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Effect of compression on water transport in gas diffusion layer of polymer electrolyte membrane fuel cell using lattice Boltzmann method

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HIGHLIGHTS

- We simulate the water transport dynamics in the GDL using LBM.
- We investigate the effect of compression ratio on water transport.
- We discuss the mechanism of water transport in the GDL.

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ABSTRACT

The effect of the compression ratio on the dynamic behavior of liquid water transport in a gas diffusion layer (GDL) is studied both experimentally and numerically. We experimentally study the emergence and growth of liquid droplets in a channel at various compression ratios by adopting a direct visualization device. The results of the experiment show that water breakthrough occurs at the channel for a low compression ratio, whereas it is observed at the channel/rib interface for a high compression ratio. To determine the mechanism of water transport in the GDL, a multiphase lattice Boltzmann method (LBM) is developed for a simplified porous structure of the GDL. The observation of lattice Boltzmann (LB) simulation shows that the compression ratio significantly affects the water transport in the GDL. The results indicate that the lower compression ratio reduces the water saturation in the GDL. The simulation and experimental result are similar.

1. Introduction

Polymer electrolyte membrane fuel cells (PEMFCs) are assembled under compressive loads to prevent gas leakage and to minimize contact resistance. A bipolar plate and gas diffusion layer (GDL) are clamped together in the assembly process. In the clamping process, the GDL experiences deformation that causes a variation of its microstructure with respective to permeability and pore size. Consequently, the dynamics of liquid water transport within the GDL could be affected by the compression. It is well known that the performance of a fuel cell changes considerably when the cell is disassembled and re-assembled [1]. This is due to compressive loads that are repeatedly placed on the GDL and membrane electrode assembly (MEA). Excessive compression will increase mass transfer resistance and change the holdup of water in the GDL, resulting in poor performance. Unreasonably low clamping pressure can cause high contact resistance and gases leakage.

During the past decade, a number of experiments have been conducted to investigate the effect of GDL compression on water transport. Lee et al. [2], Chang et al. [3], Ge et al. [1], and Zhou et al. [4] studied cell performance as a function of compression pressure for various GDLs. Their experimental results showed that the cell performance increases at a low compression ratio, and decreases at a high compression ratio. They suggested that the different cell performance could be due to the change in mass transfer resistance, contact resistance, and water contents of the GDL. Ge et al. [1] and Zhou et al. [4] suggested that there exists an optimal clamping force to obtain the highest performance. Chi et al. [5] investigated both

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experimentally and numerically the effect of non-uniform GDL structure on cell performance caused by uneven compression. They reported that GDL compression results in an oscillation of heat flux, species concentration, current density and saturation between the channel and rib. The fluctuation amplitude depends on the compression ratio. Roshandel et al. [6] considered the sine wave porosity distribution of a GDL in their simulation. They reported that any change in porosity can lead to a substantial effect on cell performance due to the change of diffusion overpotential. Saha et al. [7] observed that permeability has a strong effect on the pressure drop. Nitta et al. [8] found that GDL is compressed very little under the channel, and the change of GDL thickness under the rib is mostly due to the loss of porosity. Bazylak et al. [9] examined the effect of compression on liquid water transport through the GDL using Fluorescence microscopy. They reported that the compressed GDL provides preferential pathways for water transport and breakthrough caused by localized hydrophilic pathways in the compressed GDL. These studies provide basic understanding of the effects of GDL compression on water transport, but they are ambiguous in quantifying the water saturation in a GDL due to the difficulty in measuring the liquid water distribution. Despite extensive studies of the effects of GDL deformation, less attention has been paid to pore-scale water transport behavior in compressed GDLs. The dependence of the compression ratio on the water transport inside a GDL is quite uncertain according to reports from the literature.

Direct visualization of the liquid water transport through the micro-pores of a GDL has yet to be reported. This is mainly due to the immense difficulty associated with making *in situ* measurements during the operation of PEM fuel cells. This difficulty is compounded by the requirements for micro-scale flow visualization, which include optical accessibility. However there has been some process using *ex situ* visualization techniques or *in situ* water measurement techniques (e.g., magnetic resonance images, the beam technique, transparent fuel cells, residence time distribution, pressure drop, and membrane monitoring) to macroscopically visualize water distribution within an operational fuel cell. *Ex situ* visualization offers insight into the local motion of water droplets at the channel, but it does not provide visualization of liquid water transport inside the GDL. *In situ* techniques have shown potential for visual inspection of liquid water transport in an operating fuel cell. However, this technique presents difficulties in resolution of their images as well as cost. Nevertheless these techniques offer the opportunity of identifying locations where the water breaks through the GDL.

