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Three-dimensional two-phase flow model of proton exchange membrane fuel cell with parallel gas distributors

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ABSTRACT

A non-isothermal, steady-state, three-dimensional (3D), two-phase, multicomponent transport model is developed for proton exchange membrane (PEM) fuel cell with parallel gas distributors. A key feature of this work is that a detailed membrane model is developed for the liquid water transport with a two-mode water transfer condition, accounting for the non-equilibrium humidification of membrane with the replacement of an equilibrium assumption. Another key feature is that water transport processes inside electrodes are coupled and the balance of water flux is insured between anode and cathode during the modeling. The model is validated by the comparison of predicted cell polarization curve with experimental data. The simulation is performed for water vapor concentration field of reactant gases, water content distribution in the membrane, liquid water velocity field and liquid water saturation distribution inside the cathode. The net water flux and net water transport coefficient values are obtained at different current densities in this work, which are seldom discussed in other modeling works. The temperature distribution inside the cell is also simulated by this model.

1. Introduction

Proton exchange membrane (PEM) fuel cells are supposed to be the most promising candidate for powering of electric vehicles due to their high power density, short response time, low operating temperature and pollution free. Modeling and simulation are being used extensively in researches and industrial applications across the world to gain better understanding of the fundamental processes and to optimize fuel cell designs before building a prototype for engineering application.

The importance of water management to PEM fuel cell performance is repeatedly expressed in the early published work [1–5]. Despite several studies on water management in the cell within the past decade, effective water management has remained imperfect. This is partly due to the fact that liquid water is transported within the membrane-electrode-assembly (MEA) by the several coexisting and comparable forces. They are electro-osmotic drag due to the electrical potential, back diffusion from the cathode due to nonuniform concentration, diffusion and hydraulic permeation due to the pressure difference. The other complication results from the conflict that while liquid water is necessary to ensure good ionic conductivity of the membrane, excessive water can result in flooding of the electrodes at high current. Thus it is neither desirable to remove the water completely, nor is it desirable to have excessive water. The difficulty of water management exists in this.

Over the past few years, some modeling works of liquid water formation and transport were published in the literature. Baschuk and Li [6] proposed the one-dimensional steady-state model in which the degree of water flooding was determined by matching the predictions to the experimental polarization curve. He et al. [7] developed a two-dimensional (2D) two-phase model for cathode of PEM fuel cell with interdigitated flow field. The model included capillary transport of liquid water in a completely wetted gas diffusion layer (GDL). Wang et al. [8] classified four regimes of water transport in the PEMFC air cathode and presented a 2D two-phase flow model based on the multiphase mixing model (M^2 model) formulation of Wang and Cheng [9]. Subsequently, You and Liu [10] published a similar work investigating the effects of several operating parameters on two-phase transport. Berning and Djilali [11] developed a non-isothermal water transport model, in their work, the water formed at the cathode catalyst layer (CL) by electrochemical reactions was assumed to be in the liquid phase and any phase-change phenomena was neglected. The works of Van Zee and co-workers [12,13] have introduced water transport models, in which phase change is assumed to occur only at the interface between the membrane and the electrode, and two-phase transport effects are neglects. Transport of water occurs by means of vapor motion only. Mazumder and Cole [14] presented a rigorous

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3D mathematical model to treat formation and transport of liquid water in PEM. Results show that the inclusion of liquid water transport greatly enhances the predictive capability of the model and is necessary to match experimental data at high current density. Luo et al. [15] presented a three-dimensional, two-phase isothermal model based on the M^2 model formulation for investigating the condensation and/or evaporation interface, and successfully predicted the important feature of the dry–wet–dry transition in the PEM fuel cell. Zhang et al. [16] studied liquid water transport and its removal from the GDL and gas channel of PEM fuel cells both experimentally and theoretically. Wang and Wang [17] expanded the M^2 model to permit investigation of the interaction between the two-phase flow and thermal transport due to non-isothermal effects. They also developed an unsteady two-phase model to study the dynamics of the GDL dewetting and its impact on PEM fuel cell performance [18]. A comprehensive two-phase non-isothermal steady model for PEM fuel cell was developed by Basu et al. [19] to investigate two-phase flow and maldistribution in the gas channels.

Recently, other fundamental modeling studies have been reported to investigate water transport phenomena in GDLs based on the Lattice–Boltzmann method [20,21] and the pore-network model [22–24]. Also, experimental investigations have been conducted for the visualization of two-phase flow or quantification of the liquid water content in GDLs within an operating polymer electrolyte fuel cell, using transparent fuel cells [16,25], a fluorescein dye solution [26], and neutron radiography [27–29].

In an earlier publication, our research group has presented an isothermal, three-dimensional comprehensive model of a complete single cell [30]. Phase-change and multiphase flow, however, could not be addressed with that model.

