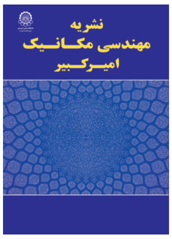

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A Parametric Investigation of Two Phase Flow in the Cathode Side of Polymer Electrolyte Membrane Fuel Cell

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ABSTRACT: In this study, performance of polymer electrolyte membrane fuel cell was investigated using a two-phase, transient and three-dimensional model of the cathode side of the polymer electrolyte membrane fuel cell. At first a comprehensive model was presented for two-phase flow simulation. Then, the governing equations were discretized by a finite volume method and were solved numerically using an in-house developed FORTRAN program. A parametric study on the liquid water formation in porous medium and the performance of the polymer electrolyte membrane fuel cell was conducted. Among effective parameters on the performance of polymer electrolyte membrane fuel cell, porosity and permeability of porous medium, contact angle between water and solid surface, were studied. The results showed that the reduction of porosity, permeability and contact angle will increase the amount of liquid water in porous media. Permeability and contact angle are most effective and by variation of permeability from 10^{-9} m^2 to 2×10^{-14} m^2 , average of the liquid water saturation in the catalyst layer changes from 0.04 to 0.16 and by variation of contact angle from 91 to 140, average of the liquid water saturation in the catalyst layer changes from 0.058 to 0.15. Finally, in order to study the influence of capillary diffusion coefficient on the amount of liquid water in the catalyst layer and polymer electrolyte membrane fuel cell performance in the different cell voltage, a unit parameter is defined in a way to be just function of gas diffusion layer properties and effect of this parameter on average of water liquid saturation in the catalyst layer was studied.

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1- Introduction

In recent years, several one-dimensional and two (or three)-dimensional models were presented for studying the Polymer Electrolyte Membrane (PEM) fuel cell performance. These models assumed that water in PEM fuel cell is only in the vapor phase and there is no liquid water in the cell; whereas water can be formed in the liquid phase. Since at high current density, the influence of the water liquid production is significant, these models were not able to make a good prediction of the PEM fuel cell performance. Hence, two-phase flow models were developed for PEM fuel cells to account for the liquid phase formation.

Wang et al. [1] presented one of the earliest two-phase, two-dimensional model for the cathode side of Proton-Exchange Membrane Fuel Cell (PEMFC). This model was based on traditional mixture model [2]. In this model, conservation equations were solved for the mixture, then at post processing step, each phase velocities were determined. You and Liu [3] further developed the previous model and studied the effect of different membrane on PEM fuel cell performance. They reported that the net water transport from anode side toward cathode side depends on the operating current density, the water activity, the water partial pressure on two sides, and the membrane properties. Baboli and Kermani [4] used a two-phase and transient model similar to the model presented by Wang *et al.* considering that fluid flow in the cell is compressible. Liu et al. [5] employed a two-fluid, steady state, three-dimensional and non-isothermal model for both anode, cathode and membrane of PEM fuel cell. They reported that the water content in the membrane near of anode side is higher than that of the cathode side under small current density, while it is lower under higher current density. Qin et al. [6] considered liquid water in the gas channel of the PEM fuel cell using a similar method to one presented by Wang et al. [7]. They show that ignoring the gas channel flooding leads to the incorrect prediction of the liquid water distribution in the porous medium.

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2- Methodology

In the present study, a two-phase, transient, two-dimensional, multicomponent model is considered for the cathode side of PEM fuel cell. The governing equations of the model were solved by an in-house developed FORTRAN code. The main purpose of this investigation is to study the effect of gas diffusion layer and porous medium properties on the water production and cell performance. A detailed parametric study is performed to investigate the effect of Gas Diffusion Layer (GDL) properties. Then a unit parameter that is just a function of GDL properties is defined to predict the average water liquid saturation in the Catalyst Layer (CL).

2- 1- Numerical procedure

Governing equations have been discretized by Finite Volume Method (FVM). For velocity-pressure coupling, we have employed the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm [11, 12]. Collocated grid and the Rhie-Chow interpolation has been implemented to avoid the checkerboard pressure [13]. A FORTRAN program was developed to perform the numerical solution. Also, Tri-Diagonal Matrix Algorithm (TDMA) algorithm was used to solve the algebraic equations that result from the FVM discretization.

3- Results and Discussion

Contact angle between water liquid and solid surface at the porous medium is one of the important parameters in the two-phase flow of PEM fuel cell. This parameter can affect the water liquid production. The effect of the GDL contact angle on the average liquid water saturation in the CL and the average cell current density is shown in Fig. 1 for the cell voltage of 0.16V.

Fig. 1 shows that for hydrophobic porous media, increasing the GDL contact angle leads to a decrease in the average liquid water saturation in the CL and conversely, an increase in the average current density. Under these operating conditions, the liquid water saturation varied from 0.058 to 0.15 and cell current density from 0.88 A/cm^2 to 0.98 A/cm^2. In addition, it was observed that when the GDL contact angle is close to 90, the capillary diffusion coefficient will be reduced; the water generated due to the phase change is much more accumulated in the CL.

GDL permeability influences on the velocity profile, mass fraction of the components and the liquid water saturation. In order to investigate the effect of GDL permeability, the average of liquid water saturation in the CL and the average current density at different GDL permeability was shown in Fig. 2.

