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Liquid water distribution in hydrophobic gas-diffusion layers with interconnect rib geometry: An invasion-percolation pore network analysis

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ABSTRACT

Water distribution in gas diffusion layers (GDLs) of polymer electrolyte membrane fuel cells (PEMFCs) is determined by the pore morphology of the GDL as well as the flow conditions between the GDL and the gas flow field, where interconnect ribs and gas channels are placed side-by-side. The present study employs a steady state pore network model based on the invasion-percolation (IP) process to investigate the water transport in the under-rib region, in the under-channel region, and in between those regions inside the GDL. The interconnect rib partially blocks the outlet surface of the GDL, which forces water transport paths from the under-rib region to grow towards the gas channel through an extra IP process. The pore network model predicts spatially non-uniform water distributions inside the GDL due to the interconnect ribs, especially with an increased saturation level in the under-rib region. Parametric studies are also conducted to investigate the effects of several geometrical factors, such as width of the rib and the channel, thickness of the GDL, and water intruding condition at the inlet surface of the GDL.

1. Introduction

Polymer electrolyte membrane fuel cell (PEMFC) is a promising replacement for internal combustion engines in vehicles due to high efficiency and zero-CO_2 emission [1]. Successful application of PEMFCs to automobile systems has been challenged by high cost of platinum catalyst, performance loss at low temperature, low durability, etc. Water management is among the most significant issues concerning the commercialization of PEMFCs because it is related with high power performance, essential for automobile powertrains. While a PEMFC system requires an adequate amount of water in the polymer membrane for fast proton exchange, excessive liquid water flooding in the porous components hinders reactant gas flow passages, resulting in limited current generation [2].

In order to address the water management problem, polymer membrane is humidified by supplying reactant gases

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with saturated water vapor in gas channels whereas the gas diffusion layers (GDLs) are coated with hydrophobic polymer (PTFE) for repelling liquid water [3]. When a PEMFC operates at high power conditions, the water generation rate often exceeds to the water removal rate resulting in the flooding of the GDL and the catalyst layer (CL). Thus, various efforts have been made to mitigate the flooding in porous media by proper management methods on the basis of the knowledge of water transport mechanisms [4–6]. Many experimental and numerical studies have been conducted to reveal the water transport mechanisms in the GDL and in the CL and thus to predict liquid water distributions in PEMFC systems [7–14]. For numerical model studies, the continuum two-phase flow models have been widely used, which incorporate the Darcy's law for flow in porous media and the experimentally determined correlations for capillary pressure and relative permeability [8,10–12]. However, recent numerical studies [15–20] suggested that the continuum transport theory may not be applicable or should be significantly modified since liquid water transport through hydrophobic GDLs is driven by the capillary fingering flow (capillary fingering regime) [21]. Previous pore network results of Lee et al. [15] proposed that the capillarity is the main driving force for the water transport in GDLs. The consecutive study [22] showed that pore morphological factors of GDLs, such as pore connectivity, pore size distribution, etc. play a major role on water distribution because the capillary fingering flow is governed by the invasion-percolation process which makes the liquid water to preferentially occupy a pore with the largest size in hydrophobic porous media.

Experimental studies adopted in-situ visualization techniques such as X-ray tomography [23–25] and neutron radiography [26,27] to measure liquid water distribution inside the GDL, in the in-plane or through-plane directions. Using the high resolution neutron radiography, Turhan et al. [27] presented that water distribution in a cathode GDL is rather independent of the water production rates under the operating currents of 0.2 A m^{-2} and 1.0 A m^{-2}. Their observation, i.e., the weak influences of the water flow rate on the invasion-percolation process, supports the proposition of Lee et al. [15] that the capillary fingering flow is the dominant mechanism for the water transport in the cathode GDL. The observation by Hartnig et al. [23] using the synchrotron X-ray tomography seems to be opposite to the results of Turhan et al. [27], indicating strong dependence of the water distribution in a GDL on the water production rate. However, in their experiments, gas in flow channels was relatively dry so that water could be removed as vapor; this results in low water accumulation in the cathode GDL at low current conditions.

It has been observed in many experiments that water accumulation in the GDL is more severe under an interconnect rib than under a gas channel [28–32]. Kowal et al. [28] quantified the water volume in a carbon paper GDL and obtained a volume ratio of 6:4 for liquid water stored under ribs to that under channels (the rib width was the same as the channel width). Boillat et al. [29] obtained high resolution images for water distribution across the MEA structure using neutron radiography and showed strong variation of water content under the ribs and channels. Deevanhxay et al. [30] discovered in their soft X-ray radiography images that, at low current density, liquid water accumulated under the rib but not under the channel. They attributed the localized water generation to the enhanced oxygen reduction reaction in the under-rib region due to faster electron transfer. Deevanhxay et al. [31,32] also investigated the transient liquid water transport in a microporous layer (MPL) and a GDL under interconnect ribs and reported that pore morphology significantly impacts on water accumulation behaviors. Despite of technological advances for visualizing water distributions in the GDL, water transport mechanism with interconnect rib geometries has not been well understood. Improving the configuration of gas flow field plates of PEMFCs cannot be achieved without understanding how the rib design influences liquid water distribution inside GDLs. Thus, experimental studies have been conducted for the practical purposes related with gas flow field designs. Yoon et al. [33] performed several experimental tests to investigate the effects of channel and rib widths on the performance of a PEMFC and concluded that the narrower ribs lead to a better cell performance. Numerical models [34,35] also have been developed for exploring the channel and rib designs of PEMFCs; however, these models generally failed to capture the microscopic liquid water transport in GDLs which can significantly influence the performance of PEMFC at high current conditions.

This study investigates the water transport and saturation distribution in the GDL under the interconnect rib and under the channel. A pore network model based on an invasion-percolation path-finding process, developed in the previous studies [22,36], is used for the calculation. Parametric studies are also conducted to clarify the effects of pore geometrical factors, such as width of the rib and the channel, thickness of the GDL, and water intruding condition at the inlet surface of the GDL (at the CL/GDL interface).

2. Theory and calculation

2.1. *Pore network generation*

The pore network geometries developed in the previous studies [22,36] are used to simulate the pore morphology of GDLs. The calculation domain is presented in Fig. 1(a) as the network of regularly stacked cubic cells where pores and throats are enclosed. The boundary conditions (BCs) are also shown in Fig. 1(a), where the bottom plane of the domain is the inlet boundary through which liquid water enters the pore network. The outlet boundary is corresponding to the central part of the top plane, which is open to the gas channel under a constant air pressure. The top plane underneath the interconnect rib is regarded as the closed wall boundary because the interconnect rib does not allow liquid water exhaust out of the GDL. Cyclic connectivity is assumed for side planes to extend the calculation domain infinitely in planar x and y directions.

At the inlet boundary, a spatially uniform flux of liquid water is assumed to enter the GDL from the CL. That is, liquid water is assumed to randomly invade into the pores adjacent to the inlet boundary while the number of those water-invaded pores is prescribed according to the inlet invaded