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Numerical simulations of water droplet dynamics in hydrogen fuel cell gas channel

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HIGHLIGHTS

- We investigated the droplet dynamics from two pores, using a 3D VOF model.
- Hydrophilic sidewall shows more effective fuel transport to the reaction site.
- Clogging was more likely to occur for hydrophobic channel wall.

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ABSTRACT

The droplet dynamics in the cathode gas flow channel of a hydrogen fuel cell has been numerically investigated to obtain ideas for designing a flow channel to effectively prevent flooding. Three-dimensional two-phase flow simulations employing the volume of fluid method have been performed. Liquid droplets emerging from two adjacent pores at the hydrophobic bottom wall are subjected to airflow in the bulk of the gas flow channel. The effects of various parameters (pore distance, locations, sidewall contact angle, and airflow rate) on the liquid water removal from the gas channel have been investigated in terms of liquid water saturation, coverage of liquid water on the gas diffusion layer (GDL) surface, and change in the pressure drop in the channel. The numerical results show that the coalescence of two adjacent droplets enhances the water removal as compared to two separate, small droplets. It is also observed that droplets generated near the hydrophilic sidewall can be attached to the upper corner of the channel walls, which prevents the liquid water from covering the GDL surface, whereas the hydrophobic sidewall may cause clogging of the gas channel with liquid water at a low airflow rate.

1. Introduction

A polymer electrolyte membrane fuel cell (PEMFC) has a wide range of applications because of its diverse advantages, including high power density, relatively simple structure, rapid start-up and response capability, and excellent durability in comparison to other types of fuel cells. Further, it has attracted considerable attention as an attractive source of clean energy because of its electrochemical mechanism capable of generating electrical power directly from an electrochemical process. In addition to electricity, a PEMFC produces water as a byproduct. Water is generated through the electrochemical reaction between the oxygen fed through the gas flow channel and the hydrogen ions traveling through the electrolyte, whereby flooding may result from an inadequate liquid water discharge in the channel, thus impeding the fuel transport to the reaction site and leading to problems of diminished fuel cell function. Therefore, to improve the PEMFC performance, it is important to control and manage the water generated during the electrochemical process.

From this perspective, the study of the droplet behaviors in the gas flow channel is of vital importance for enhancing fuel cell performance, and hence, related research has been conducted extensively. Table 1 lists several recent experimental studies on liquid water behaviors in a fuel cell gas channel (GC). Most studies have been performed using a transparent fuel cell to visualize the liquid water behavior in the flow channel. Zhang et al. [1] showed different flow patterns of liquid water for airflow rates in the gas channel and reported that the corner flow pattern leads to efficient water removal from the gas channel with a relatively low parasitic power. Ous et al. [2] investigated the effects that the operating conditions of a transparent PEMFC, such as reactant stoichiometry,

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Nomenclature

A	area (m^2)
A_w	relative coverage of liquid water on the GDL surface
d	droplet diameter (m)
F	force (N), momentum source (N m^{-3})
g	gravitational acceleration (m s^{-2})
H	channel height (m)
n	unit normal vector
p	pressure (Pa)
R_{dp}	relative change in the pressure drop in the gas channel
S_w	liquid water saturation in the gas channel
t	time (s)
V	velocity (m s^{-1})

Greek letters

α	volume fraction
δ	distance (m)
κ	local curvature of the interface surface (m^{-1})
μ	viscosity (kg (m s)$^{-1}$)
θ	contact angle (rad, °)
ρ	density (kg m^{-3})
σ	surface tension (N m^{-1})

Subscript

0	single phase flow
d	drag
k	fluid index
w	water, wall

cell temperature, and electric load, have on the liquid water formation and extraction in serpentine flow channels. Further, Hsieh et al. [3] examined different channel configurations in addition to diverse operating conditions and reported that a uniform current distribution may be obtained in an interdigitated flow channel despite a considerable pressure drop. Zhan et al. [4] conducted an in-depth study on water transport, taking into account the operating conditions, including current density, temperature, air stoichiometry, and relative humidity. On the other hand, there was a study investigating, along with the water transport in an active fuel cell, the dynamic evolution of a water droplet by feeding water from a pore at a predetermined velocity [5].

In parallel with experimental studies, a number of studies based on numerical simulation have also been carried out (Table 2). Most studies have revolved around the GC or PEMFC cathode [6–17], and of late, there have been studies investigating the liquid water transport in the PEMFC itself including the membrane electrode assembly (MEA) and the gas diffusion layer (GDL) [18–20]. Some such studies included a simulation of the conditions in which liquid water is gradually fed from the GDL pore to GC [9,12–14], whereas others involved a simulation with a given liquid water distribution as the initial condition [6–8,18]. Therein, a smooth hydrophobic surface was used as the GC bottom surface to express the GDL, and a hydrophilic condition was provided for the top and sidewall surfaces of the GC. Chen et al. [9] went further and introduced a hybrid structure model cube simulating a realistic GDL structure. The majority of these studies focused on the liquid water dynamics from the perspective of fluid dynamics, and some recent papers conducted in-depth studies on the coupled process of liquid water transport and reactant transfer [9,15,19]. According to their study results, the transport of liquid water in the GC follows the route of the droplets generated from the pores as they are detached from pores and travel at the airflow rate; this process is influenced by the channel design and the channel surface. Further, factors influencing the liquid water dynamics in the GC are very diverse, such as operating conditions, geometrical shapes of the channel, and the interactions among droplets.

However, most of the existing studies on the droplet behaviors in a channel are limited to a single droplet generated from a single pore in the channel, and the mechanism of inter-droplet interaction is difficult to understand. Moreover, there is a lack of studies closely investigating the interaction between multiple droplets and the channel wall. Therefore, this study investigated the inter-droplet interactions under the condition of discharging water from two pores into the airflow stream of the cathode channel, using a 3D volume of fluid (VOF) model. The droplet dynamics was analyzed in the spatiotemporal context with respect to various cases dependent on the distance between the pores, distance from the gas channel sidewall, contact angle of sidewalls, and airflow rate change. Further, a comparative analysis was carried out on the liquid water saturation and the liquid water coverage on the GDL surface in the channel and on the time-dependent change in the pressure drop.

2. Computational details

The flow in the GC was assumed as being unsteady, isothermal, and laminar 3D flows, with negligible heat generation and heat transfer. This study employed a VOF model of a two-phase flow. VOF is a surface-tracking method employed to study the location of the interface between two unmixable fluids. The equations governing the two-phase fluid flow are the continuity equation and the Navier–Stokes equation expressed as follows:

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

Table 1
Experimental studies on droplet dynamics in fuel cell gas channels.

Authors and published year	GC shape	Research aspects	Condition
Zhang et al., 2006	Transparent PEFC	Effects of gas flow velocity on water droplet dynamic behaviors	Electrochemical reaction
Ous et al., 2009	Transparent PEMFC	Effect of air stoichiometry, hydrogen stoichiometry, temperature, and electric road on the accumulation of liquid water in PEMFC flow channels	Electrochemical reaction
Hsieh et al., 2011	Four different flow channels	Effects of pressure drop, hydrogen, airflow rates, cell temperatures, water accumulation, and current density distribution on the cathode of a PEMFC	Electrochemical reaction
Zhan et al., 2012	Transparent PEMFC	Transport process of liquid water with different operating conditions	Electrochemical reaction
Wu et al., 2012	Transparent channel with water inlet pore	Flow regimes under different air and water velocities; effect of air velocity on the dynamic contact angle of the droplet	Injection of water from a small pore