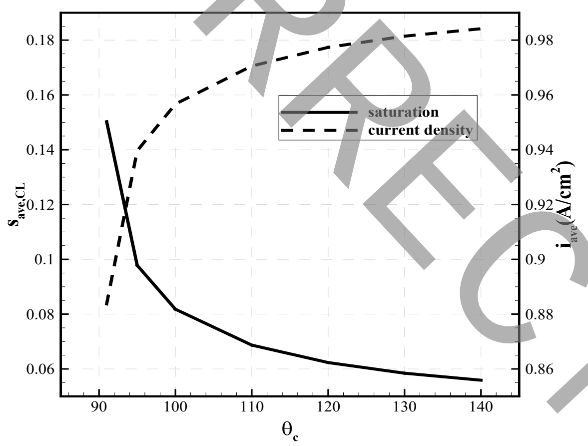

Fig. 1. The effect of GDL contact angle on the average liquid water saturation at the CL and the average current density (V_{cell}=0.16 V).

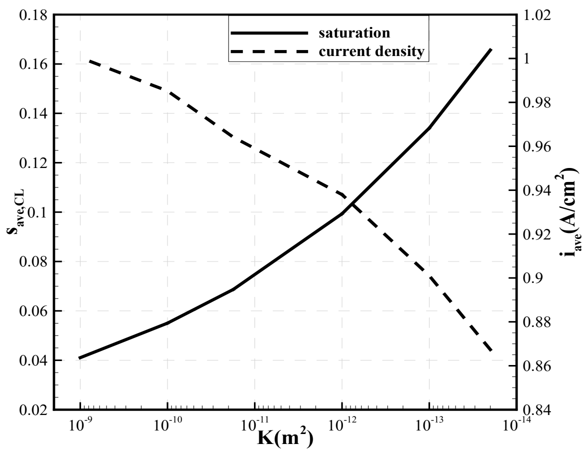

Fig. 2. The effect of GDL permeability on the average liquid water saturation at the CL and the average current density (V_{cell}=0.16 V).

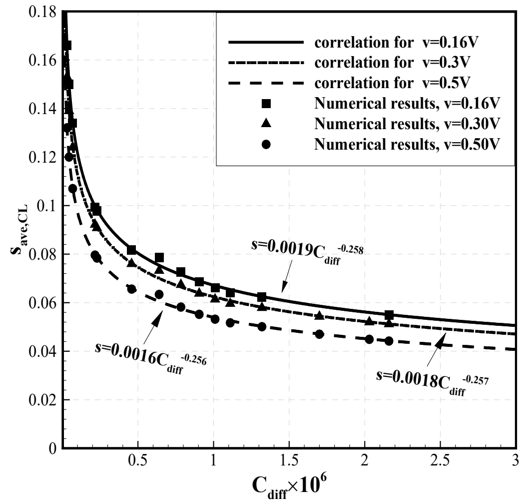

Fig. 3. The effect of C_{diff} on average of liquid water saturation at the catalyst layer.

In Fig. 2, the horizontal axis is logarithmic to allow observing better the variations. As the GDL permeability is lower, the average of liquid water saturation is increased; while, average current density is reduced. The liquid water saturation was is changed from 0.04 to 0.16 and cell current density from 0.86 A/cm^2 to 1.005 A/cm^2. Although at low permeability, capillary pressure is increased; however, the diffusion of liquid water in the porous medium is reduced. Also, the liquid water has less ability to diffuse into other parts such as the gas channel. We define $C_{diff} = (eK)^{0.5} cosq$ as a unit parameter that is just related to the GDL characteristics. C_{diff} represents the effect of GDL material on the two-phase flow in the PEM fuel cell. Variation of average liquid water saturation versus C_{diff} is shown in Fig. 3 voltage of 0.16V, 0.3V and 0.5V. The results show that if capillary diffusion coefficient increases, the amount of water liquid saturation in the CL will decrease. For C_{diff} near to 0, variation of liquid water saturation in CL is very intense and for C_{diff} more than 2, the slope of variation approximately is constant. For the operating condition tested here, average of liquid water saturation in the CL can be estimated by fractional or exponential functions. For example at cell volt tion is $s_{ave,CL} = 0.0019C_{diff}^{-0.258}$ $s = 0.0016C_{diff}^{-0.254}$ which was resulted by performing a curve fit using the least square method. Although, this function is just true for this operation condition, but this relation causes an insight for the reader about variation of the amount of liquid water saturation in the CL versus C_{diff} or characteristic parameter of GDL. For other voltage, the functionality of the variation is the same with different constant coefficients.

4- Conclusions

In this research, the effects of several parameters on the PEM fuel cell performance were studied using a two-phase flow, two-dimensional, transient and isothermal model. The results can be summarized in some points.

1. GDL properties such as porosity, permeability and

contact angle are effective on the resulting amount of water liquid in the cell.

2. At low GDL porosity and GDL permeability, liquid water in the CL will increase; while, cell current density will reduce.
3. At contact angles near 90, liquid water in the CL will increase and cell current density will reduce rapidly. At higher contact angles, the intensity of variation will decrease.
4. The capillary diffusion coefficient of liquid water in the porous media is the most important characteristic parameter of the two-phase flow in PEM fuel cells. If the capillary diffusion increases, more liquid water is transferred from the CL to the gas channel. Moreover, the amount of liquid water in the CL decreases and the cell performance is improved.

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