]. Fei and Hong [7] presented an all-angle Lattice-Boltzmann model to simulate the two-phase (gas and liquid), two-component (CO_2 bubble in methanol solution) flow. A micro channel with blocks on both sides of the wall was intended to simulate the critical gap of the flow channel in the porous diffusion layer.

This work investigated the CO_2 bubble dynamics in micro fluidics of a μDMFC from the microscopic perspective. The hydrophilicity of channel wall surface was conducted, and results of the simulation based on Lattice-Boltzmann method exhibited a better cell performance because of the improved CO_2 expelling and fuel supply. A comparison test was carried out to verify the simulation results. Polarization test results showed that the hydrophilic flow field indeed enhanced the power density output at high current density.

2. Modeling and simulation

Solid, liquid and gas interfacial interaction has a complex gas–liquid two-phase dynamic behavior in the anode channel of μDMFC. Most of the dynamic behaviors can be elaborated in micro scale level by modeling and simulation. Considering most of the actual operating situation, the method of Lattice-Boltzmann is applied in the modeling and simulation.

There are two steps in the method of Lattice-Boltzmann analyses: collision and propagation.

$$\text{Collision}: f_i'(x,t) = f_i(x,t) + \Omega_i(f(x,t)) \quad (1)$$

$$\text{Propagation}: f_i(x + c_i\delta_t, t + \delta_t) = f_i'(x,t) \quad (2)$$

where $f_i(x,t)$ is the distribution function of the particle with velocity $\vec{e_i}$ at position x and time t, Ω_i is the collision function, and δ_t represents the time increment.

The boundary conditions are associated with the adjacent grid points and all the calculation of the collision is localized because

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of the migration step. Typical Lattice-Boltzmann simulation includes a discrete-velocity model, equilibrium distribution functions and evolution equation of the distribution functions, which can be shown as follows:

$$f_i(\vec{X}+\vec{e_i}\delta_t, t+\delta_t) - f_i(\vec{X}, t) = -\frac{1}{\tau}[f_i(\vec{X}, t) - f_i^{(eq)}(X, t)] + \delta_t F_i \quad (3)$$

where τ represents dimensionless collision relaxation time, and $f_i^{(eq)}(X, t)$ represents the equilibrium distribution function.

In this paper, the D_2Q_9 model was used to simulate the anode multiphase flow of the μDMFC, and the repeat unit of the model was shown in Fig. 1. In this model, there is a nine-point lattice model in two-dimensional space and a stationary particle on each node. The model unit has 9 lattice speeds, in which speed with $i = 0$ represents static particle. Speeds with $i = 1$–8 represent other 8 speed directions.

Speeds in the D_2Q_9 model can be described as follows:

$$e_i = \begin{cases} (0,0) & i = 0 \\ e\left[\cos\frac{(i-1)\pi}{2}, \sin\frac{(i-1)\pi}{2}\right] & i = 1,2,3,4 \\ \sqrt{2}e\left[\cos\frac{(2i-9)\pi}{4}, \sin\frac{(2i-9)\pi}{4}\right] & i = 5,6,7,8 \end{cases} \quad (4)$$

The function of equilibrium distribution can be expressed as:

$$f_i^{(eq)} = \frac{4}{9}\rho\left[1 - \frac{3}{2}\frac{U^2}{e^2}\right] \quad i = 0 \quad (5)$$

$$f_i^{(eq)} = \frac{1}{9}\rho\left[1 - 3\frac{e_i \cdot U}{e^2} + \frac{9}{2}\frac{(e_i \cdot U)e^2}{e^4} - \frac{3}{2}\frac{U^2}{e^2}\right] \quad i = 1,2,3,4 \quad (6)$$

$$f_i^{(eq)} = \frac{1}{36}\rho\left[1 + 3\frac{e_i \cdot U}{e^2} + \frac{9}{2}\frac{(e_i \cdot U)e^2}{e^4} - \frac{3}{2}\frac{U^2}{e^2}\right] \quad i = 5,6,7,8 \quad (7)$$

where U is the particle velocity vector, which can be decomposed into the x and y directions, and ρ is the macroscopic physical quantity density of the lattice fluid in each direction. The unit volume momentum can be expressed as:

$$\rho^\sigma(X, t) = \sum_r f_i^\sigma(X, t) \quad (8)$$

$$\vec{u} = \frac{\vec{v}}{c_0 + \sqrt{c_0^2 + c_1|\vec{v}|}} \quad (9)$$

$$\rho^\sigma(X, t)U^\sigma(X, t) = \sum_i f_i^\sigma(X, t)e_i + F_{total}^\sigma(X, t) \quad (10)$$

