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Short communication

Liquid water breakthrough location distances on a gas diffusion layer of polymer electrolyte membrane fuel cells

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HIGHLIGHTS

- 22 realizations of stochastic gas diffusion layer model are applied in simulations.
- Two kinds of water breakthrough location distances are analyzed statistically.
- Water breakthrough location distances (BLD) are described by normal distribution.
- Shortest neighbour breakthrough location distance (SN-BLD) is geometry independent.
- SN-BLD bridges the gap for multiple scale simulations in PEMFC.

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ABSTRACT

The lattice Boltzmann method is adopted to simulate the three dimensional dynamic process of liquid water breaking through the gas diffusion layer (GDL) in the polymer electrolyte membrane fuel cell. 22 micro-structures of Toray GDL are built based on a stochastic geometry model. It is found that more than one breakthrough locations are formed randomly on the GDL surface. Breakthrough location distance (BLD) are analyzed statistically in two ways. The distribution is evaluated statistically by the Lilliefors test. It is concluded that the BLD can be described by the normal distribution with certain statistic characteristics. Information of the shortest neighbor breakthrough location distance can be the input modeling setups on the cell-scale simulations in the field of fuel cell simulation.

1. Introduction

The polymer electrolyte membrane fuel cell (PEMFC) plays a major role in future energy devices because of its zero emissions [1]. The two-phase problem is an important feature that affect cell performance [2]. One of the most important aspects on simulating two-phase flow for PEMFC is to bridge the gap between mesoscale and cell-scales simulations.

To date, there is rare simulation work bridging multiscales simulations. Instead, some works focused on cell-scale (in mm or higher range) and mesoscale two-phase simulations of PEMFC independently. The cell-scale two-phase simulations of fuel cell was focusing on the single cell or gas channel (GC). Ding et al. [3] did volume of fluid (VOF) simulation on water droplet emerging from a GDL in GC. Some regular shaped water breakthrough location (BL) were artificially set. Zhu et al. [4] did VOF simulations of water droplet dynamics in GC and a single circle BL with fixed area was defined on the GC-GDL interface. Qin et al. [5] studied the effects of water maldistribution on cell performance by combination of analytical water production model and VOF. The mesoscale two-phase flow simulations were focusing on the GDL (in μm range). Sinha and Wang [6,7] did pore-network model (PNM) simulations of two-phase flow though GDL with the different wetabilities and compressions. Tao's group [8] and Zhou et al. [9] did 2D lattice Boltzmann (LB) simulations on water transport and distribution in the cross section of a reconstructed GDL, and the effects of carbon fiber distribution and spatial mixed-wetability were discussed. Niu et al. [10] did LB simulations on water and gas transport in a 3D reconstructed GDL.

In multi-scales simulations, the result from mesoscale simulations can be the input of cell-scale simulations. The BL position can be part of output from mesoscopic two-phase simulations in GDL, and input modeling setups in cell-scale simulations (like VOF) in GC [11]. BLs

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were also observed in experiments. Djilali's group [12,13] observed liquid water transport through GDL under different wetability and compression. Santamaria et al. [14] observed a series of BLs with varying water flux, GDL thickness and inject penetration area. Bazylak et al. [15] observed dynamic BLs in an ex-situ experiment. Gao et al. [16] and Shahraeeni [17] observed the breakthrough location distribution in different kinds of GDL from in-situ experiments by image postprocess.

In summary, the liquid water BLs on GDL were observed in experiments but there is still lack of simulation studies. It is necessary to provide the details to cell-scale simulations from mesoscale simulations in GDL. In our previous work, Yu et al. [18] presented liquid water transport through the microstructures of Toray 090 GDL. The focus of this work was on the statistical evaluation of local contact angles at the rough surface of the GDL adjacent to the air channel. Like in our previous studies [18], the LB method is adopted to simulate liquid water through GDL in this work. Two kinds of liquid water breakthrough location distance (BLD) are discussed statistically and their distribution is evaluated by the Lilliefors test. The LB model is reviewed in section 2. Then simulation setups and conditions are presented in section 3. Finally, results are shown and discussed in section 4. Conclusions are summarized in section 5.

2. Lattice Boltzmann model

The multi-relaxation time (MRT) D3Q19 ShanChen multicomponent LB model was used [19]. We provide a brief model description below and we refer readers to our previous work for the additional details [18,20,21]. The evolution equation for αth component with the MRT collision operator is

$$f_i^\alpha(\mathbf{x}+\mathbf{e}_i\Delta t, t+\Delta t) = f_i^\alpha(\mathbf{x}, t) - \mathbf{M}^{-1}\mathbf{S}^\alpha\mathbf{M}[f_i^\alpha(\mathbf{x}, t) - f_i^{\alpha,eq}(\mathbf{x}, t)] + \beta^\alpha(\mathbf{x}, t) \quad (1)$$

with $f_i^\alpha(\mathbf{x}, t)$ is the distribution function of the αth component and time step $\Delta t = 1$. $\mathbf{M}$ is a transformation matrix [22] and $\mathbf{S}^\alpha$ is a diagonal matrix, while $f_i^{\alpha,eq}(\mathbf{x}, t)$ is the equilibrium distribution function, their formula and set are the same as our previous work [18]. The source term $\beta^\alpha(\mathbf{x}, t)$ in Eq. (1) is represented by the exact difference method (EDM) force scheme as

$$\beta^\alpha(\mathbf{x}, t) = f_i^{\alpha,eq}(\rho_\alpha, \mathbf{u}^{\alpha,eq}(\mathbf{x}, t) + \Delta\mathbf{u}^\alpha(\mathbf{x}, t)) - f_i^{\alpha,eq}(\rho_\alpha, \mathbf{u}^{\alpha,eq}(\mathbf{x}, t)) \quad (2)$$

where ρ_α, $\mathbf{u}^{\alpha,eq}(\mathbf{x}, t)$ and $\Delta\mathbf{u}^\alpha(\mathbf{x}, t)$ are the density, equilibrium velocity and velocity difference of αth component. The lattice Boltzmann model was validated in one of our previous work [18]. The errors from the lattice and the algorithm were observed.

