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Model prediction of effects of operating parameters on proton exchange membrane fuel cell performance

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ABSTRACT

The performance of a proton exchange membrane (PEM) fuel cell is greatly affected by the operating parameters. Appropriate operating parameters are necessary for PEM fuel cells to maintain stable performance. A three-dimensional multi-phase fuel cell model (FCM) is developed to predict the effects of operating parameters (e.g. operating pressure, fuel cell temperature, relative humidity of reactant gases, and air stoichiometric ratio) on the performance of PEM fuel cells. The model presented in this paper is a typical nine-layer FCM that consists of current collectors, flow channels, gas diffusion layers, catalysts layers at the anode and the cathode as well as the membrane. A commercial Computational Fluid Dynamics (CFD) software package Fluent is used to solve this predictive model through SIMPLE algorithm and the modeling results are illustrated via polarization curves including *I–V* and *I–P* curves. The results indicate that the cell performance can be enhanced by increasing operating pressure and operating temperature. The anode humidification has more significant influences on the cell performance than the cathode humidification, and the best performance occurs at moderate air relative humidity while the hydrogen is fully humidified. In addition, the cell performance proves to be improved with the increase of air stoichiometric ratio. Based on these conclusions, several suggestions for engineering practice are also provided.

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1. Introduction

The proton exchange membrane (PEM) fuel cell has been the most attractive energy conversion technology because of high efficiency, low operating temperature, zero emission and quick start-up. These advantages make it a promising candidate to be the power sources for portable and transportation applications as well as for distributed power stations [1–3]. A basic schematic of a PEM fuel cell is shown in Fig. 1. At the anode, hydrogen flows into the gas channels of the current collector, and diffuses through the gas diffusion layer (GDL). Then hydrogen gets to the catalyst layer (CL) where it is split into electrons and protons through chemical reaction. The electrons flow to the cathode side through external circuit while the protons pass through the polymer electrolyte membrane. At the cathode, air also arrives at CL through current collector and GDL. Subsequently, the electrons, protons and oxygen combine to form the byproduct of water.

Fuel cell models (FCMs) play an important role in the development of PEM fuel cell technology, which facilitate understanding the electro-chemical reaction, thermal dynamic phenomena, and fluid transfer mechanism in PEM fuel cells. In recent years, many FCMs based on computational fluid dynamics (CFD) software packages have been established which involve multi-phase, multi-component and multi-dimensional flow, heat and mass transfer with electro-chemical reaction occurring in irregular geometries including porous medium [4,5]. These models greatly benefit R&D work in the areas of flow field design, transport mechanism, water and thermal management in PEM fuel cells.

It is widely known that the PEM fuel cell performance highly depends on the hydration level of the polymer membrane. Humidification of the reactant gas is usually essential to keep the membrane under well-hydrated condition. However, this approach brings negative influences that cannot be neglected such as electrode flooding [6–9] and complicated design process of humidifiers. Thus, the performance of PEM fuel cells without any humidification (i.e. dry operation) has drawn more attention because it can be improved by optimizing cell design and water management [10–24]. In a PEM fuel cell, water molecules are driven in following three ways: the electro-osmotic drag from the anode to the cathode due to potential difference, the back diffusion from the cathode to the anode due to concentration gradient and the pressure differences between the cathode and anode. These water transport mechanisms result in

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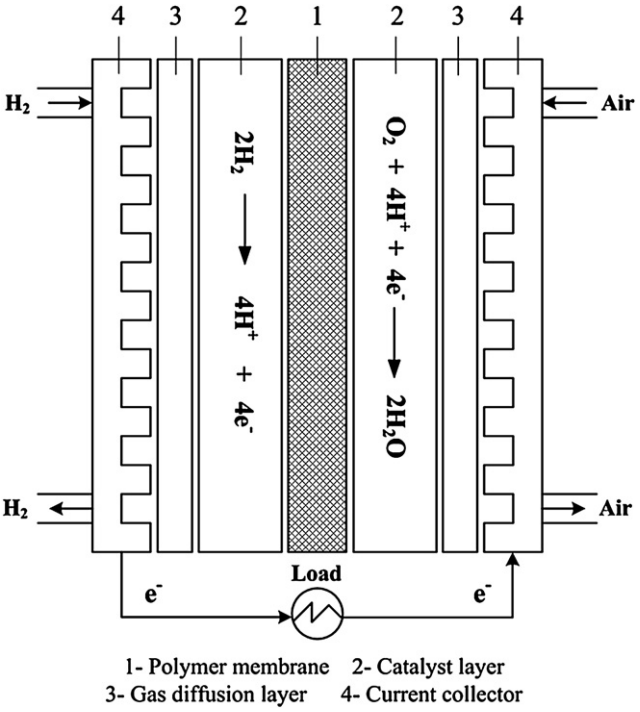