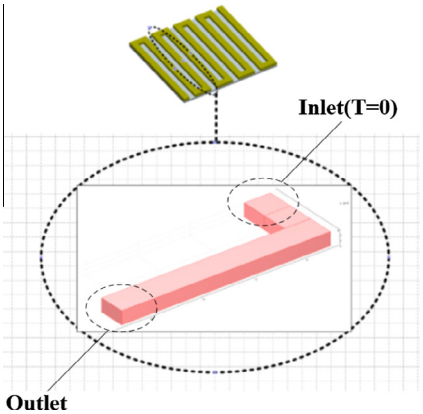

Fig. 1. Simulation domain of the model.

In which $\vec{v}$ can be expressed as:

$$\rho v = \sum_i \vec{e_i} f_i + \frac{\delta_t}{2}\varepsilon\rho\vec{G} \quad (11)$$

c_0 and c_1 in the Eq. (9) can be expressed as:

$$c_0 = \left(1 + \varepsilon\frac{\varepsilon_t}{2}\frac{v}{K}\right) \quad c_1 = \varepsilon\frac{\varepsilon_t}{2}\frac{F_\varepsilon}{\sqrt{K}} \quad (12)$$

Superscripts of the formula (8) represent the different compositions, which are methanol solution and CO_2 bubbles respectively.

Indeed, there should be many external forces in the momentum equation. Surface tension, fluid–solid interaction and buoyancy force are the key forces of the external forces. Therefore, the external $F_{total}^\sigma(X, t)$ in Eq. (10) can be expressed as:

$$F_{total}^\sigma(X, t) = F_{surface\ tension}^\sigma(X, t) + F_{solid}^\sigma(X, t) + F_{buoyancy}^\sigma(X, t) \quad (13)$$

The force from the surface tension can be expressed as:

$$F_{surface\ tension}^\sigma(X, t) = -\tau^\sigma\left[\psi^\sigma(X, t)\sum_{\sigma'} G^{\sigma\sigma'}\sum_i \psi^{\sigma'}(X + e_i\Delta t, t)e_i\right] \quad (14)$$

where $\psi^\sigma(X,t)$ is the function of the position vector and time, which can be expressed as $\psi^\sigma(X,t) = A\exp(-\rho_0/\rho)$.

The collision between methanol solution and the inner wall of micro channel can be expressed as:

$$F_{solid}^\sigma(X, t) = -\rho^\sigma(X, t)\sum_i G_i^\sigma s(X + e_i\Delta t)e_i \quad (15)$$

where G^σ represents solid–liquid relative station parameter, which is proportional to the solid–liquid contact angle. And $s = 0$ or $s = 1$ represents liquid particles or solid–liquid contact surface particles respectively.

The buoyancy in the expression comes from the density difference between the poly-phase components, which can be expressed as:

$$F_{buoyancy}^\sigma(X, t) = g\sum_i \rho^\sigma(X + e_i\Delta t, t)e_i \quad (16)$$

In which g represents the non-dimensional gravitational constant and ρ^σ represents the density of the specie σ. The direction of buoyancy in the effective simulation domain is vertically upward. When the bubble moved to the horizontal channel, the effect of buoyancy made the CO_2 contact with the upper wall, and the hydrophobic properties of channel decreased the gas velocity. When the bubble moved to the vertical channel, the effect of buoyancy made a reverse influence on the CO_2 emission.

Fig. 2(a) and (b) illustrate inlet and boundary conditions respectively in this model. In Fig. 2(a), the solid lines and dotted lines represent the known diffusion equations (f_0, f_1, f_3, f_4, f_7 and f_8) and the unknown ones (f_2, f_5 and f_6) respectively. The bounce-back assumes that the particle velocity is equal and opposite after collision with the wall. The relationship can be expressed as follows coupled the unknown velocity vectors, the known ones and the inlet condition:

$$f_2 + f_5 + f_6 = \rho_{in} - (f_0 + f_1 + f_3 + f_4 + f_7 + f_8) \quad (17)$$

$$e(f_2 + f_5 + f_6) = \rho_{in}v + e(f_4 + f_7 + f_8) \quad (18)$$

$$f_5 - f_6 = -f_1 + f_3 + f_7 - f_8 \quad (19)$$

where ρ_{in} represents the inlet methanol density and the vertical component of the velocity is zero.

In the boundary setting of Fig. 2(b), using bounce-back boundary condition to represent no-slip boundary condition, take the upper channel wall as the example, the unknown functions f_4, f_7 and f_8 could be calculated by given functions f_2, f_5 and f_6