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Influences of the perforation on effective transport properties of gas diffusion layers

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ABSTRACT

In this paper, the through-plane and in-plane effective transport properties, including permeability, diffusivity and thermal conductivity, of the perforated gas diffusion layer (GDL) are predicted using multiple-relaxation-time (MRT) lattice Boltzmann method (LBM) based on stochastic reconstructed microstructures. When predicting effective thermal conductivities of GDL, the effect of anisotropic conductive property of fibers is considered. The effective transport properties of dry perforated GDL are fitted as a function of perforation diameter and porosity. It is found that the permeability and effective diffusivity of GDL increase with perforation diameter and porosity while the effective thermal conductivity decreases. The two-phase LBM is adopted to simulate water distributions in perforated GDLs, and dependences of effective transport properties on saturation are then obtained. The results show that: the existence of the perforation significantly affects the water transport in hydrophobic perforated GDLs if its diameter is larger than the average pore size of GDL. The effective permeability and diffusivity of GDL decrease while effective thermal conductivity increases with saturation. The effective transport properties of perforated GDLs change less significantly with saturation than those of non-perforated GDL if the water droplet intruding into the perforation is displaced, while change more rapidly with saturation if the water droplet remains inside the perforation.

1. Introduction

The proton exchange membrane fuel cell (PEMFC) is a promising power source for automotive and stationary applications due to its high power densities apart from its other advantages. The gas diffusion layer (GDL) plays an important role on the reactant gas transport, water and thermal management in PEMFCs [1–3]. The most widely adopted GDL material is the carbon paper which is composed of fibers randomly distributed in the plane, resulting in the anisotropy of GDLs with different transport properties in the in-plane and through-plane directions [4,5]. In recent years, the effective transport properties of GDL, including gas permeability [6–9], effective diffusivity [10–13] and thermal conductivity [14–17], are widely investigated by experimental measurements or numerical simulations. The presence of liquid water in GDLs impedes reactant gas transport to the active sites, resulting in a significant loss in the performance of PEMFCs, especially at the high current density. Therefore, the dependence of effective transport properties on the saturation of GDL have also been a focus and widely studied by many researchers [10,13,18–20].

To avoid the water flooding problem in the PEMFC, Gerteisen et al. [21,22] first proposed a perforated GDL in which the laser-perforation (80 μm in diameter) is made in the through-plane direction. The test cell with the perforated GDL shows a higher current density than the cell with original GDL. After that, many scholars started to investigate influences of the perforation on water transport in GDL. Manahan et al. [23,24] conducted neutron radiography experiments to observe the changes in liquid water behaviors due to the perforation. Markötter et al. [25] performed the in-situ X-ray radiography experiments to observe the water distribution in perforated GDL. Subsequently, his cooperators Hauβϖ mann et al. [26] verified the improvement of water transport in perforated GDL and achieved the highest performance with the perforation diameter of 60 μm among three different diameters (30 μm, 60 μm and 150 μm). Okuhata et al. [27] also investigated the effect of perforation structure on liquid water transport by optically visualized technique. However, due to the high costs of experiments, the above studies only focused on some kinds of perforated GDLs, and could not obtain the correlations of effective transport properties with the perforation diameter and porosity.

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In this aspect, numerical simulations have a great advantage over the experimental studies. During the past few decades, the lattice Boltzmann method (LBM) has developed as an alternative and powerful technique to simulate fluid flows and transport processes, especially in applications involving complex geometries and interfacial dynamics [28–30]. The LBM allows to simulate pore-scale single-phase flow [7,8], mass or heat transports [17,31], and two-phase (water-gas) flow [32–35] in GDL considering the real structures of GDL. It is reported that with the single-relaxation-time LBM to deal with fluid-solid boundaries, the predicted effective transport coefficients are viscosity dependent. Then, the multiple-relaxation-time (MRT) LBM is developed to overcome this drawback and improve the numerical stability [8,36].

In most previous studies, when predicting the effective thermal conductivity of GDL, the solid fibers are assumed to be isotropic [14–17]. However, the fiber is anisotropic with different thermal conductivities in axial and radius directions. A D3Q7 MRT LB model with off-diagonal components in the relaxation time matrix was developed to predict the effective thermal conductivity of heterogeneous materials with anisotropic components [37,38]. However, as indicated in Ref. [30], a reduced LB model (D3Q7) is insufficient for the complex porous medium, and therefore a D3Q19 model is extended in this paper.

