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Numerical simulation of two-phase cross flow in microstructure of gas diffusion layer with variable contact angle

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ABSTRACT

For a gas diffusion layer (GDL) with hydrophobic treatment, its hydrophobicity (contact angle) may change along the through-plane direction, and lead to different two-phase transport characteristics. In this study, such variable contact angle is implemented in a three-dimensional unsteady two-phase model based on the microstructure of GDL to study the liquid water transport characteristics along the in-plane direction caused by cross flow. It is found that during a liquid water intrusion process, the liquid water first moves through some of the pores that are easy to penetrate, forming a "fingering transport" mode; and after that, with more liquid water accumulated, the rest of the pores can also be filled, forming a "steady transport" mode. Increasing the differential pressure or decreasing the contact angle of GDL accelerates the liquid water intrusion, and this effect is weakened at higher differential pressures and contact angles. For a GDL with variable contact angle, the water transport characteristics in different cross sections normal to the through-plane direction with different contact angles are similar to the corresponding fixed contact angle cases in these cross sections, and the overall process of water intrusion with variable contact angle is similar to its corresponding average fixed contact angle case.

Introduction

Fuel cell is an eco-friendly device that converts the chemical energy in certain fuel to electrical energy directly. During the past two decades, fuel cell has attracted increasing attention due to its outstanding merits such as zero/low emission, high efficiency, and low noise. However, the high cost and insufficient durability hindered the wide application of fuel cell. The proton exchange membrane (PEM) fuel cell was firstly developed by General Electric Company in 1950s [1]. With active ongoing research, it has been found that an effective control of the dynamic balance between liquid water removal and hydration plays an important role on the improvement of performance and durability, as well as cost reduction [2].

During the operation of a PEM fuel cell, besides the reaction-generated water in the catalyst layer (CL), external water is usually provided from the hydrated gas flow to humidify the membrane-electrode assembly (MEA), which can reduce the ohmic resistance of membrane. On the other hand, especially for cathode, extra water needs to be removed by the gas flow from the channel, to avoid flooding in which liquid

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Nomenclature

F	source term of surface tension, kg m^{-2} s^{-2}
g	gravitational acceleration, m s^{-2}
P	static pressure, Pa
υ	velocity, m s^{-1}

Greek letters

α	volume fraction
θ	contact angle, °
κ	surface curvature, m
μ	viscosity, N s m^{-2}
ρ	density, kg m^{-3}
σ	surface tension coefficient, N m^{-1}

Subscripts and superscripts

1	air
2	liquid water

water could block the micro pores of gas diffusion layer (GDL) and CL and hinder the reactant transport toward CL. The water and reactant in GDL can transport along the through-plane direction as shown in Fig. 1(a); and it can also move along the in-plane direction through the porous material of GDL as shown in Fig. 1(b), which is called cross flow [2–6]. Among different types of channels, the serpentine and interdigitated flow channels exhibit excellent performance on water removal due to the noticeable effects from cross flow compared with the other flow channels [2–6].

Due to the important role of cross flow, a lot of researches have been conducted to study the effects of this phenomenon on water transport. Sun et al. [7] developed a numerical model to study the effect of channel designs on the cross flow in serpentine flow channel case. It is found that the cross flow can reduce the pressure drop between the adjacent channels, and it can be enhanced by increasing of the Reynolds number. Park et al. [8] developed a three-dimensional two-phase model based on the microstructure of GDL, and numerically investigated the two-phase transport processes along the in-plane direction. Tehlar et al. [9] developed a numerical model to investigate the effect of cross flow on the PEM fuel cell performance, and they reported that the cross flow from channel to channel can enhance the current density, which becomes more significant with thicker GDL. Williams et al. [10] found that the cross flow can enhance the limiting current density in their experiments. Chen et al. [11] investigated the effect of porous structure and channel design on the pore-scale mass transfer by lattice Boltzmann method (LBM), and they found that narrow land can enhance the water removal ability but the high contact angle dose not. Suresh et al. [12] concluded that the transport of water in microstructure of GDL is by the means of fingering and channeling type, and the cross flow can enhance the water removal. Didari et al. [13] showed that the pressure variation in GDL is very small, and the main factor affecting the water transport is capillary action. Wargo et al. [14] reconstructed the three-dimensional structure of a GDL by the means of in-house structural analysis protocols and a full pore morphology model, and they found that the porous material has a more favorable transport along the through-plane direction. Park et al. [3,15] have experimentally studied the cross flow in GDL by visualization of liquid water transport. The effects of GDL deformation [16] and dynamic wettability [17] on the transport characteristics and performance were also investigated.

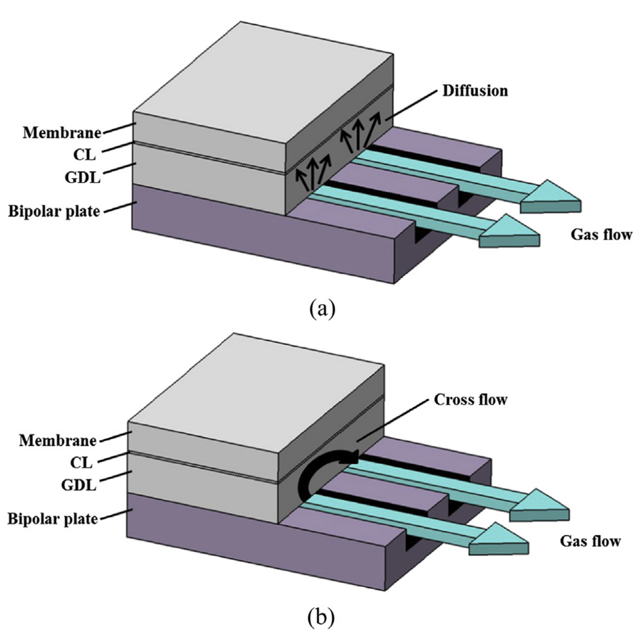

Fig. 1 – Schematic of through-plane (a) and in-plane (b) transport.

During fabrication process, GDL material should be treated for hydrophobization. In the process of hydrophobization, GDL material is typically put into polytetrafluoroethylene (PTFE) solution for full immersion, which is aimed to decrease the mass transfer loss [18] and enhance conductivity [19]. Then it is dried and sintered, which can lead to a smaller hydrophobicity in average inside the GDL than that at the surface [20]. Therefore, this process could result in a non-uniform contact angle of GDL, which is smaller inside the GDL. However, there are not many studies in the effect of non-uniform contact angle on the process of water transport.

In order to investigate the process of water intrusion in GDL, a three-dimensional two-phase unsteady volume of fluid (VOF) model of the microstructure of GDL has been developed in this study. To simulate the realistic situation of water transport with cross flow in GDL, contact angle gradient in GDL is established. In addition, the effects of pressure gradient and different variations of contact angle gradient on the process of water intrusion are investigated based on the model simulation.

Numerical model

Computational domain

In this study, a three-dimensional fibrous porous structure of GDL is reconstructed by three-dimensional solid cylinders, and the computational domain is shown in Fig. 2. The related