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Advanced control of liquid water region in diffusion media of polymer electrolyte fuel cells through a dimensionless number

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HIGHLIGHTS

- A 3-D model is employed to investigate the non-isothermal 2-phase flow in GDLs.
- The GDL's liquid water (or liquid-free) region is determined by the Da_0 number.
- A liquid-free GDL zone is created though the channel is subject to two-phase flow.
- Such a liquid-free zone benefits water management, avoiding flooding and dryness.

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ABSTRACT

In the present work, a three-dimension (3-D) model of polymer electrolyte fuel cells (PEFCs) is employed to investigate the complex, non-isothermal, two-phase flow in the gas diffusion layer (GDL). Phase change in gas flow channels is explained, and a simplified approach accounting for phase change is incorporated into the fuel cell model. It is found that the liquid water contours in the GDL are similar along flow channels when the channels are subject to two-phase flow. Analysis is performed on a dimensionless parameter Da_0 introduced in our previous paper [Y. Wang and K. S. Chen, Chemical Engineering Science 66 (2011) 3557–3567] and the parameter is further evaluated in a realistic fuel cell. We found that the GDL's liquid water (or liquid-free) region is determined by the Da_0 number which lumps several parameters, including the thermal conductivity and operating temperature. By adjusting these factors, a liquid-free GDL zone can be created even though the channel stream is two-phase flow. Such a liquid-free zone is adjacent to the two-phase region, benefiting local water management, namely avoiding both severe flooding and dryness.

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1. Introduction

Water management is a central issue in the development of polymer electrolyte fuel cells (PEFCs): liquid water may considerably increase the oxygen transport resistance and hence the transport polarization whereas dryness dehydrates the electrolyte membrane, raising the Ohmic voltage loss. PEFCs produce water during operation and the electro-osmosis enlarges the water imbalance between the anode and cathode sides, making water management a complex operation that requires a careful treatment. Issues such as diffusion media dewetting, anode rehydration, and internal humidification have received much attention in recent years [1]. Modeling and numerical simulation are capable of revealing details of transport phenomena, and is a powerful tool for elucidating water management.

Modeling two-phase transport in PEFCs is an active area of research [1–5]. Springer et al. [6], Nguyen and White [7], Fuller and Newman [8], and Bernardi and Verbrugge [9], to name just a few, represent an early pioneering effort dated back in 1990s. In their studies, the through-plane direction is the focus with both electrochemical and transport activities accounted for. Multi-dimensional models, based on conservation equations (continuity, fluid flow, energy and so on) in conjunction with electrochemical reactions, were attempted by later studies such as the two-dimensional models of Yi and Nguyen [10] and Gurau et al. [11] and the three dimensional models of Dutta et al. [12], Zhou and

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Liu [13], Berning et al. [14], Mazumber and Cole [15], Um and Wang [16] and Wang and Wang [17], to name just a few. These models mostly neglected liquid water formation and transport and assumed water exists in a super saturated state. Two-phase models were developed by He et al. [18], Natarajan and Nguyen [19], Berning and Djilali [20], Mazumber and Cole [21], Wang and co-workers [22–24], You and Liu [25], Hu and Fan [26], and Webber and Newman [27], to name just a few. They considered vapor and liquid water moving at different velocities. Other liquid water behaviors including the surface tension and flooding effects were also taken into account. Liquid water originates from water production by fuel cell electrochemistry. When fed-in reactants are dry, no liquid will appear at the beginning. As the water vapor is saturated down the channel, vapor condensation takes place, leading to liquid water formation. Capturing the point where two-phase flows emerge is important because the portion further downstream this onset point requires liquid water removal, as described by Luo et al. [28] and Wang [29], which numerically captured the regime of two-phase flow downstream. In the in-plane direction, water produced under the solid lands must reach the channel stream in order to be removed. Wang and Chen [30] investigated the liquid water profiles in both through-plane and in-plane direction and validated their predictions against experimental data, showing how GDL-property spatial variation and land compression influence liquid water distribution. Most of previous modeling studies excluded the channel two-phase flow and phase change. In the channel, liquid will accumulate along the flow direction due to water production and two-phase flow plays an important role in fuel cell operation [31–35]. Wang et al. [36] and Wang [37] modeled the two-phase flow in the along-channel direction, and analytically obtained the liquid saturation profiles in channels. The model [37] was further adopted to compare with experimental measurements for both hydrophilic and hydrophilic-hydrophobic micro channels [38,39]. In addition to two-phase flow, droplet formation at the cathode GDL/channel interface may greatly impact fuel cell performance [40–44]. At the microscale, transport in GDLs takes place in the interconnected pore structure. Pore-level transport in GDLs was modeled and investigated by Sinha et al. [45], Park and Li [46], and Wang et al. [47], to name just a few. In the two-phase regime, the heat pipe effect may occur and contribute to both water and heat removals [5,48,49]. Wang and Gundevia [48] carried out experiments in which heat pipe effect in carbon paper was measured and the impact of material wetting property was evaluated.

