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Numerical simulation of water droplet dynamics in a right angle gas channel of a polymer electrolyte membrane fuel cell

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ABSTRACT

The dynamics of liquid water emerging from a micro pore on a gas diffusion layer (GDL) surface into a right angle gas channel of a polymer electrolyte membrane (PEM) fuel cell is investigated numerically with the volume of fluid method. As the GDL surface contact angle decreases, droplets from the outer and inner pores tend to move along the side walls or the lower edges and droplets from the center pore show complex patterns of behavior. As the hydrophobicity of the side and top walls increases, the GDL surface water coverage ratio increases, while the water volume fraction decreases. While the higher GDL surface water coverage ratio hinders the diffusion of reactants to reaction sites, the lower water volume fraction is advantageous in preventing water flooding in the gas channel. Therefore, in general gas channel geometry, the GDL surface water coverage ratio and the water volume fraction may compete with each other to determine the performance of PEM fuel cells, while changing the hydrophobicity of the side and top walls. As the air inlet velocity increases, liquid water moves faster and the water volume fraction decreases. As the water injection velocity increases, the moving speed of the water and the water volume fraction increase.

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Introduction

The polymer electrolyte membrane (PEM) fuel cell has been considered to be a promising candidate for solving future energy and environmental problems due to its zero/low emission, low operating temperature, low noise/vibration, and high power density. PEM fuel cells have a wide range of applications for portable, mobile, and stationary power systems including automobiles, and combined heat and power generation units [1–3]. Compared with other types of fuel cells, much research has been carried out by various groups to improve the performance, durability, and cost of PEM fuel cells [4–8]. Especially, the water management in the gas channels is one of the most important issues in PEM fuel cell studies because the level of membrane hydration must be in a proper range for the best performance and sufficient amounts of reactants should be delivered to the cathode reactions sites [5,6]. Without a sufficient level of water, membrane dehydration results in performance degradation and may cause

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Nomenclature

Bo	Bond number
Ca	capillary number
$\vec{F}$	momentum source term due to surface tension
$\vec{g}$	gravitational acceleration vector
$\vec{n}_2$	unit normal vector computed from local gradients in surface normal at gas–liquid interface
p	pressure
Re_1	Reynolds number of gas phase
Re_2	Reynolds number of liquid phase
t	time
$\vec{u}$	velocity vector of mixture
$\vec{u}_1$	velocity vector of gas phase
$\vec{u}_2$	velocity vector of liquid phase
$V_{in,air}$	air inlet velocity
$V_{in,water}$	water inlet velocity
We	Weber number

Greek letters

α_1	volume fraction of gas phase
α_2	volume fraction of liquid phase
θ	contact angle
κ_2	surface curvature of liquid phase
μ	viscosity of mixture
μ_1	viscosity of gas phase
μ_2	viscosity of liquid phase
ρ	density of mixture
ρ_1	density of gas phase
ρ_2	density of liquid phase
σ	surface tension coefficient

Subscripts

1	gas phase
2	liquid phase

permanent material damage [8]. On the other hand, excess water causes the so-called water flooding phenomena due to water production from the electrochemical reactions and water condensation at the low operating temperature (typically about 80 °C) of PEM fuel cells. Water flooding is a critical problem in automotive applications of PEM fuel cells, where high current density is required. With increasing current density, excessive liquid water severely reduces the rate of reactant supply to the reaction sites and degrades the performance of PEM fuel cells [6,7]. In addition, water flooding can also cause ineffective heat removal, non-uniform current density distribution, membrane swelling, and the delamination of fuel cell components due to repeated thermal cycling [8].

In practical applications, a number of single PEM fuel cells are usually connected in series to form a PEM fuel cell stack that can meet sufficient power requirements. A single PEM fuel cell has a polymer electrolyte membrane at the center. Catalyst layers (CL), gas diffusion layers (GDL), and bipolar plates (BP) are attached on the membrane, in that order, on both the anode and cathode sides. Gas channels (GC) are grooved on the bipolar plates to supply fuel and oxidant, which are typically hydrogen gas and air. At the anode, hydrogen gas flows into the GC through the GDL to the CL. In the anode CL, hydrogen decomposes into protons and electrons. The protons move to the cathode CL through the membrane and the electrons travel to the cathode through an external circuit. At the cathode, oxygen gas flows into the GC through the GDL to the CL. In the cathode CL, oxygen reacts with the protons and electrons from the anode, producing water and heat. To maintain the high proton conductivity of the PEM, membrane hydration is controlled by supplying externally humidified reactant gases. Liquid water accumulation in the GC or GDL results in water flooding and reactant transport to the CL is hindered. Water flooding is most severe near the cathode CL because water is produced in this layer and electro-osmotic drag (EOD) causes water migration from the anode CL to the cathode CL. Back diffusion of water from the cathode to the anode is also possible depending on the relative concentrations of water [6].

A number of experimental techniques have been used to understand the behavior of liquid water in the GCs and GDLs of PEM fuel cells. As an important diagnostic tool, the two-phase pressure drop in the reactant GCs can be used to measure the effectiveness of water management [5,9]. The pressure drop increases with current density, which is proportional to reactant flow rates and water production rates. Liu et al. showed that the total pressure drop mainly depended on the resistance of the liquid water to the gas flow and could be used to distinguish the different flow patterns [9]. However, pressure drop measurements do not provide information regarding the location of water flooding. Various fuel cell visualization techniques explain the qualitative and quantitative features of the two-phase flow patterns. Bazylak reviewed on both in situ and ex situ liquid water visualization techniques for PEM fuel cells, including direct optical photography, nuclear magnetic resonance (NMR) imaging, neutron imaging, X-ray microtomography, synchrotron X-ray radiography, and scanning electron microscopy (SEM) [8]. Direct optical visualization techniques provide high temporal and spatial resolution information about the liquid water behavior in the GCs and upper layers of the GDL [10,11]. Yang et al. visualized a variety of phenomena in the GC such as the sporadic appearance of droplets from the GDL surface, liquid film formation along the channels, and channel clogging [10]. Spernjak et al. investigated the effect of varying GDL properties on liquid water removal with a transparent single serpentine PEMFC [11]. In addition, fluorescence microscopy in conjunction with optical photography is a useful tool to visualize the microscale transport of liquid water near and on the surface of the GDL [12]. Despite the advantages of optical imaging methods, they suffer several disadvantages such as changes of the channel surface properties due to the adoption of optically transparent windows and fogging of the windows due to high temperature and a fully saturated gas stream in the GCs. To overcome these disadvantages of the conventional optical imaging methods, more advanced imaging techniques have recently been applied to provide in-situ visualization of liquid water dynamics in PEMFCs [13–23].

Tsushima et al. used NMR imaging to measure the spatial distribution of water in a Nafion membrane of an operating

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