Fig. 1. Schematic of a PEM fuel cell.

a conflict that on the anode side, the membrane tends to dry out owing to electro-osmotic transport while on the cathode side, flooding emerges so that excessive water may block the pores of the catalyst layers, the gas diffusion layers or even the gas channels. Moreover, water formation and distribution along with phase change are also important processes concerned with water management. A detailed schematic of water behavior in a PEM fuel cell is illustrated in Fig. 2. Springer et al. [10,11] incorporated water diffusion coefficients, electro-osmotic drag coefficients, water sorption isotherms and membrane conductivities into the model equations. But the model does not include the water transport due to pressure differences between both sides of the membrane. Fuller and Newman [12,13] concentrated on transport number of water in Nafion 117 membrane experimentally and also developed a mathematical model indicating that equilibrium sorption of water between the gas phase and the polymer electrolyte depends strongly on temperature. Based on Ref. [12,13], Zawodzinski et al. [14] investigated a variety of polymer membranes and discovered that the electro-osmotic coefficients do not obviously depend on the microscopic structure of the membranes. However detailed reasons for this phenomenon were not given in the paper. Eikerling et al. [15] proposed a model which accounts for electro-osmotic drag and the counterflow in a hydraulic pressure gradient. Okada et al. [16] demonstrated that the membrane thickness and humidifying conditions both influenced water content in PEM fuel cells. Mazumder and Cole [17] treated formation and transport of liquid water in PEM fuel cells utilizing a three-dimensional CFD model, in which the phase change process is regarded as an equilibrium process, while the transport of liquid water is governed by surface tension, gravity besides pressure and electro-osmotic drag. Sui and Djilali [18] and Janssen [19] both discussed water transport problem by means of Phenomenological Models.

It is evident that the performance of PEM fuel cells is mainly determined by water management especially when fuel cells operate under higher current densities. Meanwhile, the heat and gas management should be also taken into account because they are closely related with water management. Matamoros and Brüggemann [20,21] solved the water and thermal management through modeling and simulation of the water transport in polymer membrane, phase change of water in the cathode porous medium and capillary flow to the gas channels. Impacts of the geometry parameters on cell performance under different humidifying conditions were also evaluated. Nguyen and White [22] set up a water and heat management model to describe the electro-osmotic drag and back diffusion process, heat transfer from solid phase to gas phase, latent heat associated with water evaporation and condensation in the flow channels. Yan et al. [23] computed water distribution in the membrane under different operating conditions. It was shown that temperature distribution changed greatly when the current densities reach higher levels and dehydration of the membrane on the anode side deteriorated cell performance. Djilali and Lu [24] assessed the characteristics of gas and water transport associated with heat formation and transfer. The results showed that non-uniform distribution of temperature and pressure interfered water transport in PEM fuel cells. Li et al. [25] presented a numerical model coupling the heat/mass transfer and electro-chemical reaction in which the latent heat from the condensation of water vapor in cathode channel was considered. Hwang [26] predicted local thermal nonequilibrium between the solid matrices and the fluids in the gas diffusion layers using a thermal-electrochemical coupled model. Yu and Jung [27] explored the thermal management strategy by presenting three sub-models including a water transport model, an agglomerate

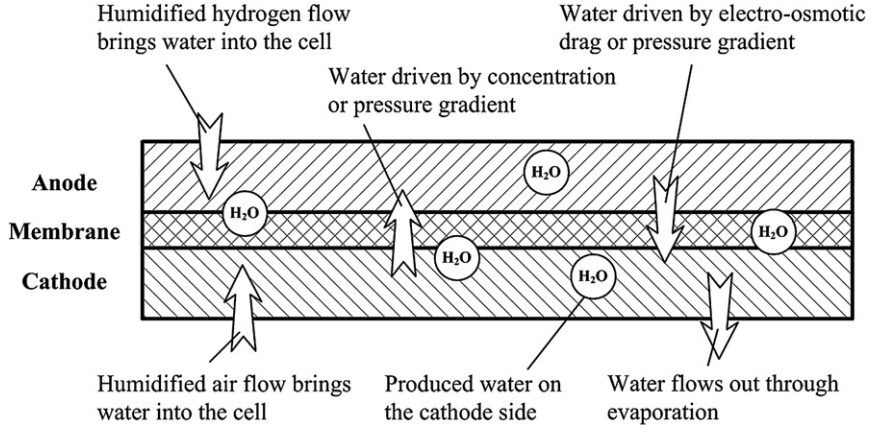

Fig. 2. Schematic of detailed water behavior in a PEM fuel cell.

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