Although many empirical correlations of permeability, effective diffusivity and thermal conductivities of GDLs are proposed, they usually ignore the effects of real structure and water droplet distributions on the estimations of effective transport properties, which further reduces the accuracy of PEMFC modeling. As for the perforated GDL, there exist few correlations for predicting effective transport properties. In the present paper, the effective transport properties of perforated GDL, including permeability, diffusivity, thermal conductivity, are predicted by MRT D3Q19 LBM accounting for the microstructure of GDL. Based on a large number of predicted data, the correlations of effective transport properties of dry perforated GDL are fitted as a function of porosity and perforation diameter. Then, the two-phase LBM is adopted to simulate the water distribution in perforated GDL. Finally, the effective transport properties as a function of porosity, perforation diameter and water saturation are obtained. To reveal the effects of perforation, comparisons of effective transport properties of perforated GDL and non-perforated GDL are also made in this paper.

This paper is organized as follows. In Section 2, the LBM including single-phase and two-phase flows and transport models with specified boundary conditions are introduced. In Section 3, the accuracy of the models is verified. In Section 4.1, the effective transport properties of dry perforated GDL are obtained. The water droplet distributions are simulated by two-phase LB model in Section 4.2, and the effective transport properties of partially saturated perforated GDL are obtained in Section 4.3. Finally, some conclusions are drawn in Section 5.

2. Lattice Boltzmann method

2.1. MRT lattice Boltzmann method

In the present paper, a D3Q19 MRT LB model is adopted to simulate the gas flow, diffusion and heat transport in the GDL. The evolution equation of the particle distribution function is [31]:

$$f_i(\mathbf{x}+\mathbf{e}_i\delta t,\ t+\delta t)-f_i(\mathbf{x},\ t)=-(\mathbf{M}^{-1}\mathbf{S}\mathbf{M})_{ij}[f_j-f_j^{eq}] \tag{1}$$

where f_i is the density distribution function; $\boldsymbol{x}$ denotes the position; t is the time; δt is the time step, $\boldsymbol{e}_i$ is the discrete velocity along the ith direction:

$$[e_i]=\begin{bmatrix}0,1,-1,0,0,0,0,1,-1,1,-1,1,-1,1,-1,0,0,0,0\\0,0,0,1,-1,0,0,1,1,-1,-1,0,0,0,0,1,-1,1,-1\\0,0,0,0,0,1,-1,0,0,0,0,1,1,-1,-1,1,1,-1,-1\end{bmatrix} \tag{2}$$

In Eq. (1), $\mathbf{M}$ is an orthogonal transformation matrix, defined as:

$$\mathbf{M}=\begin{bmatrix}
1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1\\
-30, & -11, & -11, & -11, & -11, & -11, & -11, & 8, & 8, & 8, & 8, & 8, & 8, & 8, & 8, & 8, & 8, & 8, & 8\\
12, & -4, & -4, & -4, & -4, & -4, & -4, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1\\
0, & 1, & -1, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1, & 1, & -1, & 1, & -1, & 0, & 0, & 0, & 0\\
0, & -4, & 4, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1, & 1, & -1, & 1, & -1, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & 1, & -1, & 0, & 0, & 1, & 1, & -1, & -1, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1\\
0, & 0, & 0, & -4, & 4, & 0, & 0, & 1, & 1, & -1, & -1, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1\\
0, & 0, & 0, & 0, & 0, & 1, & -1, & 0, & 0, & 0, & 0, & 1, & 1, & -1, & -1, & 1, & 1, & -1, & -1\\
0, & 0, & 0, & 0, & 0, & -4, & 4, & 0, & 0, & 0, & 0, & 1, & 1, & -1, & -1, & 1, & 1, & -1, & -1\\
0, & 2, & 2, & -1, & -1, & -1, & -1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & -2, & -2, & -2, & -2\\
0, & -4, & -4, & 2, & 2, & 2, & 2, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & 1, & -2, & -2, & -2, & -2\\
0, & 0, & 0, & 1, & 1, & -1, & -1, & 1, & 1, & 1, & 1, & -1, & -1, & -1, & -1, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & -2, & -2, & 2, & 2, & 1, & 1, & 1, & 1, & -1, & -1, & -1, & -1, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & 1, & -1, & -1, & 1, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 1, & -1, & -1, & 1\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 1, & -1, & -1, & 1, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1, & -1, & 1, & -1, & 1, & 0, & 0, & 0, & 0\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & -1, & -1, & 1, & 1, & 0, & 0, & 0, & 0, & 1, & -1, & 1, & -1\\
0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 1, & 1, & -1, & -1, & -1, & -1, & 1, & 1
\end{bmatrix} \tag{3}$$