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Short Communication

Numerical studies of interfacial phenomena in liquid water transport in polymer electrolyte membrane fuel cells using the lattice Boltzmann method

*Bo Han, Hua Meng**

School of Aeronautics and Astronautics, Zhejiang University, Hangzhou, Zhejiang 310027, China

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ABSTRACT

Water management is an important issue in the polymer electrolyte membrane (PEM) fuel cell, which is considered as a promising alternative power source for future automotive applications. In this article, lattice Boltzmann simulations are conducted to examine the interfacial phenomena in liquid water transport in porous materials of a PEM fuel cell. Numerical results clearly indicate that large perforated pores through the porous diffusion layers can serve as a convenient liquid water transport pathway and thus assist in liquid water removal. An interconnected horizontal and vertical pore combination is especially beneficial to liquid water transport through the porous layers in flooding conditions. Therefore, liquid water transport in a PEM fuel cell may be effectively managed through well engineered interfacial structures in porous materials.

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1. Introduction

The polymer electrolyte membrane (PEM) fuel cell has been considered as a promising alternative power source for automotive applications due mainly to its high energy efficiency and environment-friendly operations. Water management, particularly liquid water transport, plays a crucial role in maintaining PEM fuel cell performance, stability, and durability. Many experimental [1–6] and numerical [7–17] studies on liquid water transport phenomena in PEM fuel cells have been extensively conducted in the past decade. Meso- [18–22] and micro-scale [23–25] numerical simulations were recently carried out to obtain fundamental understanding of the underlying transport mechanisms. Good progress has been achieved in this field.

From these existing studies, interfacial effect is identified to be one of the important phenomena in controlling transport processes and liquid water distribution in the porous materials of PEM fuel cells, including the catalyst layer (CL), micro-porous layer (MPL), and gas diffusion layer (GDL). Meng and Wang [11] showed that the liquid water droplet coverage at the interface of GDL/gas channel (GC) can hinder liquid water transport inside the porous materials and thus dictate the flooding dynamics in PEM fuel cells. Nam et al. [23] examined the presence and coverage of liquid droplets at the CL/MPL and MPL/GDL interfaces, and based on

* *Corresponding author*. Tel.: +86 571 87952990.
E-mail address: menghua@zju.edu.cn (H. Meng).

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experimental observations and numerical modeling results, they proposed an explanation for the significant role that the MPL plays in controlling water transport and fuel cell performance. Mench et al. [26–29] conducted thorough investigations on the interfacial phenomena between CL and MPL. The interfacial morphology was experimentally characterized [26,27] while its effects on cell performance were both analytically [27] and numerically [28] studied. The effects of the interfacial cracks on cell performance were also experimentally examined [29]. Recent experimental studies [30–34] further demonstrated that large laser perforated pores through the gas diffusion media can change liquid water distribution and enhance liquid water transport in the porous materials, and therefore, lead to improved water management and PEM fuel cell performance.

In this short technical note, numerical studies are conducted to examine the interfacial effects on liquid water transport in the porous diffusion layers of PEM fuel cells. Because of the complex and meso-scale geometric structures of the porous materials, a two-phase lattice Boltzmann method is employed herein as a robust and efficient numerical simulation tool. Results obtained in this paper can assist in optimizing and engineering the gas diffusion materials for efficient water management in PEM fuel cells.

2. Model description

The present numerical simulations are carried out using the lattice Boltzmann model with a single relaxation time collision operator (the so-called LBGK model), which further incorporates the Shan–Chen multi-phase approach [35,36] to handle liquid water transport processes in the porous diffusion media of a PEM fuel cell. This numerical method simulates multi-phase fluid flows, mainly liquid water transport processes in the present studies, through direct evolution of the particle density distribution functions on fixed lattices and proceeds in two steps: collision and streaming. The collision procedure relaxes the density distribution functions on a lattice toward the equilibrium states, while the streaming step moves the particle distributions to the immediate neighboring lattices. In the Shan–Chen two-phase model, extra forces are introduced in the equilibrium distribution functions to account for fluid inter-particle and fluid–solid interactions. Because of the simple collision and streaming procedures in the lattice Boltzmann method, it is proved to be a very convenient and robust numerical tool for handling fluid flows in complex geometric structures, e.g., the porous materials [18,19,37].

This two-phase LBGK model has been programmed into a computational software package in our research group and rigorously validated using various test cases concerning the liquid–gas interaction [21], which leads to phase separation and surface tension, the liquid–solid interaction [21], which reveals different wetting characteristics of a solid surface, and a single liquid water droplet emerging from a micropore and its subsequent movement on a hydrophobic channel surface [22]. More details concerning this two-phase LBGK model and model validations can be found in our prior publications [21,22], which clearly indicate that this method is capable of accurately handling liquid–gas and liquid–solid interactions. Therefore, the two-phase lattice Boltzmann model briefly described in this section is next employed to numerically examine liquid water transport processes in porous diffusion media of PEM fuel cells, focusing mainly on the interfacial phenomena.

3. Results and discussion

The problem of concern is liquid water transport through a two-layer (MPL and GDL) porous media in a PEM fuel cell, as shown in Fig. 1. The porous structures are randomly generated in the present lattice Boltzmann simulations for fundamental understanding of the underlying physics. The numerical studies are conducted in a two-dimensional configuration to maintain computational efficiency. The physical size of the computational domain in Fig. 1 is 500 * 200 μm in the horizontal (width) and vertical (depth) directions. The depths of MPL and GDL are set at 20 μm and 130 μm, respectively. The porosities in MPL and GDL are maintained at 0.4 and 0.65 [16,23], while the micropore sizes in the two layers are around 0.5 μm and 5 μm, respectively. The hydrophobic contact angle of the solid materials in the two porous layers is set at 160° for a simplified numerical treatment and qualitative studies. More accurate micro structures and wetting properties of the porous materials should be used in future quantitative investigations. After careful grid independence studies, the computational lattices are chosen as 1000 * 400 in the horizontal and vertical directions.

The effect of a large perforated pore and/or crack through the two porous layers on liquid water transport is first numerically investigated, as shown in Fig. 2. The size of the large perforated pore is around 10 μm. A thin layer of liquid water reservoir is constantly maintained under the MPL to supply liquid water. Therefore, the present numerical studies focus mainly on liquid water transport in flooding conditions. A small upward flow velocity at $0.5 * 10^{-5}$ ms^{-1} is initially defined to start numerical simulations. Once the liquid water enters the porous regions, its movement is mainly driven by the capillary force through interaction with the solid material. Numerical results obtained with and without the perforated pore in the porous layers are clearly compared in Fig. 2. Without the large perforated pore, liquid water randomly penetrates through the porous regions and eventually emerges as two small droplets at the top channel

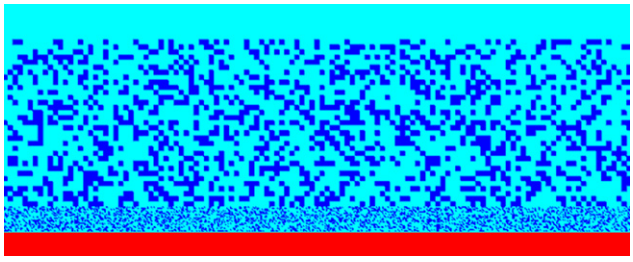

Fig. 1 – Schematic of the computational domain with two porous layers.

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