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Optimization and parametric analysis of PEMFC based on an agglomerate model for catalyst layer

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ABSTRACT

A one-dimensional, non-isothermal, single-phase, steady-state comprehensive model is developed to investigate the effects of different parameters of catalyst layer and operational case as relative humidity on the proton exchange membrane fuel cell (PEMFC) performance, then to optimize the design and operation of PEMFC. The agglomerate model with thin film of polymer and liquid water was employed to describe electrochemical reaction in catalyst layers. The model considers the effect of different production ratio of water vapor and liquid water in the reaction on the fuel cell performance. The effects of operational case as temperature, relative humidity of reactants and catalyst layer structure parameters as Pt loading, agglomerate radius and Pt radius on cell performance are computed and discussed in detail. The results indicate that agglomerate radius, Pt loading and Pt particle radius, operation temperature and pressure have different kinds of effects on performance, and the performance can be improved by suitable operational case and catalyst layer structure. Results can provide good reference for optimization design of the catalyst layer and the whole cell.

1. Introduction

Proton exchange membrane fuel cell (PEMFC) is a promising candidate for power sources of portable equipments and vehicles for its advantage characteristics as high-energy conversion efficiency and fast startup at ordinary temperature. However, high cost and low durability are still two main barriers to its mass productions and applications. The appropriate design of catalyst layer structure, operational case, and water and heat management in the core component membrane electrode assembly (MEA) of PEMFC is significantly important to the performance optimization because they will greatly affect cell performance, stability and durability of fuel cell.

During the past two decades, many researchers were involved in developing different computational models for PEMFC [1–13]. The developed models were from simple to complex; from one-dimensional [1–3], two-dimensional [4–6] to three-dimensional [7–10]; from single-phase to two-phase; from macro-scale to meso-scale [11], and even micro-scale [12,13]. Water management of PEMFC plays an important role for operation and performance optimization of PEMFC. Thus, many models focused on the water management. Bernardi et al. [2] developed a hydraulic model with assumptions that the membrane is fully hydrated with liquid water. However, this model is not suitable for a partially dry membrane. Yi et al. [14] developed one model for interdigitated flow fields considering liquid water. However the liquid water flow induced by capillary forces and gas flow induced drag was addressed by semi-heuristic equations. Natarajan et al. [15] developed a pseudo-three-dimensional model by extending their two-dimensional isothermal model. This model can be used to obtain qualitative insight into the distribution of liquid water in the backing layer. Janssen et al. [16] developed a two-dimensional, phenomenological model based on concentrated solution theory to describe the transport of water in the membrane, and of water vapor and liquid water in the electrodes. Two-phase flow modeling in the porous air cathode of a PEMFC was attempted by Wang et al. [17]. The transport coefficients in the stationary numerical two-phase model are parameterized as functions of the liquid water saturation. However, this model only considered the cathode half cell. Later, this model was further developed to include the whole cell by You et al. [18]. Berning et al. [7] developed a 3D, two-phase PEMFC model based on computational fluid dynamics multiphase. Transport of liquid water inside the gas-

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diffusion layers is modeled using viscous forces and capillary pressure terms. Shimpalee et al. [19] developed a complete three-dimensional model, which treated the liquid water as component of the gas mixture. Steinkamp et al. [20] presented a 2D dynamic two-phase flow model accounting for all important transport processes in a PEM fuel cell. Unfortunately, the computational cost for simulation was quite high because of the high complexity of the model. Siegal et al. [21] presented a 2D model to account for the transport of liquid water in the electrode and treat all three forms of water as a separate phase and allow mass transport among them. Zhang et al. [22] developed a model including three forms of water: dissolved water in the electrolyte or membrane, and liquid water and water vapor in the void space. A one-dimensional model of water transport across the entire cell is presented for the proton exchange membrane fuel cell [23]. In the model, the water vapor in the pore is coupled with liquid water in the ionomer phase by the isotherm sorption. A one-dimensional analytic solution of liquid water transport across the CCL is derived from the fundamental transport equations [24]. Based on a dimensionless time constants analysis, it has been shown that liquid water production from the phase change process is negligible comparing to water production from the electrochemical process.

