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Two-dimensional analytical model of a proton exchange membrane fuel cell



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ABSTRACT

In this study, a two-dimensional full cell analytical model of a proton exchange membrane fuel cell is developed. The analytical model describes electrochemical reactions on the anode and cathode catalyst layer, reactants diffusion in the gas diffusion layer, and gases flow in the gas channel, etc. The analytical solution is derived according to the basic physical equations. The performance predicted by the model is in good agreement with the experimental data. The results show that the polarization mainly occurs in the cathode side of the proton exchange membrane fuel cell. The anodic overpotential cannot be neglected. The hydrogen and oxygen concentrations decrease along the channel flow direction. The hydrogen and oxygen concentrations in the catalyst layer decrease with the current density. As predicted by the model, concentration polarization mainly occurs in the cathode side.

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1. Introduction

The proton exchange membrane fuel cell (PEMFC) is considered as one of the most promising power sources and has attracted much attention in recent years because of its advantages such as high efficiency and low emissions [1-3]. The PEMFC has potential applications in many fields, such as hybrid power supply system [4,5], electric vehicle [6-8], and space mission [9]. Abundant works have been done on the PEMFC. The major approaches for investigating the PEMFC are experiments and numerical simulations. Only a few researchers have used analytical models to study the PEMFC.

A number of studies have been done on the polarization curves of PEMFCs with semi-empirical or empirical analytical equations [10–13]. This kind of model used empirical equations to fit the measured polarization curve. Modification, considering species transport, has been done to modify the expression to be a more complicated function of current [14,15]. However, these models cannot yield true mechanistic behavior and they are not good for predicting the performance of fuel cells [16]. Moreover, these models are zero-dimensional. No spatial dimensions of the fuel cell are considered in these models.

In addition, one-dimensional (1D) analytical models of PEMFCs have been developed. Most of 1D analytical models focus on particular components of PEMFCs, such as the cathode catalyst layer [17–27], the gas channel [28], the membrane [29–32], and the membrane humidifier [33,34]. Besides, polarization curve [35–38], electrical contact resistance [39], proton resistance [40], membrane resistance [41], and impedance [42] have also been concerned. Bernardi et al. [43] developed a model of a PEMFC to investigate the transport phenomena in the fuel cell. This model ignored the anode and cathode gas channels. Only the species transport along the direction normal to the plane of each layer was considered. Springer et al. [44] presented a 1D model for the cathode side of a PEMFC. Basic equations of the model can be solved analytically. Perry et al. [45] developed a 1D model for the gasdiffusion electrodes. They solved the model with combined numerical techniques and analytical approach. The solution could be used as a diagnostic tool for fuel cells cathode. Eikerling et al. [46,47] presented macrohomogeneous models of PEMFCs. The models were developed for the cathode catalyst layer. However,





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analytical expressions were obtained under restrictive conditions. Gurau et al. [48] developed a 1D analytical model of a PEMFC. This model focused on the cathode side and took into account oxygen transport and current density. The diffusion layer was divided into several layers because of different liquid water contents. In order to study the heat transport in a PEMFC, a 1D analytical model was developed by Kulikovsky [49]. The analysis domain included the anode catalyst layer, the membrane, and the cathode catalyst layer. Relations for the temperature on both sides of the membrane was obtained because of the analytical solutions. Kulikovsky [50] also developed a dead spot model in the anode catalyst layer to obtain the potential and current distributions in and around the spot. Cylindrical coordinates was used in the model. The twodimensional (2D) equation for membrane potential problem became a 1D expression with simplification. Analytical models for the cathode overpotential [51], membrane potential [52], and oxygen consumptions [53] were also studied. 1D models usually take into account species transport or other kinetic phenomena across the fuel cell and ignore species transport along the surface of each layer in the fuel cell. Therefore, 1D models are insufficient to describe the phenomena in PEMFCs.

Comparing with 1D models, 2D models give a more comprehensive view of PEMFCs. Shamardina et al. [54] developed a pseudo 2D model of a high temperature PEMFC. This model mainly concentrated on the cathode side of the PEMFC and studied the crossover of gases through the membrane. Moreover, they proposed a more accurate model of a high temperature PEMFC cathode to study the dynamic behavior of the cell [55]. Tsai et al. [56] developed a 2D analytical model for the oxygen transport in the cathode gas diffusion layer of a PEMFC. Analytical solution was derived to analyze the effect of gas diffusion layer. Lin et al. [57] presented a quasi 2D analytical model of a PEMFC. They discussed the distribution of the oxygen mass fraction, the solid polymer electrolyte potential, and the current density with the analytical solutions derived from the half cell model. This model was only for the cathode side. Kulikovsky [58] proposed a semianalytical model of a PEMFC. This analytical model considered 1D oxygen and water transport across the cell and 1D flow description of species along the fuel supply channels. Other 2D models on the performance of PEMFCs were also developed by Kulikovsky [59,60]. Whereas, these models are for the cathode. Khakpour et al. [61] presented analytical solutions for the species transport in a PEMFC. The solutions contained 2D convection and diffusion process in the porous layers of the PEMFC. The solutions were derived by using matched asymptotic expansion and Laplace transform. He et al. [62] simply discussed a 2D analytical model of a PEMFC. However, the solution was so complicated that most practical issues cannot be answered by the solution.

Although a number of 2D analytical models of PEMFC have been developed, even quasi three-dimensional model [63] has been built, these models are mainly for the cathode. To the best of our knowledge, 2D full cell analytical model of the PEMFC considering species transport, voltage, and current density has not been developed. A previous study [64] built a 2D full cell analytical model of a direct methanol fuel cell. In this work, a 2D full cell analytical model of a PEMFC has been developed and the solution to the model equations for the voltage and current density is presented. The anode overpotential has been neglected in abundant literature e.g. Ref. [54]. However, Herrera et al. [65] suggested that the anode overpotentials cannot be ignored. Therefore, both the anode and cathode overpotentials have been taken into account in the model. The solution is derived from the basic physical equations which describe the species transport in the PEMFC. The results show that the performance of the fuel cell predicted by the model agrees well with the experimental data in literature [66].

The previous 2D analytical models considering current density and voltage are for the cathode of PEMFCs. Therefore, the main contributions of this work are: 1) to develop a 2D full cell analytical model for a PEMFC, 2) to derive the analytical solution for the cell voltage and current density, 3) to obtain the species distribution in both anode and cathode side of the PEMFC using the model. The rest of the work is organized as follows. Section 2 develops the 2D full cell analytical model and deduces the solution of the model. The validation of the model and species distribution are evaluated in Section 3. The conclusions are given in Section 4.

2. Analytical model and solution

2.1. Assumptions

Fig. 1 shows the system of coordinates for the analytical model. The model takes into account the channel, the gas diffusion layer, the catalyst layer, and the membrane. The water transport in the fuel cell is neglected for simplicity. Reactants diffusion in the membrane is not considered because the membrane is supposed to be impermeable for hydrogen and oxygen. The other assumptions which are commonly made in literature e.g. Refs. [17,54,58–60] are presented as follows:

- 1. The flow in the fuel cell is steady.
- 2. The flow velocities of fluids in channel are constant and uniform.
- 3. Pressure drop in the flow channel is ignored.
- 4. The overpotential is constant along the direction of channel.
- 5. The cell temperature is uniform and the electrochemical reaction occurs under constant temperature.
- 6. Transport of reactants in the catalyst layer along the y-direction is ignored because the thickness of the catalyst layer is two orders of magnitude smaller than its size along the channel direction.
- 7. The reactants concentration change across the catalyst layer is not taken into account because the catalyst layer is very thin. As



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