In this study, the effect of GDL compression on the behavior of liquid water transport in a GDL is investigated using a two-dimensional LBM approach. The LBM, which is widely used numerical tool for simulating multiphase flow in porous media, can generally describe the realistic pore-scale dynamic behavior of water in a GDL. Moreover, the LBM is more appropriate for micro-scale simulation because it is formulated on the basis of the kinetic theory and the Boltzmann equation. On the other hand, the LBM requires large and even prohibitive computational resources. Thus, this study is limited to two-dimensional analysis. 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. Therefore, the advantages of the LBM are fully used, leading to the resolution of microscopic behavior in a complex porous structure with acceptable computational cost. Our LBM study provides cross-sectional liquid water distribution and saturation profiles in the GDL. Substantial changes in GDL characteristics can have a remarkable effect on the behavior of micro-scale water transport. Thus, it is important to determine how the variation of the GDL structure goes through under different compression ratios, targeting to elucidate the intrinsic characteristics. Although many research groups have studied the dynamic behavior of water transport using the LBM, they did not validate their results with experimental work [10–14]. Therefore, their studies have difficulty in thorough understanding of water transport behavior inside a GDL. In the present study, an experiment is conducted for comparison with the results of LB simulation by visualizing cross-sectional water droplet emergence and growth in the channel. The LB simulation provides the water transport behavior inside the GDL, and *ex situ* experiment is used to visualize the water transport of post breakthrough and validate the LB simulation. Water transport research both with LB simulation and *ex situ* experimental results has not previously been described on the literature. We focused on a comparison of liquid water transport behavior in a GDL at various compression ratios. Our results can contribute to a more comprehensive understanding of liquid water transport phenomena.

2. Experiment

2.1. Experimental setup

In order to visualize the liquid water accumulation at the flow channel/GDL interface and droplet growth in the channel, a specially designed cell module was devised. Fig. 1 shows the experimental setup and main components used in the experimental work. The experimental apparatus consists of a cell device, syringe pump, halogen lamp, and charge coupled device (CCD) camera controlled by a personal computer (PC). To supply the desired flow rate of water into the bottom of the tested GDL, a water injection region with a rectangular cross-section (3 mm × 0.5 mm) was installed at the bottom plate. A flow rate of 1 μL min^{-1} was supplied by a capillary tube connected to a syringe pump. The supplied flow rate was determined by the water production rate corresponding to a current density of 2 A cm^{-2}. To provide sufficient illumination on the back side of a GDL, a halogen lamp was adopted. Images of a droplet's occurrence and its growth were captured and recorded at a time interval of 1/30 s by the CCD camera. The experiments were carried out at room temperature. In an operating PEM fuel cell, humidified air is supplied into the cathode channels. Hence, the humidified air has some additional effect on the water droplet emergence and growth. In this study, both ends of the channels were exposed to atmospheric conditions in order to exclude the additional effect of air flow.

Fig. 2 shows the geometrical configuration of the experimental device adopted for the observation of liquid water behavior in the channel. To understand droplet behavior in the channel, cross-sectional observation is essential. For this purpose, the main observation area was a cross-sectional cut with a transparent acrylic cell. The channel has a width of 1 mm and depth of 1 mm, and the rib has a width of 1 mm. Teflon coating was applied to the rib to exhibit the surface wetting characteristics, which is similar to an actual bipolar plate in a PEM fuel cell.

o investigate the effect of compression on water droplet behavior, GDL compression was done by adjusting the torque applied to the upper plate using bolts. Four bolts were threaded into tapped holes on the upper plate, and hence the GDL thickness was controlled by applied compression force. The compression ratio (CR) is defined as the ratio of the reduced thickness versus the original thickness (i.e., $CR = (L-1)/L$) [5]. The compression ratio was measured with gauges, one placed on each side of the cell.

2.2. Gas diffusion layer (GDL)

A commercial GDL with 5% PTFE loading (SGL 10BA, SGL group®)