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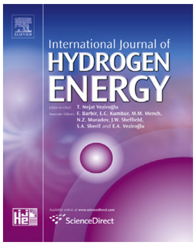

Short Communication

Effects of hydrophilic/hydrophobic properties of gas flow channels on liquid water transport in a serpentine polymer electrolyte membrane fuel cell

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ABSTRACT

The droplet dynamics in the serpentine flow channel of a hydrogen fuel cell has been numerically investigated to obtain ideas for designing a serpentine channel with the aim of effectively preventing flooding. Three-dimensional two-phase flow simulations employing the volume of fluid (VOF) method have been performed. Liquid droplets emerging from four adjacent pores at the hydrophobic bottom wall are subjected to airflow in the bulk of the serpentine flow channel. The effects of contact angle variation of the channel walls on liquid water removal have been tested in terms of liquid water saturation and coverage of liquid water on the gas diffusion layer (GDL) surface. The numerical results show that the hybrid case, which consists of hydrophilic channel walls at the straight part and hydrophobic walls at the turning part of the serpentine flow channels, enhances water removal compared with two other cases in which the channel wall is homogeneously hydrophilic or hydrophobic. The three-dimensional visualization of liquid water droplets reveals that the hydrophobic wall at the turning part reduces the water saturation in the channel and the hydrophilic wall at the straight part prevents the liquid water from covering the GDL surface.

Introduction

The polymer electrolyte membrane fuel cell (PEMFC) has been widely used because it shows high power density, rapid start-up and response capability, and excellent durability in comparison to other types of fuel cells. The PEMFC is an electrochemical device that generates electricity directly using hydrogen in the fuel and oxygen in the air and it requires a constant supply of hydrogen and oxygen in the active area. However, if the liquid water generated from the electrochemical reaction of PEMFC is not properly discharged in the channel, flooding occurs, prohibiting the fuel supply and deteriorating in performance of the fuel cell. Thus, liquid water control in the channel of the fuel cell is critical for designing and optimizing PEMFC and has been widely studied in the industry and academia [1].

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For an efficient discharge of liquid water, a variety of shapes of gas flow channels have been developed, and the functions of such flow channels include the supply and release of reaction gas, electric conductivity between cells, mechanical strength, and liquid water removal. Among several types of gas flow channels, serpentine flow channels have been most widely used in the PEMFC flow field design because they exhibit superior liquid water removal performance despite significant parasitic power loss due to the high pressure drop [2]. Serpentine flow channels consist of long straight parts and turning parts with sharp or round corners. With visualizing liquid water distribution in the serpentine flow channel using neutron imaging [3], transparent cells [4,5] or other techniques [6], it was reported that liquid water was not fully removed from the turning part. Le et al. [7] compared the results of volume of fluid (VOF) simulation of the flow channel with that of the visualization experiment and confirmed that the VOF method is suitable for estimating the flow of liquid water, subsequently suggesting that the main factors affecting liquid water removal are the airflow velocity, contact angle of the channel wall, and surface tension. Quan [8] performed a VOF simulation on a U-shaped serpentine channel and reported that the airflow velocity and wall adhesion of water droplets play an important role in the liquid water behavior at the turning part. It was also reported that flooding could occur after liquid water passed the turning part, which implies that the liquid water should properly go through the straight part as well as the turning part for effective liquid water removal in the entire serpentine channel. On the other hand, Kim et al. [9] performed numerical simulations with adjusting the contact angles of the walls in the serpentine flow channel and reported that the droplet discharge time was shorter in the hydrophobic wall than in the hydrophilic wall.

For effective discharge of liquid water in the serpentine flow channel, liquid water should flow well not only at the turning part, but also at the long straight part, which occupies most of the flow channel. Many studies on liquid water removal in the straight micro-channel have been performed through experiments and computational fluid dynamics. With flow visualization using transparent channel configurations, Zhang et al. [10] showed that the detachment of liquid droplets from the surface of gas diffusion layer (GDL) occurs via two modes; one is by the shear force of the gas flow stream and the other is by capillary wicking onto the hydrophilic side walls of the channel. Their theoretical analysis suggests that liquid water on the GDL surface can be sufficiently removed by the corner flow induced by the wicking mode under relatively low flow rate (or stoichiometry) conditions. The effects of channel wall contact angle on water removal in the straight channel have been tested by several authors. Cai et al. [11] reported that a hydrophilic channel sidewall is effective in avoiding water accumulation on the MEA surface. Recently, Kim et al. [12] also showed that droplets near a hydrophilic channel sidewall can be easily removed by corner flow along the top edge despite the reduced water discharge velocity, which results in the reduction of the GDL surface coverage by liquid water.

Based on the results of previous studies on the behaviors of liquid water in the gas channel of PEMFC, it can be expected that liquid water in the serpentine channel is discharged more effectively in a hydrophobic channel wall at the turning part and in a hydrophilic wall at the straight part. Hence, this study performed three-dimensional VOF simulations for the hybrid case which consists of hydrophilic channel walls at the straight part but hydrophobic walls at the turning part of the serpentine flow channel. In addition, numerical simulations for the reference cases in which the channel walls were either all hydrophilic or hydrophobic were carried out, and its result was compared with that of the hybrid case. For each wall type, the droplet behavior and liquid water saturation in the channel were analyzed in the spatiotemporal context, and the characteristics of the water removal in the serpentine channel were examined.

Computational details

The flow in the gas channel was assumed as being unsteady, isothermal, and laminar three-dimensional flows, and heat generation and heat transfer were considered to be negligible. In this study, the VOF model was employed for the two-phase flow simulation in the gas channel. The governing equations for the two-phase flow in the channel are the continuity equation and the Navier-Stokes equation expressed as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \tag{1}$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V}) = -\nabla p + \nabla \cdot \left(\mu\left(\nabla \mathbf{V} + \nabla \mathbf{V}^{T}\right)\right) + \rho \mathbf{g} + \mathbf{F} \tag{2}$$

where p is the pressure, ρ and μ are the averaged volume density and the coefficient of viscosity, respectively, $\mathbf{V}$ is the fluid velocity, and $\mathbf{g}$ is the gravitational acceleration. $\mathbf{F}$ denotes a momentum source term related to the surface tension and, in accordance with the continuum surface force (CSF) model [13], is expressed as follows:

$$\mathbf{F} = \sigma \kappa_k \frac{\rho \nabla \alpha_k}{\langle \rho \rangle} \tag{3}$$

where σ is the coefficient of the surface tension, $\langle \rho \rangle$ is the average density of two fluids, and κ_k denotes the local curvature of the interface surface calculated by the gradient of the surface normal vector ($\mathbf{n} = \nabla \alpha_k / |\nabla \alpha_k|$).

$$\kappa_k = \nabla \cdot \mathbf{n} \tag{4}$$

The volume fraction of fluid k, α_k is governed by volume fraction equation which is solved in every computational cell:

$$\frac{\partial \alpha_k}{\partial t} + \mathbf{V} \cdot \nabla \alpha_k = 0 \tag{5}$$

The wall adhesion is taken into account by imposing the unit normal vector of the interface at the wall as

$$\mathbf{n} = \mathbf{n}_w \cos \theta + \mathbf{t}_w \sin \theta \tag{6}$$

where $\mathbf{n}_w$ and $\mathbf{t}_w$ are unit vectors normal and tangential to the solid wall, respectively, and è is the contact angle. In the present study, all the simulations have been carried out using