3. Simulation setups and conditions

GDL plays a significant role on water management of PEMFC [23]. In this work, 22 reconstructed Toray TGP090 GDL fully covered with polytetrafluoroethylene (PTFE) (porosity is 0.8) are applied [20]. The geometry model was developed by Thiedmann et al. [24]. It described GDL by layers of straight fibers with additional binder material. The realization are locally different from each other but all of them are stochastic equivalent to the real microstructures as validated in the BESSY synchrotron in Berlin. The contact angle on PTFE is 110°. The simulation domain includes three regions: buffer space, GDL and free space in (Fig. 1 a). Initially, buffer space with 15 μm thickness is filled with water while other regions are occupied by air. The density and velocity field initialization follows the previous work [18]. The free space has the same size as GDL (600 μm × 600 μm × 195 μm in Y, Z and X directions) to form droplets in Fig. 1 a). The fixed velocity is adopted on the first layer of buffer space with Zouhe method toward X direction [18,25], while the open condition is applied on the top of domain. The periodic condition is set on other boundaries [18].

The liquid water through a GDL is assumed to be the two-phase flow in a porous media, and its behavior can be evaluated by a phase relation of dynamic viscosity ratio M against capillary number Ca (ratio of viscous force to the surface tension force) [26]. When the fuel cell is operating, $M \approx 18$ (water divide air) and $Ca \approx 10^{-9} \sim 10^{-6}$ (calculated by average water produced velocity in whole active GDL area) [18,27]. This leads to a fixed velocity applied to the inlet. Under this condition, the liquid water through GDL can be simplified as a capillary fingering process where the density ratio and viscosity ratio of water and air are negligible [26]. According to the experiment observation of Santamaria et al. [14], the Ca number and GDL thickness have effects on the water flowing through GDL process, such as the formed droplets distribution on GDL surface are different. Here $Ca \approx 10^{-4}$ based on our previous work [18] and also other ex-situ experiments setups [28]. It is chosen in a way to consider the preferred paths in to microstructures according to Markötter et al. [29] Ca is higher than the average value in the operated PEMFC but it makes sense when thinking of local produced water. The simulated domain area (0.36 mm^2) is much smaller than the whole active GDL area (range of 100 cm^2 [30]) and small cracks on the microporous layer (MPL) [14,23], the water is produced very inhomogeneously and it causes local water produced velocity is much larger than the average [31].

The liquid water through GDL is a dynamic process. The total saturation S_{total} (water fraction of total pores) changes with the evolution time. (Fig. 1 b) shows S_{total} against evolution time in one of geometries (geometry NO.1), while other 21 geometries show the similar dynamic saturation curve [18]. It is seen that S_{total} increases because the water is continuously injected to the GDL. After breakthrough time (≈ 13 ms), the slope of saturation curve decreases due to water breaking through the GDL and some BLs are formed. The BL is assumed to be independent of evolution time. A snapshot time (≈ 15 ms) is chosen for a snapshot of simulation when sphere-shape droplets are formed on GDL surface [18]. This is only a snapshot of a dynamic process as already argued by Bazylak et al. [15]. They concentrated on the dynamics of the water breakthrough process. As a consequence, the operating condition and also the choice of the snapshot time will surely affect the BLD. The focus on a fixed snapshot time draws the eye to the impact of the local geometry which is possible by the use of locally different but statistic equivalent microstructures.

4. Results and discussion

Some sphere-shape droplets are formed on the GC-GDL interface and shown in Fig. 2 a (geometry NO.15). In other geometries, droplets amounts, shapes (apparent contact angles) and positions are different [18]. The situation on the GC-GDL interface is shown in Fig. 2 b), three BLs (red) with three BLDs (yellow, I to III) are distributed on it.

BL is assumed on the geometry center of the irregular breakthrough region (blue in Fig. 2 (b)) [32]. Touching boundary breakthrough regions are not taken into account and the BLD is the distance between two BLs. The local position of a single BL on a small section (0.6 mm × 0.6 mm) is not useful for the interpretation in cell-scale applications. The distances between neighbor BLs (BLD) are evaluated statistically.

In this work, two kinds of BLD are discussed including the specific BLD (S-BLD) and the shortest neighbor BLD (SN-BLD). The S-BLD is the distance between two BLs in a specific domain (three S-BLDs are the same as BLD I to III in Fig. 2 (b)). The S-BLD is calculated only within the simulated area, neglecting the distances to mirrored BLs caused by a checker board setup due to the periodic boundary condition. The S-BLD is domain size dependent and it will be larger with the bigger GDL domain (more BLs will be formed on a bigger area). The SN-BLD is the shortest distance between one BL and its neighbor BLs, which is filtered from S-BLD data. It is independent of domain size and can be the input modeling setups on the larger cell-scale simulation (VOF simulation in GC) [33]. For example in Fig. 2 b), BLD II and III are the two SN-BLDs