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Numerical Investigation of Water Management in the Cathode and Anode Sides of Proton Exchange Membrane Fuel Cell

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ABSTRACT: Water management in a proton exchange membrane fuel cell is numerically modeled by considering the 2D, non-isothermal steady flow assumptions. Governing equations are solved in all cell layers including cathode and anode electrodes by finite volume method using a single-region approach. The effect of gas cross-over through the membrane is studied on cell performance. This consideration, not only improves the general accuracy of modeling, but also makes it possible to model energy losses due to direct reaction of reactant gases. The effect of some key variables such as liquid water diffusivity, current density, membrane thickness, etc. on PEMFC conditions such as the amount of saturated liquid water, power density, cell temperature, cross-over efficiency and so on are examined. It was observed that the amount of saturated liquid water on the anode side is considerably important. This observation addresses needs for further investigation of liquid water behavior in the anode electrode. The amount of liquid water saturation in both the cathode and anode electrodes is increased with increasing the current density. The results showed that at the current density of 0.2 A/cm^2, cross-over effect causes about 10% reduction in cell efficiency and by decreasing the current density this effect is enhanced.

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1- Introduction

In recent years, A few articles have been published in the field of anode water management. The experimental studies on Proton Exchange Membrane Fuel Cell (PEMFC) water management showed that for certain operating conditions, flooding can also occur in the anode side [1]. For the first time, the two-phase flow in an anode Gas Flow Channel (GFC) of a PEMFC was numerically investigated using Volume Of Fluid (VOF) method by Ferreira et al. [2] in 2015. In this study, the flow was assumed to be laminar, isothermal and transient, without phase-change. Moreover, since the focus of study was on simulating fluid dynamics and predicting liquid water distribution in the GFC, the electrochemical reactions occurring in PEMFC were not considered. Xing et al. [3] in 2016 described a steady, non-isothermal and two-dimensional along-the-channel Computational Fluids Dynamics (CFD) model for a PEMFC. In this, liquid water saturation was simulated inside the electrodes and channels at both the anode and cathode sides. Their results showed that water flooding, represented by liquid water saturation, was prone to occur near the downstream channel of both the anode and cathode.

The water management models developed so far have not considered effect of gas cross-over through the membrane in waste of energy. Seddiq et al. [4] in 2006 show that this effect is not always negligible especially in calculation of cell efficiency. So, in this paper the effect of gas cross-over through the membrane is investigated using a model in the GFC direction (Fig. 1). Water in the cell is considered to be in the form of vapor, but liquid and dissolved phase in the form of polymer.

2- Methodology

In all layers, the flow is assumed 2D, steady state, non-isothermal, laminar and incompressible with variable density. The main equations are mass, momentum, species (oxygen and water vapor), liquid water, proton and energy conservation which are solved in all PEMFC parts (single-region approach). Subsidiary equations for physical and electrochemical properties are also needed. Media is of porous type in all areas except for GFCs. Porosity modeling

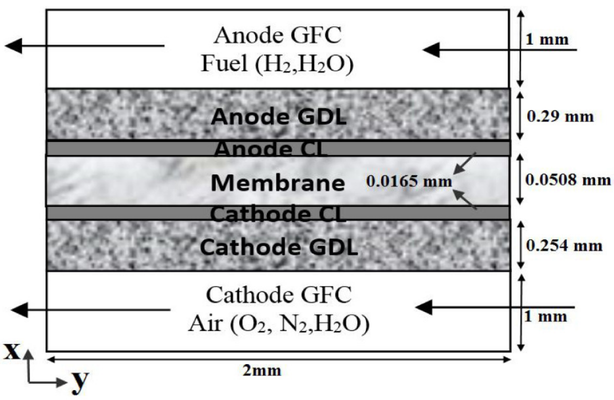

Fig. 1. Computational domain

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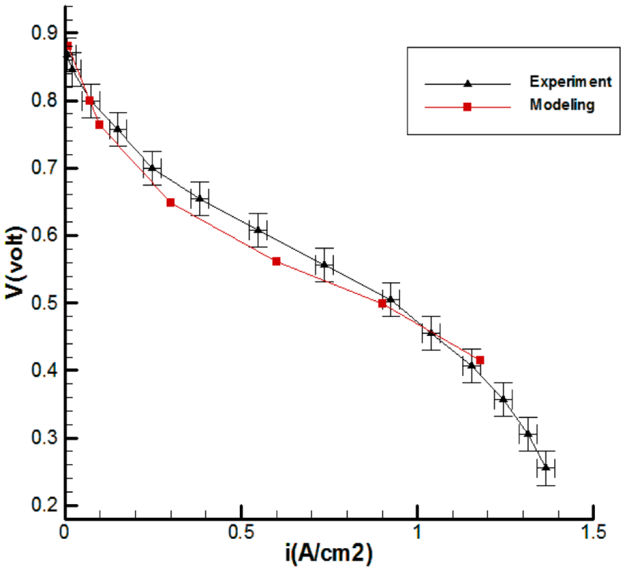


