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Two-phase flow modeling for the cathode side of a polymer electrolyte fuel cell

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ABSTRACT

Liquid water flooding in micro gas channels is an important issue in the water management of polymer electrolyte fuel cells (PEFCs). However, in most previous numerical studies liquid water transport in the gas channels (GC) has been simplified by the mist flow assumption. In this work, we present a two-phase flow model for the cathode side of a PEFC. The GC is assumed to be a structured porous medium with the porosity of 1.0. The two-phase Darcy's law is applied to both diffusion layers and GC. Based on the developed model, the liquid water flooding in the GC and its impact on the liquid water distribution in the diffusion layers are explored in detail. Furthermore, we study the effect of the immobile saturation on the predicted liquid water distribution in the diffusion layers. The results show that neglecting the GC flooding leads to an incorrect prediction of liquid water distribution in the diffusion layers and an overestimation of the cell performance. The gas flow rate in the GC can be optimized to achieve the best cell performance. Finally, when considering the immobile saturation in the model, more liquid water is predicted in the diffusion layers.

1. Introduction

In the pursuit of reduced dependence on fossil fuels, less pollution, as well as high efficiency, the polymer electrolyte fuel cell (PEFC) is regarded as one of the most promising alternative power sources in the future. It is expected to be widely employed in stationary, automotive and portable sections. However, before this can occur, several technical challenges of PEFCs must be solved, such as cell durability, system power density, fuel storage, generation and delivery, as well as system cost to ensure a proper market penetration [1–3].

In a single PEFC unit, various transport processes are intricately coupled, along with electrochemical reactions in the catalyst layers. As a consequence, water and heat issues are always ineluctable. A typical PEFC consists of four distinct constituents, namely, bipolar plate (gas channels are grooved on both sides of bipolar plate), gas diffusion layer (including the micro porous layer), catalyst layer, and polymer electrolyte membrane. On one hand, the membrane should retain high water content to transport protons effectively with low ohmic resistance. Hence, gaseous reactants (e.g. H_2, O_2) are humidified before being fed into fuel cells. On the other hand, excessive liquid water accumulation within fuel cells would block reactant pathways to reactive sites in catalyst layers, resulting in the so-called flooding situation. Thus, it is evident that there exist two conflicting requirements for liquid water. We need to have a delicate water balance inside fuel cells to ensure that the membrane is fully hydrated for high protonic conductivity, while severe flooding is avoided, especially on the cathode side. To be able to bring about this balance, a profound understanding of water transport inside fuel cells is indispensable [4–7].

It is widely recognized that the flow of two immiscible phases (gas and liquid water) within PEFCs is challenging. While PEFCs are operating under certain conditions (e.g. high current densities, humid environments, and cold start-up), liquid water is simultaneously formed in all components. The mechanisms affecting the liquid water transport are distinct in different layers. A very simple categorization of the two-phase flow in PEFCs can be as follows [8,9]: (1) liquid water accumulation and transport in the CL, (2) two-phase flow in the GDL, along with interfacial coverage at the GC–GDL interface, and (3) water transport in the GC. These three sub-processes negatively impact the performance of PEFCs. For instance, in the CL, excessive liquid water would cover active catalyst sites, acting as an additional barrier to reactants transport. Based on the preceding descriptions of water transport we can see that a proper water management plays a central role in the development and commercialization of PEFCs.

Abbreviations: GC, gas channel; GDL, gas diffusion layer; CL, catalyst layer; MEM, membrane; PEFC, polymer electrolyte fuel cell.

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Nomenclature

a	charge transfer coefficient; net water transfer coefficient
A_{gc}	cross-sectional area of gas channel (m^2)
A_m	reactive area (m^2)
C	mass fraction
D	species diffusivity ($m^2\,s^{-1}$)
F	Faraday's constant, 96487 ($C\,mol^{-1}$)
i_0	exchange current density ($A\,m^{-2}$)
I_{ave}	averaged current density ($A\,m^{-2}$)
j	volumetric current density ($A\,m^{-3}$)
k_0	intrinsic permeability (m^2)
k_{rl}	relative permeability for liquid phase
k_{rg}	relative permeability for gas phase
k_{cond}	condensation rate (s^{-1})
k_{evap}	evaporation rate ($Pa^{-1}\,s^{-1}$)
M	molecular weight ($kg\,mol^{-1}$)
$\bar{n}$	normal direction vector
n_1	exponent for the effect of liquid water saturation on species diffusivity
n_2	exponent for relative permeabilities
n_3	exponent for the effect of liquid water saturation on current density
p	pressure (Pa)
$p_{H_2O}^{sat}$	water vapor pressure (Pa)
q	switch function for phase change model
R	universal gas constant ($8.134\,J\,mol^{-1}\,K^{-1}$); mass source due to phase change ($kg\,m^{-3}\,s^{-1}$)
RH	relative humidity
s	liquid water saturation
S	source term
T	temperature (K)
$\bar{V}$	velocity vector ($m\,s^{-1}$)
$\bar{U}$	intrinsic velocity vector ($m\,s^{-1}$)
Y	molar concentration ($mol\,m^{-3}$)

