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Numerical investigation on double gas diffusion backing layer functionalized on water removal in a proton exchange membrane fuel cell

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ABSTRACT

Since flooding is a limiting factor of cell performance in a proton exchange membrane fuel cell (PEMFC), it is important to remove produced water effectively from GDL. In this study, a multi-layer GDL containing single micro porous layer (MPL) and double gas diffusion backing layer (GDBL) was introduced as a practical design and the effect of porosity and/or hydrophobicity of GDBL on water removal was investigated with one-dimensional steady-state model based on a capillary pressure–saturation relationship. The results shows that double GDBL with different porosity in a positive direction (GDBL with lower porosity near the MPL and GDBL with higher porosity near the flow channel) and/or different hydrophobicity in a negative direction (more hydrophobic GDBL near the MPL and less hydrophobic GDBL near the flow channel) enhances the water removal ability of the GDL compared with uniform single GDBL. Based on the results, the property arrangements of double GDBL were optimized to minimize the amount of liquid water remaining in GDL. It is expected that the amount of produced water remaining in ML-GDL can be reduced about 9.2% with optimized porosity arrangement and 5.6% with optimized hydrophobicity arrangement.

1. Introduction

It is expected that hydrogen energy technologies will play an important role on a future energy economy and a fuel cell has received a significant attention due to its high electrical efficiency and clean energy conversion [1,2]. Among the various types of fuel cells, a proton exchange membrane fuel cell (PEMFC) has several advantages such as low operating temperature, quick response, and high fuel utilization efficiency [3].

In PEMFCs, placed between membrane electrode assembly (MEA) and gas supplying channels, the gas diffusion layer (GDL) plays important roles on water management, gas diffusion, electron transport and membrane electrode assembly (MEA) support. Among them, water management is an important issue for fuel cell performance because the produced water remaining inside GDL occupies the pore volume and excess water blocks the reactant gases to reach the reaction sites. This phenomenon is called as flooding and, in addition to flooding in channels [4], flooding in GDL is a limiting factor of fuel cell performance [5,6]. Therefore, the water removal ability and gas diffusion kinetics of GDL should be enhanced for high cell performance.

Considering the operation condition of PEMFCs and the pore size of GDL, water transport in GDL is strongly dominated by capillary force, while viscous and inertial forces are negligible [7]. Based on the Young–Laplace equation, the capillary pressure is related to the average pore diameter and hydrophobicity of the porous material, which can be replaced by porosity and contact angle. Therefore, the cell performance can be improved with optimized property of porosity and contact angle in GDL [8,9].

For this reason, conventional GDL is composed of micro porous layer (MPL) and gas diffusion backing layer (GDBL). Placed between the catalyst layer and gas diffusion backing layer (GDBL), MPL effectively removes the produced water from the catalyst layer where the fuel cell reaction occurs so that the reactant gases can reach the reaction sites through the relatively dry pores [10]. However, since the low porosity of MPL acts as a resistance for gas

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diffusion, the MPL should be coated on GDBL as thin as possible. Then, in order to investigate the effect of GDBL porosity on cell performance, many researchers have developed flow models in porous media [11–17]. In addition, Chu et al. [18] suggested GDBL with porosity gradient and investigated the effect of average porosity on the oxygen transport. Roshandel et al. [19] evaluated the effects on PEM fuel cell performance with porosity variation resulting from the compression pressure corresponding to assembly process. Zhan et al. [20,21] analyzed the distribution of liquid water saturation in GDL containing GDBL with uniform porosity, linear porosity gradient, and parabolic porosity distribution. In their researches, the effects of continuous distribution of GDBL porosity on gas diffusion and water removal were investigated based on a simplified one-dimensional model. Chen et al. [22] developed a two-phase flow model based on the multiphase mixture concept to investigate the transport characteristics of produced water passing through the cathode GDL containing GDBL with linear porosity gradient. Moreover, Huang et al. [23] predicts the enhancement of the water transport for linear porosity gradient in the cathode GDL with a three-dimensional, two-phase, non-isothermal model. With these efforts, numerically, it has been demonstrated that a GDBL with a linear porosity gradient is more favorable than that with uniform porosity for water removal from the catalyst layer to the flow channel.

Hydrophobicity, which is represented by contact angle, is also an important parameter in terms of water management. It was found that GDL with proper hydrophobicity effectively removes the liquid water [24–30]. To date, various hydrophobic agents such as polytetrafluoroethylene (PTFE) [24–28] and fluorinated ethylene propylene (FEP) [29,30] have been employed to GDBL. Moreover, it was found that CF_4 plasma treatment is also effective to make hydrophobic materials [31]. In general, a hydrophobic treatment is conducted by dipping a GDBL into the hydrophobic agent or spraying, brushing it on the GDBL. Then, hydrophobic agent permeates through the GDBL and it makes hydrophobic gradient in GDBL. Hence, some degree of hydrophobic gradient is an inevitable phenomenon, whether it is intended or not. For example, Kumar et al. [32] developed multistage PTFE treatment to enhance the mechanical and electrochemical durability of GDLs and observed a PTFE gradient in the GDL by adopting the treatment.