Fig. 2. Polarization curve vs. experimental data [6]

in the equations is applied by defining porosity coefficient ε. For details of governing equations and boundary conditions, one can see Refs. [4] and [5]. It is worth noting that in Ref. [4] the effect of liquid water and in [5] the effect of gas cross-over is not considered. Governing equations are solved based on finite volume method implemented into a Fortran code. Discretization based on power law is used in solving all governing equations and using SIMPLE algorithm, the pressure-velocity coupling are handled. Then, all equations are solved by line by line iteration, which applies a three diagonal matrix algorithm. The computational solution procedure is given in [5].

3- Results and Discussion

A mesh independent grid size of 260×51 is used in the calculation. Obtained results for polarization curve is compared with experimental data in Fig. 2, where a good agreement can be observed. In Fig. 3, saturated liquid water contour (s) is shown. Saturation in channels is very low. Amount of liquid water in membrane is zero. Amount

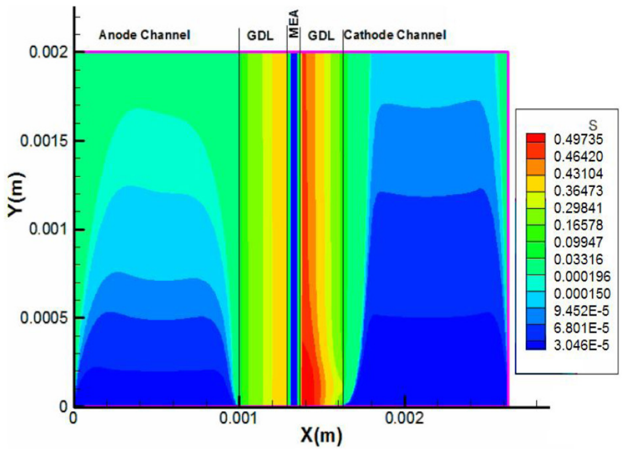


Fig. 3. Saturated liquid water contour

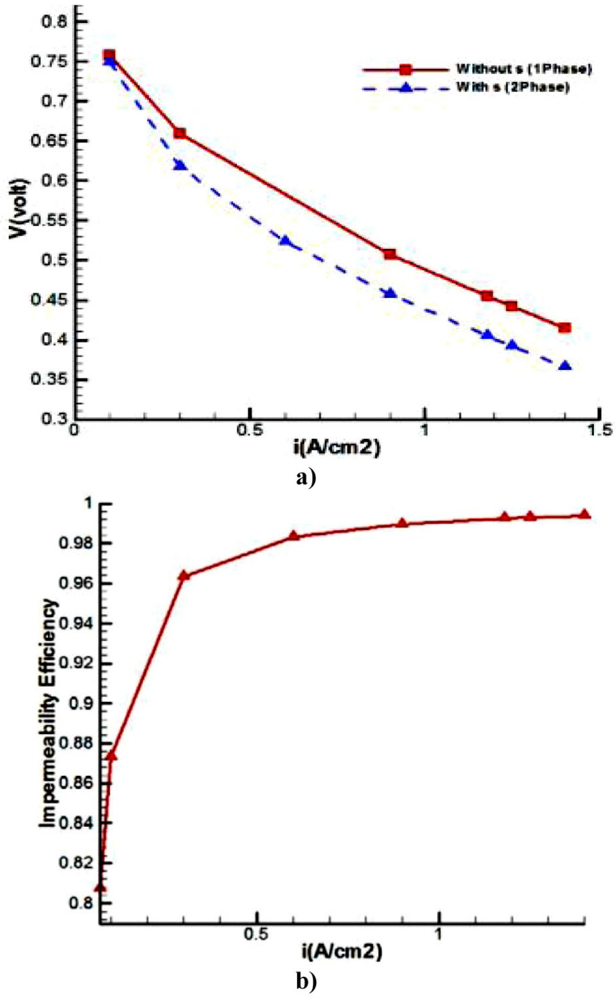


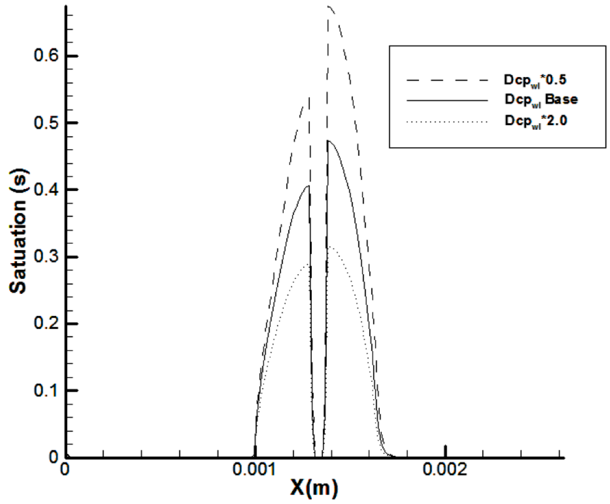
Fig. 4: a) Polarization curve; b) Cross-over efficiency curve

of liquid water in cathode is more than anode. In the initial part of channel due to higher level of reaction and water production, liquid water is more, which amount is decreased in the channel direction.

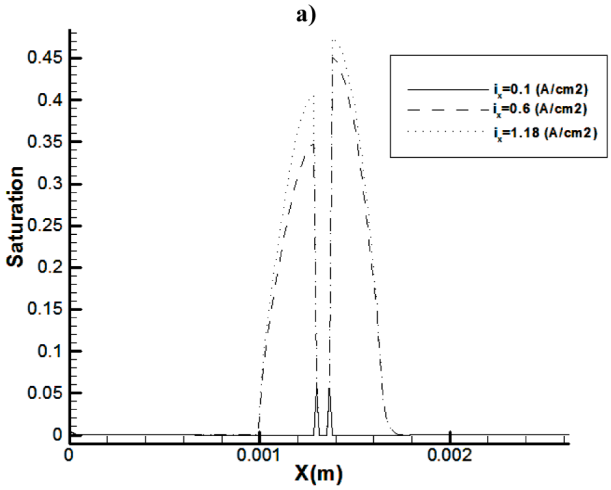
In Fig. 4, polarization curve and cross-over efficiency curve of the model are shown. As it can be seen from the curves, when effect of liquid water on PEMFC is considered, the related curves will decrease. One of the liquid water effects is effect of mass transfer by blocking gas passage in Gas Diffusion Layer (GDL) that affects diffusivity equation. Based on Fig. 4 (b) at the current density of 0.2 A/cm^2, cross-over effect causes about 10% reduction in cell efficiency and by decreasing the current density this effect increases.

Effect of liquid water diffusivity and current density on distribution of liquid water saturation is shown in Fig. 5. This distribution is shown in the middle of the channel.

