Pore-Network Simulation of Liquid Water Transport through Multi-Layer Gas Diffusion Medium

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1. Introduction

A polymer electrolyte membrane fuel cell (PEMFC) is a clean energy conversion device that can directly generate electrical power via electrochemical reaction of hydrogen and oxygen [1, 2]. Due to low operating temperature of PEMFCs below 100°C, water produced by the reaction can condense to liquid phase inside the gas diffusion layer (GDL). Water management and electrode flooding is one of crucial technical problems that should be solved to enhance the performance of PEMFC [3, 4]. In this study, pore-network simulation was conducted to study the water transport and saturation distribution in multi-layer gas diffusion medium. The previous steady pore-network model [5, 6] was extended to invasion-percolation liquid water transport through multiple porous layers, to simulate the interaction between the fine and coarse pore structures of GDL and microporous layers (MPL)

2. Theory and calculation

Liquid water does not spontaneously penetrate into pores in the hydrophobic porous media because more energy is needed to wet the hydrophobic surface. Instead, droplets and blobs are the preferential configurations for liquid water in hydrophobic porous media. The capillary pressure is defined as the pressure difference across the water/air interface.

$$P_c = P_w - P_a = \sigma\left|\cos\theta_w\right|\left(\frac{1}{R_1}+\frac{1}{R_2}\right) = \frac{2\sigma\left|\cos\theta_w\right|}{R_m} \qquad (1)$$

In Eq. (1), σ denotes the surface tension, R_1 and R_2 denote two principal radii of curvature, and R_m denotes the mean radius of curvature of water/air interface. Note that the capillary pressure in hydrophobic GDL or MPL has positive values in general. If the air pressure is constant at the atmospheric pressure, P_c is the same as the gauge pressure.

The pore-network model is a proven numerical method that has been used to study various transport phenomena in porous media. In this study, the pore-networks for GDL and MPL were constructed with box-shaped pores and throats. The geometrical parameters of GDL and MPL are summarized in Table 1. The present pore-network model first conducts search for invasion-percolation paths of liquid water transport, followed by calculation of viscous pressure drop through the invasion-percolation paths.

3. Results

Figure 1 shows that liquid saturation and capillary pressure distribution in MPL and GDL, where the jumps in the saturation and also in the capillary pressure is shown at the interface of MPL/GDL. Figures 2 and 3 illustrate the air/water interface formed in MPL and GDL, where complex interface shapes are well observed. About 80 breakthrough sites were formed at the MPL outlet, while only about 4 were formed at GDL outlet.

Table 1 Parameter for the present pore-network model.

GDL Parameters	Explanation	Value
$N_{G,x}\times N_{G,y}\times N_{G,z}$	Size of pore-network	16×16×8
$L_{G,x}\times L_{G,y}\times L_{G,z}$	Length of pore-network	400×400×200 μm^3
$L_{G,cell}$	Unit cell size	25μm
$l_{G,px}$, $l_{G,py}$, $l_{G,pz}$	Dimension of pore	17.5−22.5 μm
$l_{G,ta}$, $l_{G,tb}$	Dimension of throat	5−17.5 μm
MPL Parameters	**Explanation**	**Value**
$N_{M,x}\times N_{M,y}\times N_{M,z}$	Size of pore-network	80×80×10
$L_{M,x}\times L_{M,y}\times L_{M,z}$	Length of pore-network	400×400×50 μm^3
$L_{M,cell}$	Unit cell size	5μm
$L_{M,px}$, $l_{M,py}$, $l_{M,pz}$	Dimension of pore	3−4 μm
$L_{M,ta}$, $l_{M,tb}$	Dimension of throat	0.5−3 μm

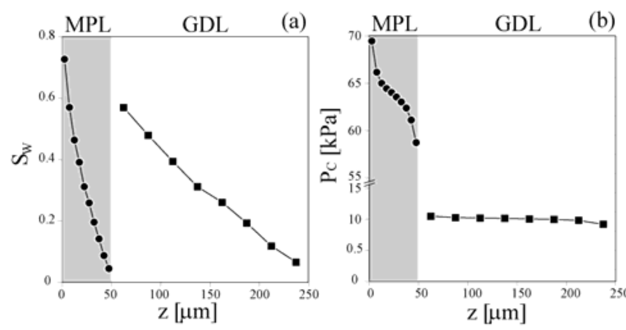

Fig. 1 The distribution of (a) liquid water saturation and (b) capillary pressure in GDL and MPL

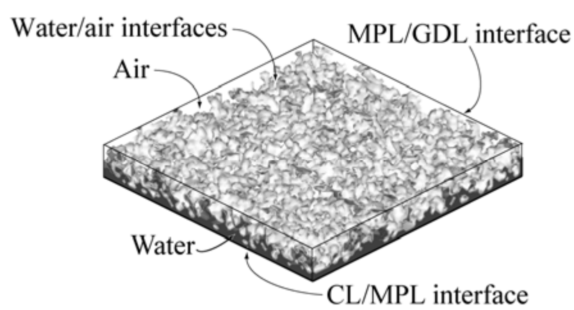

Fig. 2 The air/water interface distribution in MPL

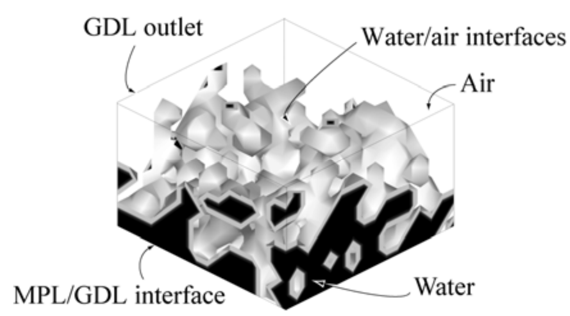

Fig. 3 The air/water interface distribution in GDL

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