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3D simulations of the impact of two-phase flow on PEM fuel cell performance

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ABSTRACT

Water management is a major issue in the operation of PEM fuel cells. Two-phase flow has been commonly observed in PEM fuel cell channels from experiments. One of the two-phase flow patterns, the slug flow, has great negative impacts on the fuel cell performance. In this work, the impact of two-phase flow patterns, especially the slug flow, on the fuel cell performance was simulated using a 3D volume fluid model (VOF) coupling with a 1D membrane electrode assembly (MEA) model. The proposed model is capable of describing the two-phase flow patterns, especially the slug flow in the cathode side gas flow channels. The comparison of fuel cell performance between single phase flow and two-phase flow shows that the presence of slug flow decreases the cell voltage output in the mass transport region, but has little effect in the kinetic and ohmic region. However, the slug flow causes great increase of overall pressure drop, which should be avoided during the PEM fuel cell operation. Effects of gas stoichiometric flow ratios on the fuel cell performance were then simulated. Increasing the gas flow rate significantly broadens the ohmic region, enabling the fuel cell to be operated at higher current densities. However, given a fixed current density during fuel cell operation, too high a gas flow rate will result in high pressure drops with little improvement in the fuel cell performance. Changing channel wall or MEA surface wettability also has great impact on the PEM fuel cell performance and two-phase flow pattern in the channel. Using a more hydrophobic MEA surface is helpful to extend the ohmic region and increase PEM fuel cell performance. Using too hydrophilic or too hydrophobic channel wall is not recommended, since either reduces the cell output voltage.

1. Introduction

Polymer electrolyte membrane fuel cells (PEMFCs) have received great attentions in recent years for their high efficiency and low operating temperatures compared to other types of fuel cells. One major issue in the design and operation of PEM fuel cells is the water management. Proper amount of water should be left in the membrane to maintain high proton conductivity; meanwhile, liquid water in the gas flow channel and gas diffusion layer (GDL) should be avoided in the fuel cell because it causes high pressure drops and blocks the reactant pathway. However, it is challenging to prevent the formation of liquid water, especially at high current densities. Liquid water in the fuel cell leads to the gas–liquid two-phase flow in the fuel cell, which was found to have great impacts on the overall fuel cell efficiency, because the presence of liquid in the gas channel causes severe damage of the cell performance (Tüber et al., 2003) and high parasitic energy loss (Anderson et al., 2010a).

Extensive work, both experimental and simulation, has been conducted on the two-phase flow in PEM fuel cell gas flow channels. A recent review (Anderson et al., 2010b) emphasized the gas–liquid two-phase flow in minichannels or microchannels related to PEM fuel cell applications, and showed that the two-phase flow in gas flow channel has great impacts on the overall fuel cell performance. However, some issues, such as the identification and prediction of two-phase flow patterns and flow regimes in an operating PEM fuel cell and the quantification of two-phase flow's impact on the fuel cell performance, are still not well documented in the literature.

From experimental observations (Dunbar and Masel, 2008; Hussaini and Wang, 2009; Liu et al., 2008; Lu et al., 2009), the presence of liquid water in gas flow channels may result in several two-phase flow patterns depending on the operating conditions, such as mist flow, droplet flow, film flow, and slug flow. However, due to the limitation of existing experimental or visualization techniques (Bazylak, 2009), it is difficult to quantify the relationship between the two-phase hydrodynamics

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Nomenclature

C_O^{m-}	Oxygen concentration at membrane (mol m^{-3})
C_O^{cl}	Oxygen concentration at catalyst layer (mol m^{-3})
C_O^{ref}	Cathode oxygen reference concentration (mol m^{-3})
$D_{O_2}^{eff}$	Oxygen diffusion coefficient (m^2 s^{-1})
E_0	Open circuit potential (V)
F	Faraday constant (C mol^{-1})
F_{vol}	Momentum sources (N m^{-3} s^{-1})
H_O	Henry's constant for oxygen (Pa m^3 mol^{-1})
I	Local current density (A m^{-2})
I_{op}	Operating current density (A m^{-2})
$i_{o,c}$	Cathode exchange current density (A m^{-2})
J_{O_2}	Oxygen molar flux (mol s^{-1} m^{-2})
L_G	Thickness of GDL (m)
N_{O_2}	Oxygen molar flow rate (mol s^{-1})
N_{H_2O}	Water molar flow rate (mol s^{-1})
p	Static pressure (Pa)
P_{op}	Operating pressure (Pa)
R	Gas constant (J K^{-1} mol^{-1})
S_A	Local GDL surface area (m^2)
S_m	Mass sources (kg m^{-3} s^{-1})
S_i	Mass sources of each species (kg m^{-3} s^{-1})
T	Temperature (K)
U	External voltage (V)
Y_i	Mass fraction of species i