Liquid water diffusivity is changed due to different factors including hydrophilicity and hydrophobicity. Based on the Fig. 5(a), if liquid water diffusivity is decreased, then liquid water transfer will also decrease. Therefore, more water liquid accumulates in cathode GDL and cell efficiency will decrease. On the contrary, the higher the hydrophobicity of cathode GDL, the more the liquid water diffusivity and the lower the water in GDL, while the more the cell efficiency. It



a)



b)

Fig. 5: Distribution of saturated liquid water in: a) different liquid water diffusivity; b) different current densities

is observed that liquid water on the cathode side is more than anode and by moving from channel to Catalyst Layer (CL), its value will increase. The amount of saturated liquid water at the anode electrode is also noteworthy that calls for further investigation of liquid water behavior in this electrode. The hydrophilic GDL can wick liquid water accumulated in the anode GFC and therefore, a smaller amount of water flooding will be observed under similar operating conditions. As it can be observed from Fig. 5 (b), the higher the consumption current, the more the produced liquid water. The higher the current consumption, the more the produced liquid water. Thus the activation voltage will increase and the cell voltage will decrease. High current density leads to higher water flux from the anode to cathode by electro-osmotic drag and thus decreases water content in the anode and reduces the tendency for liquid water formation. On the other hand, the increase in current density leads to back diffusion from the cathode to the anode. These two factors, along with the pressure difference between the two electrodes are effective in the flooding of the anode.

4- Conclusions

In this paper, the numerical investigation of water management in the PEMFC both in the cathode and anode sides are conducted and the effect of gas cross-over through the membrane is investigated. In this study, the following important results were obtained:

1) The amount of saturated liquid water at the anode GDL are considerably significant.

2) Water content in both electrodes increase with increasing current density.

3) Choosing hydrophobic GDL for cathode and hydrophilic GDL for anode can increases the cell efficiency.

4) At low current density, consideration of the permeability efficiency is essential.

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