Though modeling has been attempted by various groups to study fuel cell operation and two-phase transport, little has been done to identify dimensionless parameters that characterize two-phase flow in a fuel cell. In our previous analysis [50], we identified a dimensionless parameter Da_0 which characterizes the in-plane two-phase regime. When Da_0 is over 1, part of the GDL region is free of water due to waste heat production and evaporation. This paper examines the Da_0 number in a real fuel cell operation; especially, we will examine the Da_0 definition in a realistic fuel cell and its value along the gas flow channel. A liquid-free GDL region is defined and related to Da_0 with its benefits discussed. Impacts of operating temperatures, GDL thermal conductivities, and current densities on the region are discussed as well.

2. Theory

2.1. Along-channel water management

There is a dilemma in water management along gas flow channel: the inlet area may be subjected to dryness (when dry reactants are fed in) whereas there is a “flooding” issue near the outlet due to water production by the oxygen reduction reaction or ORR. Any strategies that alleviate the former likely worsen the latter, and vice versa. Down the channel, the reactant stream picks up water molecules from the ORR's production and increases its water content. When the stream reaches its saturated level, liquid water emerges, leading to two-phase flow. Liquid water in GDLs narrows the passage of oxygen transport toward the catalyst layer (CL), increasing transport resistance. Another issue is the liquid coverage on the GDL surface which hampers oxygen access to the reaction sites. Furthermore, the ORR is sluggish, exhibiting a large concentration loss under high current density. In this regard, liquid-free operation reduces the concentration loss by avoiding liquid blockage/narrowing of the oxygen transport passage. Dryness operation, however, leads to electrolyte dehydration, increasing the Ohmic voltage loss and raising material degradation or durability concerns.

2.2. Da_0 along gas flow channels

Water and waste heat are added to cathode GDL from CL. Water is then removed by channel gas flows; and most waste heat is taken away via lands. A dimensionless numberDa_0 as defined in our previous paper [50], describes the relative importance of water addition rate to water removal rate:

$$\mathrm{Da}_0 = \frac{\text{Rate of water addition}}{\text{Rate of water removal via diffusion \& evaporation}} = \frac{k^{eff}_{GDL,H}(1+2\alpha)}{f_{\max} F D^{eff}_w (E_o - V_{cell}) \dfrac{dC^w_{sat}(T_0)}{dT}} \left(1 + \frac{1}{Sh}\frac{H_{ch} D^{eff}_w}{H_{GDL} D_w}\right) \tag{1}$$

In the above, the Sherwood number, $Sh(=\frac{h_m H_{ch}}{D_w})$, is determined by the mass transfer in gas flow channels. Mass transfer in micro channel, analogous to momentum/heat transfer, varies in the entrance region, but remains constant in the fully developed region. In the momentum transfer, the entrance region is where the boundary layer develops near the channel walls before meeting at the centerline. For laminar flow in tubes, the entrance length is about 5 times of the channel diameter (L/D~Re/20) for Re~100 which occurs in fuel cell channels. In this case, the length is about 2.5–10 mm and after that the channel stream is fully developed. In the fully developed portion, water enters the channel from the CL's ORR production and transports across the channel and condenses over the channel's cold surface, see Fig. 1(a). Assuming the axial velocity remains constant and diffusion is the dominant through-plane transport mechanism in gas flow channel, the water flux via the vapor phase can be evaluated by:

$$G_{w,diff,\max} = \frac{\Delta C^w_{sat} + C^w_{sat}(T_0) - C^w_{ch,wall}}{\frac{H_{GDL}}{D^{eff}_w} + \frac{H_{ch}}{D_w}} = \frac{\Delta C^w_{sat} + C^w_{sat}(T_0) - C^w_{ch,wall}}{\frac{H_{GDL}}{D^{eff}_w}\left(1 + \frac{H_{ch} D^{eff}_w}{H_{GDL} D_w}\right)} \tag{2}$$

where $C^w_{ch,wall}$ is the vapor concentration at the channel bottom wall against the GDL. When the channel stream is two-phase flow, $C^w_{ch,wall}$ can be approximated to the vapor saturated concentration determined by local temperature. In addition, we assume the Sherwood number is equal to 1. In the absence of along-channel temperature variation, $C^w_{ch,wall}$ remains constant. Though defined for local GDL, the Da_0 number is also applicable to the entire GDL under the channel. Several factors affect the Da_0 number, including