Lattice Boltzmann Simulation on Water Transport in Gas Diffusion Layer of Polymer Electrolyte Membrane Fuel Cells

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Abstract. The effect of rib on the dynamic behavior of liquid water transport in gas diffusion layer (GDL) is studied. The mechanism of water transport dynamics investigated using multiphase lattice Boltzmann method (LBM). Simulation with a simplified two-dimensional model is used to predict liquid water transport processes in local regions, instead of pursuing a three-dimensional numerical analysis for the entire domain. The observation of lattice Boltzmann (LB) simulation shows that the rib changes the water transport behavior and significantly affects the water transport in GDL.

Introduction

Water management is one of the challenges in polymer electrolyte membrane fuel cells (PEMFCs) and regarded as a critical issue for achieving high performance PEMFC. While the membrane should have sufficient hydration to maintain good proton conductivity, excessive amount of water generated and accumulated in the membrane electrode assembly (MEA) can cause flooding in catalyst layer (CL).

In this study, the dynamic behavior of liquid water in the GDL is investigated numerically using a two-dimensional LBM approach. The two-phase intermolecular potential model proposed by Shan and Chen is used to examine the microscopic behavior occurring at the pore-scale in a complex porous structure. The effective permeability of GDL from two-dimensional simulation is verified by comparing the LB result with analytical solution and experimental results in the literature. The cross-sectional water distribution and water saturation profiles are presented to understand the wetting characteristic in the GDL. The effect of rib structure on the water transport behavior in the GDL is discussed.

Model Development

LBM

LBM simulates mass transport of multi-phase mixture by tracking movements of particle ensembles on a mesoscale-level. In this study, we developed the Shan-Chen pseudo-potential based two-phase LB model that allows the separation of two immiscible fluids if the interaction force between the fluids is larger than a threshold value. The time variation of distribution functions is calculated by performing a simple law of collision and streaming steps. The multiphase LB Model with a single relaxation time (SRT) for collision operator is applied in the lattice Bhatnagar-Gross-Krook (LBGK) equation. The time evolution of this model can be written as

\[ f_i^k(x+e_i \Delta t,t+\Delta t) - f_i^k(x,t) = \frac{\Delta t}{\tau_k} \left[ f_i^k(x,t) - f_i^{k,eq}(x,t) \right] \] (1)

More detailed description of the LB model can be found in Ref. [1].

Computational Domain

The schematic domain of LB model for the simulation is shown in Figure 1. The computational domain consists of channel, rib and the GDL. The dimension of calculation domain is 2000 × 1000 lu².
(lu: lattice unit). The GDL height is set to 400 lu, a rib height to 600 lu, and a channel width to 1000 lu. The porous structure of the GDL is constructed as impermeable solid particles and pore area which has void space. The commercial carbon paper SGL\textsuperscript{®} 10BA with 5% PTFE content is taken into consideration for the modeling of GDL, and thus the porosity and particle diameter are set to 0.88 and 10 lu, respectively. [2]. The boundary conditions proposed by Zou and He [3], who implemented it on the inlet/outlet boundaries and the no-slip bounce back, are applied. The inlet condition is set to the bottom boundary with the inflowing velocity of $1.0 \times 10^{-4}$ lu.

![Diagram of Computational Domain](image)

**Figure 1.** Computational domain of two-dimensional LB model.

### Results and Discussion

Figure 2 shows the liquid water distribution in the GDL. Present model consists of two fluids, i.e., liquid water and gaseous air. In the picture, blue and light grey represent the liquid water and gaseous air, respectively. A constant velocity is given for liquid water at the inlet to push gaseous air toward the outlet. Figure 2(a) presents liquid water distribution at $1.0 \times 10^6$ lattice time, and the wettability distributions are presented after each $0.5 \times 10^6$ lattice time as shown in Figure 2(b) ~ 4(e). As shown, the invaded liquid water travels through the pores between the carbon fibers, presenting complex flow patterns due to the complicated structures of GDL. Consequently, the air moves driven by the mean flow motion of the water. In Figure 2(a), liquid water is observed at the bottom, indicating that the GDL accumulates the water from the inlet. Liquid water forms several water clusters and the clustered water presents convex water fronts due to hydrophobic carbon fibers. In Figure 2(b), liquid water selects some preferential paths to flow in the in-plane or through-plane direction which has lower resistance force. Liquid water selects relatively wide throats while the linked water clusters form a single flow path through a merging process. Once the dominant path has selected, the water flows into the main branch and stretches toward the channel. In Figure 2(c), the water breakthrough occurred at the end of the dominant path. This figure indicates that the dominant path leads the water breakthrough. In Figure 2(d) and (e), the water droplet becomes larger as lattice time increases. However the water distribution inside the GDL is little changed. This is attributed to the formation of the droplet in the channel which increases the water droplet size through the dominant path, while suppressing the water spread in the GDL. These figures indicate that the large pores are mainly used as a pathway for liquid water transport, and thus the small pores can be available for gaseous reactant transport. These figures indicate that the liquid water selectively stretches toward the wider pore area as well as the channel region.
Summary

The water transport in GDL has been investigated using two-dimensional LBM simulation. The LB model is developed to simulate the dynamic behavior of liquid water and enables to visualize the water-invasion process through micro-pores in GDL. The reconstruction of GDL is established by randomly placing the particles in GDL and ignoring the GDL deformation due to clamping force. The results of LB simulation confirm that the liquid water transport inside the GDL is strongly governed by capillary force and the rib structure greatly impacts on the water transport behavior. The rib structure influences on the location of water breakthrough This is due to the higher resistance force underneath the rib, resulting in the change of flow path which preferentially selects the lower resistance force. After water breakthrough, the liquid water distribution under the channel has little change, whereas that under the rib continues to stretch. The results indicate that a careful control of rib structure would enhance the water removal from the GDL. The results of the present study would contribute to the novel design for better water removal and flooding alleviation from the GDL.

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References
