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Numerical modeling of liquid–gas two-phase flow and heat transfer in reconstructed porous media at pore scale

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ABSTRACT

The complicated multiphase flow in porous media is one important issue in the field of energy utilization. This work performed the pore-scale lattice Boltzmann modeling and simulation of liquid–gas two-phase fluid transport phenomena within porous domain. The three-dimensional porous structure was numerically reconstructed with high-resolution CT scan images. The flow and thermal parameters in porous spaces were obtained under the conditions of different contact angles. The liquid water in the porous domain with hydrophilic solid surface reaches the equilibrium state more quickly compared to that in hydrophobic one. The numerical approach established in this paper can provide detailed information of the multiphase fluid transport characteristics in complex porous media.

Introduction

The complicated multiphase flow in complex porous media is one important issue in energy utilization, in which one of challenges is how to predict the multiphase fluid flow and heat transfer processes within pore spaces [1–4]. In recent years, the application of fuel cell has attracted more and more attentions, which is one kind of hydrogen energy utilization with electrochemical conversion. The water management is the critical technique in PEM fuel cell application [5,6]. The water produced in the gas diffusion layer (GDL), which is one type of porous media, should be removed to achieve continuous operation for the fuel cell [7]. The removal of the produced water and the transport of reactant gas in porous GDL are considered as the liquid–gas flow phenomena in porous media. In the work of Jo and Kim [8], the simulation of liquid water moving from the surface pores into a rectangular channel in a PEM fuel cell was carried out with the VOF method. The results show that droplet movement is along the side walls and the lower edges, and droplets from the center pore move with a complex behavior as the wall surface is hydrophobic. In the work of Ben Amara and Ben Nasrallah [9], the droplet movement in a microchannel was predicted with a numerical approach. The droplet shape was observed for different capillary numbers and contact angles, which shows that hydrophobic boundary condition is better for droplets evacuation compared to the hydrophilic one. In the above work, the computational domain was a rectangular channel and related two-phase flow characteristic was obtained in the simple flow domain.

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As the gas diffusion layer is actually one type of porous media, the liquid–gas two-phase fluid in this complex porous media will show different flow characteristics compared to that in the domain with simplified geometry. The continuum models was normally used to calculate the flow process in porous structures relevant for fuel cells [7]. Another available approach was to develop the pore-network method to predict two-phase flow in porous domain [10,11]. For both continuum modeling and pore-network modeling, the relations among different flow parameters have to be determined with experimental or analytical method before establishing the numerical models, which is time consuming or only applicable for the porous media with simple geometry. One innovative numerical approach, which has been developed in recent ten years, is pore-scale modeling. The pore-scale modeling has been proved to be one promising technique to derive the accurate relations among different flow parameters [12–14]. The VOF model has been considered as an available tool for the immiscible two-phase flow simulation [15–17]. Park et al. [18] adopted finite volume method (FVM) with VOF to predict the unsteady water–air flow in GDL and the fibrous structure was presented by simplified solid cylinders, which were randomly arranged in the computational domain. As the flow domain becomes more complicated, the lattice Boltzmann method (LBM) is considered as one suitable approach. In the work of Xuan et al. [19], the quartet structure generation set was introduced for constructing irregular solid structure of porous wick and LBM was adopted to simulate the transport phenomena in the wick. Hao and Cheng performed pore-scale numerical simulation of liquid–gas flow in porous media with the free energy multiphase LBM, in which the stochastic generation method was adopted to reconstruct fibrous porous media [20]. The porous structure has a significant influence on the flow characteristic in the pore spaces, which means the reconstruction of realistic porous structure can lead to the accurate flow prediction in porous medium.

The reconstruction of porous media with micro-tomography images has been developed rapidly in recent years, in which the porous samples need to be scanned with micro CT equipment [14,21]. Raeini et al. [22] investigated the influence of pore-scale forces on two-phase flow using scan images of porous media with FVM method. Landry et al. [23] presented CT scan images of drainage in porous medium and the oil displacement was simulated with LBM model. In the previous work, the study of the liquid–gas flow in the reconstructed porous medium was performed with a numerical approach. The complex pore spaces are occupied by fluid with different phases. As there is a significant difference in the physical properties of liquid and gas, the velocity and temperature distributions vary differently in liquid and gas phases. But few studies on the flow and thermal characteristics of liquid–gas two-phase fluid in reconstructed porous medium have been reported in open literature till now.

