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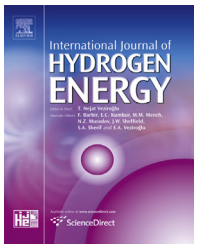

Numerical modeling of liquid water motion in a polymer electrolyte fuel cell

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ABSTRACT

A three dimensional transient model fully coupling the two phase flow, species transport, heat transport, and electrochemical processes is developed to investigate the liquid water formation and transport in a polymer electrolyte fuel cell (PEFC). This model is based on the multiphase mixture (M2) formulation with a complete treatment of two phase transport throughout the PEFC, including gas channels, enabling modeling the liquid water motion in the entire PEFC. This work particularly focuses on the liquid water accumulation and transport in gas channels. It is revealed that the liquid water accumulation in gas channels mainly relies on three mechanisms and in the anode and cathode may rely on different mechanisms. The transport of liquid water in the anode channel basically follows a condensation–evaporation mechanism, in sharp contrast to the hydrodynamic transport of liquid water in the cathode channel. Liquid water in the cathode channel can finally flow outside from the exit along with the exhaust gas. As the presence of liquid water in gas channels alters the flow regime involved, from the single phase homogeneous flow to two phase flow, the flow resistance is found to significantly increase.

1. Introduction

Two-phase flow is ubiquitous in polymer electrolyte fuel cells (PEFCs). Optical visualization experiments [1–5] have corroborated the existence of liquid water not only in the PEFC cathode, but also in the anode. Having suitable amount of liquid water remain in electrodes may be favorable to the cell performance as it improves the membrane ionic transport capability. However, liquid water remaining in catalyst layers (CL) can cover the active reaction sites and that in porous diffusion media can block the pathways of reactants, leading to reduction of cell performance or even shutdown, referred to flooding. Flooding may also occur in gas channels if liquid water accumulates in and blocks the flow path. Besides deteriorated cell performance, flooding can also bring detrimental impact at the PEFC durability as it may cause fuel starvation and ensuing carbon corrosion [6,7], resulting in accelerated aging of the membrane electrode assembly (MEA). In addition, for a PEFC stack, channel flooding (or clogging) causes flow maldistribution, and thus leads to a non-uniform, cell-to-cell reactant distribution, further exacerbating flooding effects. Therefore, water management, aiming to balance the hydration of membrane with the avoidance of flooding, plays a pivotal role to ensuring high performance and long durability of PEFCs.

Understanding the distribution and transport of liquid water is the key to PEFC water management. While

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considerable research efforts [8–13] have been expended to delineate the two phase transport in porous diffusion media and its impact on cell performance, the two-phase flow in gas channels remains intractable until a few years ago [14,15]. Almost all the mathematical modeling works [8–13] that were based on the M2 formulation [16] have an assumption of homogeneous mist flow in PEFC gas channels thereby no virtually informative results about the two phase flow in gas channels could be given. Wang et al. [14] first extended the M2 formulation to model the two phase flow in PEFC gas channels by taking the mini-channels as structured and ordered porous media. This concept was later deployed to deal with the two phase flow maldistribution in multiple gas channels of a PEFC stack by Basu et al. [15]. Another representative category of PEFC two phase flow models is the two-fluid model [17–22], which either adopts the unsaturated flow theory and solves liquid-phase equations only [17] or solves the gas-phase and liquid-phase equations [18–20] separately with some phenomenological approximations, e.g. drag and lift force [19], being introduced to account for the complex interactions between phases. The M2 model is more advantageous over the two-fluid model at computational efficiency due to much fewer primary variables involved and its capability of capturing the three dimensional dry–wet–dry transition [12] without tracking the multiple interfaces between single- and two-phase regions. The volume of fluid (VOF) method has also been used to simulate the two phase flow in PEFC air channel [23] and to investigate the dynamic behavior of liquid water entering into PEFC gas channels from gas diffusion layer (GDL) pores [24]. This method needs to solve additionally a scalar transport equation for liquid volume fraction, and in order to accurately reconstruct the interfaces between single- and two-phase regions fine mesh is critically needed. The extremely intensive computational cost hinders its practical application to PEFC modeling. In the present work, a three dimensional transient model is developed using the M2 formulation. A salient feature of this model is the complete treatment of two-phase transport throughout a PEFC, including gas channels, thus enabling detailed studies on the liquid water formation, transport, and flooding in CLs, GDLs and channels, and furthermore the channel clogging and flow maldistribution.