Greek letters

ρ	mass density ($kg\,m^{-3}$)
ε	porosity
μ	dynamic viscosity ($kg\,m^{-1}\,s^{-1}$)
$\bar{\bar{\tau}}$	stress tensor ($N\,m^{-2}$)
σ	surface tension ($N\,m^{-1}$)
θ	contact angle (°)
α	cathode catalyst specific area ($m^2\,m^{-3}$)
η_c	cathode overpotential (V)
ξ	stoichiometric ratio

Superscripts and subscripts

g	gas phase
l	liquid phase
m	momentum
i	gaseous species index
eff	effective value
c	capillary
ref	reference value
im	immobile
H_2O	water vapor
O_2	oxygen
sat	saturation
in	inlet

Over the past two decades, the two-phase flow and flooding phenomena in PEFCs have been intensively investigated via both experimental [10–15] and numerical methods [16–25]. To date, several macroscopic computational fluid dynamics (CFD) models for the two-phase flow in PEFCs are available in literature, which are all based on the so-called two-phase Darcy's law [26]. He et al. [27] developed a two-phase flow model for the cathode GDL. They solved a steady-state transport equation of liquid water flow that derived from the two-phase Darcy's law. The equation strongly resembled a general scalar transport equation with convective and diffusive terms. The authors also assumed both capillary diffusivity and convective coefficient to be constants for numerical stability. Following He's method, Ye and Nguyen [29] also derived a similar liquid water transport equation. Single-phase flow methodology was employed to model gas flow, and two phases were coupled by phase change. The effect of the presence of liquid water on gas flow was taken into account only by correcting gaseous species diffusivities. Another popular two-phase model for PEFCs is called multiphase mixture (M^2) model, which has been employed widely by fuel cell researchers [30–34]. Based on the two-phase Darcy's law, the M^2 model for multiphase, multi-component transport in capillary porous media was firstly developed by Wang and coworkers [35,36]. However, several researchers [28,37] used volume-weighted mixture dynamic viscosity and mass-weighted mixture velocity to simplify the M^2 model. So, the applications of this modified M^2 model would be limited. Berning et al. [38] used the so-called multi-fluid model to study liquid water transport in the cathode porous layers. Since this model requires a multiphase solver, and needs to be capable of coupling species transport, phase change, and chemical reactions simultaneously, it entails lots of computational efforts and is prone to being numerically instable.

In an operating PEFC, liquid water emerges from the GDL into the GC, in the form of small droplets and slugs [6]. These droplets and slugs cover the GDL surface and block the GC, in turn, influence the flooding level inside the diffusion layers. In order to capture this important physical phenomenon, an interactive model of liquid water transport between the GC and GDL should be developed. In most previous studies, a value of interfacial saturation or capillary pressure at the GC–GDL interface was specified. Normally, this value was assigned to zero, corresponding to the mist flow assumption in the GC. However, the mist flow assumption is only valid under high gas flow rates in the GC, which are not encountered in practice. So far, only a few researchers have numerically studied the water coverage effect on cell performance. Song et al. [39] developed a one-dimensional two-phase analytical model to address the effect of liquid water saturation at the GC–GDL interface on the transient behavior of liquid water transport inside the cathode GDL. Results showed that this parameter had a big impact on the calculated water saturation inside the GDL. A more elaborate interfacial coverage model was proposed by Meng and Wang [40]. In their work, the interfacial liquid saturation at the GC–GDL interface was assumed to be a simple function of the GDL surface contact angle, current density, as well as gas inlet velocity. This was not based on a derivation and they also used the mist flow assumption in the GC. The results showed that the interfacial coverage leaded to higher flooding levels inside the GDL and CL. Berning et al. [38] used the Hagen–Poiseuille equation to relate the interfacial water saturation with local pore velocity of liquid water in the GDL. Recently Basu et al. [9] proposed to apply the M^2 model into the GC directly. In this approach, the GC was assumed to be a structured porous medium, and then the two-phase coupling between the GDL and GC became straightforward.

In this work, we develop a two-phase flow model for the cathode side of a PEFC. The GC is assumed to be a structured porous medium with the porosity of 1.0; then, the two-phase Darcy's law is applied to the GC. Based on this model, we study the liquid water flooding