However, considering the manufacturing difficulties, A GDL with intended linear gradient of property is more about hope than reality in the near future. Recently, in order to overcome the manufacturing difficulties of linear gradient of porosity and/or hydrophobicity, double GDBL structure was suggested [33–35]. For convenience, Kong et al. [33,34] prepared double GDBL by stacking conventional uniform GDBLs and investigated the effect of the double GDBL on water retention for self-humidified PEM fuel cell. On the other hand, Oh et al. [35] developed double GDBL by mixing two different fibers for each layer and observed that the cell performances was improved with double GDBL under various humidity conditions. However, despite the practicality and usefulness of double GDBL on water management, there have been little discussions on the optimal design of double GDBL for water removal.

In this study, in order to improve the water removal ability of GDL, the optimal design of double GDBL was investigated with one-dimensional steady-state model based on the capillary pressure–saturation relationship. As shown in Fig. 1, it was assumed that each layer has uniform porosity and contact angle. Also, total thickness of GDBL-1 and GDBL-2 was fixed, while the thickness ratio of each GDBL can be changed (if the thickness ratio of GDBL-1 is 20%, the thickness ratio of GDBL-2 is 80%). With this model, the effect of porosity and contact angle arrangements of double GDBL was investigated under varied thickness ratio of GDBL-1 (0–100%). Then, in order to minimize the amount of residual water in GDL,

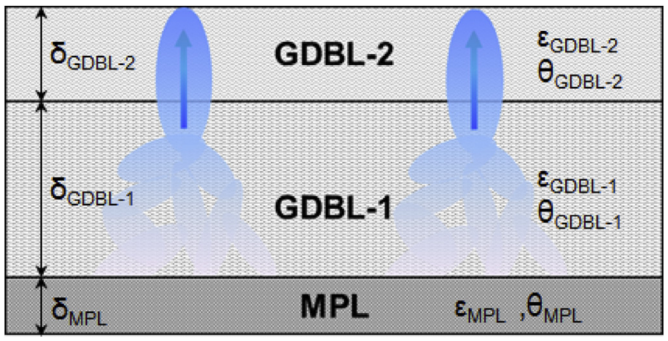

Fig. 1. Schematic design of the GDL composed of single MPL and double GDBL.

GDBL properties were optimized. This study provides an inspiration on the design of double GDBL functionalized on water removal to prevent flooding, especially under high current densities.

2. Numerical model

2.1. Liquid water saturation and water flux

As mentioned, water transport in GDL is strongly dominated by capillary force (multiplication of capillary pressure and active area). Then, the capillary pressure is defined as the difference in pressure across the interface between the non-wetting phase and the wetting phase. For the GDL, gas and liquid phases correspond to non-wetting phase and the wetting phase, respectively.

$$P_c = P_{nw} - P_w = P_l - P_g \tag{1}$$

In porous media, the capillary pressure is expressed as [13,14,20–23,36].

$$P_c = -\frac{\sigma \cos\theta}{(K/\varepsilon)^{0.5}} J(S) \tag{2}$$

where σ is surface tension (N m^{-1}), θ is contact angle (°), K is permeability (m^2), ε is porosity, and S is the liquid water saturation defined as the ratio of the pore volume occupied by water to the entire pore volume of ($S = V_l/V_p$). If S = 0, it means that the entire pore volume of GDL is fully dried. On the other hand, if S = 1, it means that the entire pore volume of GDL is filled with water. Then, Leverett J-function, J(S) can be obtained as a dimensionless function of liquid water saturation.

$$J(S) = \begin{cases} 1.417(1-S) - 2.120(1-S)^2 + 1.263(1-S)^3 & (\theta < 90^\circ) \\ 1.417S - 2.120S^2 + 1.263S^3 & (\theta > 90^\circ) \end{cases} \tag{3}$$

In hydrophobic GDL ($\theta > 90^\circ$), liquid phase pressure is higher than gas phase pressure ($P_c > 0$) and the produced water is transported from catalyst layer to channel passing through the GDL.

In recent years, various attempts have been made to relate the permeability to other more readily measurable properties and the most broadly known is the Kozeny-Carman relation [37]. Tomadakis and Robertson [37] also proposed a more comprehensive relation to predict the anisotropic permeability. Tamayol and Bahrami [38,39] related the permeability of porous media to the microstructure geometrical parameters. In addition, they modified their result to accommodate the effects of mechanical compression and PTFE contents. Among them, Kozeny-Carman equation is used in this study because of its simplicity and wide usage [20,21]. For random nonoverlapping fiber structures [37], the Kozeny-Carman

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