This work focuses only on elucidating the liquid water motion in a single-channel PEFC with particular interest on the liquid water accumulation and transport in gas channels. In the next section is brought out a three dimensional, transient, non-isothermal, two phase flow PEFC model. The third section presents detailed simulation results and discussion. Major conclusions are then summarized in the final section.

2. The PEFC model

We consider a PEFC consisting of nine sub-regions: two flow plates in the anode and cathode respectively, an anode channel, an anode gas diffusion layer, an anode catalyst layer, an ionomeric membrane, a cathode catalyst layer, a cathode gas diffusion layer, and a cathode channel, as schematically shown in Fig. 1. No anode and cathode micro-pore layers are included, since of particular interest here is the liquid water accumulation and transport in gas channels and we do not want to get involved in the disputation [25–27] about the effects of micro- pore layers on PEFC performance. Humidified air and hydrogen are fed into the cathode and anode channels, respectively, in counter flow. A constant current density is prescribed at the outer surface of the cathode flow plate. Model development is based on the works by Wang and Wang [10,13]. The developed three dimensional PEFC model fully accounts for the transient transport and electrochemical processes with a complete treatment of two phase flow throughout the PEFC, and can be concisely summarized in the form of the following governing equations:

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\vec{u}}{\varepsilon} \right) = 0 \tag{1}$$

Momentum conservation equation

$$\frac{\partial (\rho \vec{u}/\varepsilon)}{\partial t} + \nabla \cdot \left(\frac{\rho \vec{u}\,\vec{u}}{\varepsilon^2} \right) = \nabla \cdot (\mu \nabla \vec{u}) - \nabla P + S_u \tag{2}$$

Energy conservation equation

$$\frac{\partial \left[\overline{\rho c_p} T \right]}{\partial t} + \nabla \cdot \left[\gamma_T \rho c_p \vec{u} T \right] = \nabla \cdot \left(k^{\mathrm{eff}} \nabla T \right) + S_T \tag{3}$$

Species conservation equation

$$\frac{\partial \left(\varepsilon^{\mathrm{eff}} C^i \right)}{\partial t} + \nabla \cdot \left(\gamma_C \vec{u} C^i \right) = \nabla \cdot \left(D_g^{i,\mathrm{eff}} \nabla C_g^i \right) - \nabla \cdot \left[\left(\frac{m f_l^i}{M^i} - \frac{C_g^i}{\rho_g} \right) \vec{j}_l \right] + S_C^i \tag{4}$$

Charge conservation (electrons) equation

$$0 = \nabla \cdot \left(\sigma_s^{\mathrm{eff}} \nabla \Phi_s \right) + S_{\phi_s} \tag{5}$$

Charge conservation (protons) equation

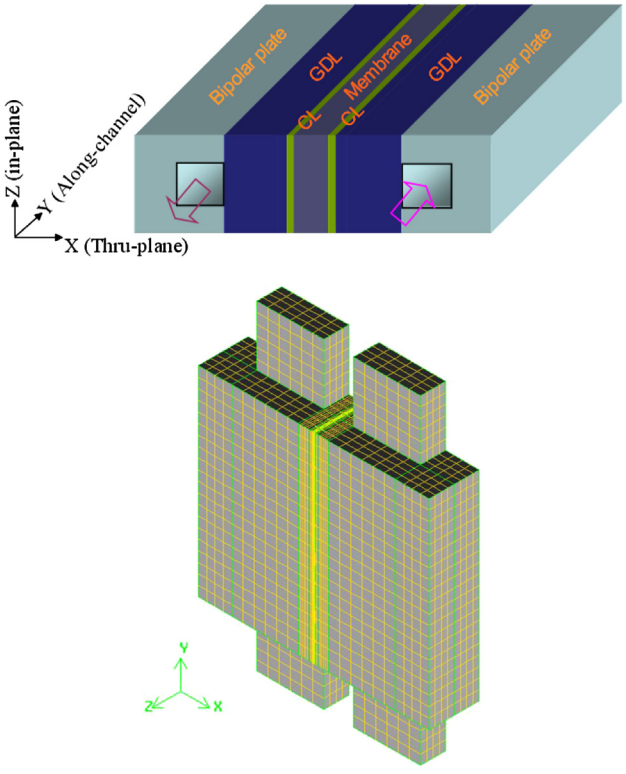

Fig. 1 – Geometry and mesh of a single-channel PEFC.