In this paper, a non-isothermal, steady-state, 3D, two-phase, multicomponent transport model is proposed for PEM fuel cell with parallel gas distributors, and numerically solved with a code developed by the authors. In addition to three-dimensionality and the inclusions of both anode and cathode, the present model differs substantially from earlier studies in that the liquid water transport in the electrode and membrane is accounted for via the liquid saturation equation and mass continuity equation, respectively. A detailed membrane model is developed for the liquid water transport with a two-mode water transfer condition, accounting for the non-equilibrium humidification with the replacement of an equilibrium assumption. Also it should be noted that the anode and cathode transport processes are coupled and the water flux balance between anode and cathode sides is insured during the modeling. In the following presentation, the model description will first be stated in detail, including the governing equations and the related boundary conditions, followed by a brief presentation of the numerical algorithm adopted, then detail discussion will be made on the numerical results. Finally some conclusions will be drawn.

2. Model description

The framework of the single-phase PEM fuel cell model in reference [30] is used. A detailed description of the single-phase model has been published and shall not be repeated here. In this paper we focus on modeling of two-phase transport and the prediction of the flooding electrode under operating conditions.

2.1. Model assumptions

In order to make the numerical simulation manageable, some assumptions are to be made as follows.

(1) All phases are assumed to be continuous so that the continuum approach is applicable.
(2) The cell operates under steady-state condition.
(3) The gas mixtures are assumed to be well mixed and can be regarded as the ideal gases. The gas species dissolved in the water is neglected.
(4) The electrode is treated as an isotropic and homogenous porous medium and the properties such as porosity and the permeability are uniform. The membrane is impermeable for gas phase.
(5) Ohmic losses in the GDL and current collector (or bipolar plate) are neglected.
(6) Thermal equilibrium is assumed among gas, liquid and solid phases in the local micro-volume unit of porous electrodes.

2.2. Governing equations

2.2.1. Transport equations of gas mixtures

Generally, the transport of gas mixtures in the flow channels and in the diffusion layers conforms to the mass, momentum, and species conservation principles. The corresponding governing equations are written as follows:

Mass conservation equation

$$\nabla \cdot (\rho \boldsymbol{u}_g) = S_m \tag{1}$$

where $\mathbf{u}_g$ is the superficial velocity vector of gas mixture, which is proportional to the intrinsic fluid velocity vector $\mathbf{U}$ by the following expression:

$$\boldsymbol{u}_g = \varepsilon(1-s)\boldsymbol{U} \tag{2}$$

where ε is porosity of the porous electrode, and s is the saturation of liquid water indicating the fraction of the void volume occupied by liquid phase in the electrode. In the gas channels, ε is unity and s is zero, then the superficial velocity vector is reduced to the real fluid velocity vector.

Momentum equation

$$\frac{1}{\varepsilon^2(1-s)^2}\nabla \cdot (\rho_g \boldsymbol{u}_g \boldsymbol{u}_g) = -\nabla p_g + \frac{1}{\varepsilon(1-s)}\nabla \cdot (\eta_g \nabla \boldsymbol{u}_g) + \frac{\eta_g}{KK_{rg}}\boldsymbol{u}_g \tag{3}$$

Species mass fraction conservation equations

$$\nabla \cdot (\rho \boldsymbol{u}_g \omega_h) = \nabla \cdot (\rho D_{h,eff} \nabla \omega_h) + S_h \tag{4}$$

$$\nabla \cdot (\rho \boldsymbol{u}_g \omega_o) = \nabla \cdot (\rho D_{o,eff} \nabla \omega_o) + S_o \tag{5}$$

$$\nabla \cdot (\rho_g \boldsymbol{u}_g \omega_w) = \nabla \cdot (\rho_g D_{w,eff} \nabla \omega_w) + S_{w1} + S_{w2} \tag{6}$$

The above governing equations are assumed to be applicable for both flow channel and porous electrode. In these equations, ρ, p and η are the density, pressure and the viscosity of the fluid, respectively; K is the absolute permeability and K_{rg} is the relative permeability for the gas in the porous electrode. The subscript 'g' denotes gas phase. The symbols of ω_h, ω_o and ω_w are the mass fraction of hydrogen, oxygen and water vapor in the gas mixtures, respectively. $D_{i,eff}$ is the effective diffusivity and the subscript 'i' represents the gas species. The last terms existing in Eqs. (1) and (4)–(6) are the volumetric sink or source terms due to the electrochemical reactions or phase change in the electrode, and they are zero in other region of the domain.

Some explanations are given below for the above governing equations. In the general form of momentum equation, Eq. (3), the last term on the right side represents Darcy's drag force imposed by the pore walls on the fluid within the pores, which usually results in a significant pressure drop across the porous medium. It is often called as the micro-scale viscous term or Darcy's viscous term. As indicated above, the general momentum equation is valid in both the porous electrode and the flow channel. In the porous medium, it reduces to the extended Darcy's law for the flow in porous media with a small permeability. While inside the gas channels, it recovers the standard Navier–Stokes equation with the porosity being unity and the permeability being infiniteness.