Among the abovementioned modeling studies on water management, some researchers assumed that the generated water is in liquid form, some believed that water is generated in vapor form. Because it is almost impossible to detect which form the generated water is by current experimental technology, in this paper, we introduce a parameter, Γ, which is percentage of water vapor in all of the generated water [25]. Using this one-dimensional, non-isothermal MEA model, the effects of the proportion of water vapor in generated water on water transport and cell performance can be investigated.

In order to know well the basic work process and optimize the cell design, computer simulation [26–31] has been adopted more and more besides the experimental study. Recent years, more and more researchers focus on the catalyst layer modeling and numerical simulation; analyze the effect of catalyst layer thickness, layer structure, control of catalyst distribution, diameter of carbon, Pt loading and polymer content on the catalyst layer and cell performance. Wang et al. [27] presented a spherical water-filled agglomerate model for the catalyst layer, investigated the effect of structure parameters as oxygen diffusion, proton conductivity, porosity and agglomerate diameter on agglomerate structure. Furthermore, different types of agglomerate structure and performance were studied [28]. Song et al. [29] built a one-dimensional steady multi-layer agglomerate model in order to analyze the performance of non-uniform catalyst layer, the catalyst layer is separated into three layers artificially, and the effect of different characteristics as thickness, porosity and agglomerate diameter on the cell performance was studied. Khajeh-Hosseini-Dalasm et al. [30] developed a comprehensive cathode catalyst layer mathematical model, studied the effect factors of activation overpotential as saturation and structure parameters polymer thickness, agglomerate diameter, Pt loading and polymer volume fraction; the effect of single parameter and interaction between different parameters on the cell performance were investigated. At last, the optimization algorithm was presented. Rao et al. [31] presented two different optimization methodologies for minimum Pt loading and maximum current based on spherical agglomerate model of cathode catalyst layer, and then the reasonable scheme scaling single agglomerate to the whole catalyst layer was presented. Recently, some other agglomerate model based catalyst layer models were presented to investigate the effects of cathode catalyst layer parameters on the cell performance [32,33]. Hutzenlaub et al. [34] compared a hydrophilic and a hydrophobic CCL by calculating an effective diffusivity of oxygen in nitrogen and a specific, GDL-connected surface area.

Catalyst layer is the core component of PEMFC, which has the complicated structure and determines the performance and durability of PEMFC. The objectives of this paper are to obtain the effect of different parameters of catalyst layer and operational case on the cell performance. A comprehensive model based on the agglomerate model is developed, and the solution of conservation equation system is conducted by software COMSOL.

2. Model description

A one-dimensional, non-isothermal model of a MEA including five subdomains: anode gas diffusion layer, anode catalyst layers, cathode gas diffusion layers, cathode catalyst layer and polymer membrane is presented. The schematic of computation domain is showed in Fig. 1.

Following assumptions are considered during the model development:

(1) The PEM fuel cell operates under steady state.
(2) A one-dimensional approximation is used in the model formulation by neglecting the variation of reactant concentrations along flow channels.
(3) The porous media such as gas diffusion layers and catalyst layers are isotropic and homogeneous, characterized by effective permeability and uniform porosity.

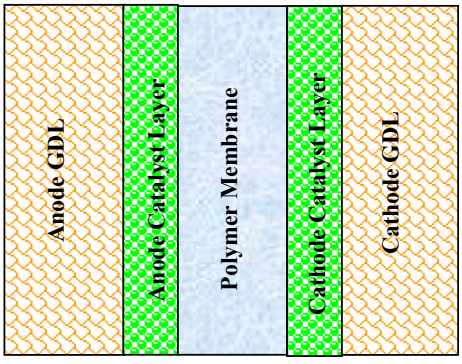

Fig. 1. Schematic of computation domain.