Greek symbols

α	Membrane water transfer coefficient
α_c	Cathode transfer coefficient
δ	Oxygen mass transfer coefficient (s mol m^{-1} C^{-1})
ε	Volume fraction
η_c	Cathode overpotential (V)
λ	Gas stoichiometric ratio
μ	Viscosity (kg m^{-1} s^{-1})
θ_w	Static contact angle
ρ	Density (kg m^{-3})
$\overline{\sigma}$	Effective conductivity (S m^{-2})

and PEM fuel cell performance. Computational modeling and simulation, alternatively, are capable of giving more details and quantitative results inside the fuel cells. The pioneer work of PEM fuel cell modeling can be traced back to 1991 from Springer (1991) and Bernardi and Verbrugge (1991). Those early PEM fuel cell models usually assumed that water only existed in the gas phase, i.e., the two-phase flow was not considered. Since 2000, two-phase flow models began to be incorporated in the PEM fuel cell modeling (Weber and Newman, 2004), and so far several two-phase models have been applied at various length scales, including the multi-fluid model, mixture model, volume of fluid method (VOF), pore-network model and Lattice Boltzmann method (Anderson et al., 2010b).

To better understand the impact of two-phase flow on the PEM fuel cell performance, a two-phase flow model must first be able to reproduce the two-phase flow patterns at the channel length scale. Multi-fluid and mixture models are not capable of tracking the gas–liquid interface, thus the two main flow patterns, i.e., droplet flow and slug flow (Theodorakakos et al., 2006a), cannot be obtained. Pore-network model and Lattice Boltzmann method, on the other hand, are only applicable at micro-scale so far, therefore not suitable for large-scale simulations. The VOF method is perhaps the most potential model for its capacity of gas–liquid interface tracking at large scale. One application of the VOF method is to study the droplet behaviors in PEM fuel cell gas flow channels. Theodorakakos et al. (2006a) studied the detachment of a single water droplet from carbon porous material surfaces under various gas flow rate and the simulation results showed good agreement with experimental data. Single or multiple droplet motion was also simulated by several groups (Bazylak et al., 2008; Cai et al., 2006; Fang et al., 2008; Jiao et al., 2006a, b; Le et al., 2010; Quan and Lai, 2007; Quan et al., 2005; Shirani and Masoomi, 2008; Zhan et al., 2006; Zhu et al., 2007, 2008a, 2008b) in either two-dimensional or three-dimensional channels. Although effects of material wettability, gas or liquid velocity, contact angle, surface tension, and flow channel designs on two-phase flow have been widely investigated, those studies only focused on one or several droplets initially located in channels or injected from one water inlet into gas channels. Those studies are useful for understanding the droplet behavior, but cannot represent the two-phase flow patterns in gas channels, since water in an operating PEM fuel cell is constantly emerged into gas channels through the porous GDL. It has been shown that the microstructure of the GDL has great impacts on the droplet behavior, therefore the microstructure must be considered explicitly in order to simulate the two-phase flow pattern in gas channels (Ding et al., 2010).

Coupling the VOF method with an electrochemical reaction model is another challenge. Le and Zhou (2008, 2009a, 2009b) developed a general model that included electrochemical reactions, heat transfer and species transport in the VOF method. However, they treated the MEA as a homogenous layer without a microstructure, with the liquid droplets being initially located in gas flow channels. Therefore, such an approach can only provide some initial or transient information about the impact of droplets on PEM fuel cell performance. Limited by the computational capacity, full reconstruction of porous media in PEM fuel cells is still impractical, especially when coupling with gas flow channels, of which the characteristic length is two orders of magnitude higher than that of the porous media. The different spatial scales in different parts of PEM fuel cells also give rise to much difficulty in meshing and the selection of time steps. Too small a mesh size requires large computational time and too large a mesh size cannot resolve the phenomena occurring at micro scales. One compromise to deal with this issue is to simplify the MEA. Cheddie and Munroe (2008) simplified the MEA by analytically solving the governing equations in catalyst layers and the membrane, then the flow in GDLs and gas flow channels was simulated numerically. Furthermore, the whole MEA can be decoupled from the gas channel, since the species transport inside the MEA is relatively slow. Berg et al. (2004) developed a 1+1D PEM fuel cell model, in which the first 1D accounts for the through-the-MEA variation, and the other 1D accounts for the along-the-channel variation. Their simulation results agreed well with their experimental results. Kim et al. (2010) developed a 2+1D model, and compared this model to a full 3D model. It was found that the 2+1D model was far less time consuming and could achieve a comparable level of accuracy. However, all of the above work assumed that no liquid water existed in the gas channel.

In the present work, a 1+3D two-phase flow model is developed to study the impact of two-phase flow on PEM fuel cell performance. The VOF method was employed to account for the two-phase flow and species transports in a 3D cathode-side gas flow channel, coupling with a 1D MEA model to account for the