This paper presents the pore-scale modeling and prediction of liquid–gas two-phase transport phenomena in reconstructed porous medium with the LB method. The three-dimensional realistic porous domain was reconstructed with micro CT equipment. The numerical simulations were carried out under the conditions of different contact angles, and the flow and thermal parameters in porous spaces were obtained. The numerical approach proposed in this work can be extended to provide detailed information for multiphase transport modeling in complex porous media at field scale.

Numerical model

The numerical simulation was performed with the LB method, which adopted a double-population function to consider flow and heat transfer phenomena, which included a Shan-Chen multiphase model for the two-phase flow [24,25]. The D3G15 flow LB model was adopted to predict the multiphase flow and the D3Q6 thermal LB model was used to calculate the heat transfer process. The lattice velocity descriptions of D3G15 and D3Q6 models can be found in Fig. 1.

The probability of a particle at a velocity of ξ is introduced as particle distribution function $f(t,\mathbf{x},\xi)$, and the related Boltzmann equation can be used to describe its evolution:

$$\frac{\partial f(t,\mathbf{x},\xi)}{\partial t}+\xi\cdot\frac{\partial f(t,\mathbf{x},\xi)}{\partial \mathbf{x}}=\Omega \tag{1}$$

Ω is the collision operator. And Eq. (1) can be simplified with the directional particle velocities $\boldsymbol{e}_\alpha$:

$$\frac{\partial f_\alpha(t,\mathbf{x})}{\partial t}+\boldsymbol{e}_\alpha\cdot\frac{\partial f_\alpha(t,\mathbf{x})}{\partial \mathbf{x}}=\Omega_\alpha \tag{2}$$

$\alpha = 0, \ldots, 14$. In D3Q15 model for fluid flow, fourteen particle velocities are in the direction towards neighboring nodes and one particle velocity is zero. The above equation is then discretized (in both time and space) and the LB equation can be described as:

$$f_\alpha(t+\Delta t,\mathbf{x}+c\boldsymbol{e}_\alpha\Delta t)-f_\alpha(t,\mathbf{x})=-\frac{1}{\tau_v}\left(f_\alpha(t,\mathbf{x})-f_\alpha^{eq}(t,\mathbf{x})\right) \tag{3}$$

τ_v is the velocity relaxation time and c is node spacing $\Delta\mathbf{x}$ divided by time step Δt. f_α^{eq} is the equilibrium distribution function:

$$f_\alpha^{eq}(t,\mathbf{x})=\begin{cases}-4\sigma\dfrac{p}{c^2}+s_0(\mathbf{V}) & (i=0)\\ \lambda\dfrac{p}{c^2}+s_\alpha(\mathbf{V}) & (i=1-6)\\ \gamma\dfrac{p}{c^2}+s_\alpha(\mathbf{V}) & (i=7-14)\end{cases} \tag{4}$$

In Eq. (4), $s_\alpha(\mathbf{V})$ can be calculated by:

$$s_\alpha(\mathbf{V})=\omega_\alpha\left[\frac{c\boldsymbol{e}_\alpha\cdot\mathbf{V}}{c_s^2}+\frac{(c\boldsymbol{e}_\alpha\cdot\mathbf{V})^2}{2c_s^4}-\frac{|\mathbf{V}|^2}{2c_s^2}\right] \tag{5}$$

where $\omega_0 = 2/9$, $\omega_\alpha = 1/9$ for $\alpha = 1–6$, $\omega_\alpha = 1/71$ for $\alpha = 7–14$, and the pseudo sound speed $c_s=\sqrt{1/3}c$. And σ, λ and γ in Eq. (4) can be determined by solving Eqs. (6)–(8):

$$\sum_{\alpha=0}^{14} f_\alpha^{eq}=0 \tag{6}$$

$$\sum_{\alpha=0}^{14} c\boldsymbol{e}_\alpha f_\alpha^{eq}=\mathbf{V} \tag{7}$$

$$\sum_{\alpha=0}^{14} c^2\boldsymbol{e}_\alpha\boldsymbol{e}_\alpha f_\alpha^{eq}=pI+\mathbf{VV} \tag{8}$$

Then $\sigma = 7/12$, $\lambda = 1/3$, $\gamma = 1/24$.

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