MODELING OF LIQUID WATER TRANSPORT IN A PEMFC

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ABSTRACT:

A two-dimensional CFD model of PEM fuel cell is developed by taking into account the mass and heat transfer occurring in all of its regions simultaneously. The catalyst layers and membrane are each considered as distinct porous regions with finite thicknesses and calculated properties such permeability, local protonic conductivity, and local dissolved water diffusion.. This model takes into account the effects of liquid water content in the catalyst and gas diffusion layers. The model for the liquid water flow takes into account the capillary effects due to the interaction between the hydrophobic solid matrix and the liquid. The liquid water transfer is included in the porous structure though the saturation field which is solved for using the continuity equation of the liquid phase.

NOMENCLATURE

K	Permeability	(m^2)
p	Pressure	(Pa)
S	Saturation	
u	x-direction velocity	(m/s)
v	y-direction velocity	(m/s)
Greek		
ε	Porosity	
μ	Dynamic viscosity	$(N.s/m^2)$
θ	Contact angle	(rad)
Subscript		
c	capillary	
g	gas	
l	liquid	

1. INTRODUCTION

As energy demands for sustained development of mankind keeps increasing, hydrogen will be a significant source of energy to meet these demands. Hydrogen is used as a fuel in the proton exchange membrane fuel cell (PEMFC) which one of the widely used fuel cell technologies due to its adaptability to many applications such as the automotive industry. Therefore, it is essential to fully characterize the PEMFC for the wide range of variables that may affect its performance. One of the advantages of the fuel cell is its clean byproducts, which are mainly water and heat. However, water when produced in its liquid phase tends to hinder the performance of the PEMFC. Hence it is essential optimize the liquid water management inside the fuel cell in order to achieve the highest power density especially when high currents are needed during steady state applications. In general both the GDL and CL are sprayed with a hydrophobic coating in order to facilitate water removal.

The principal components in a PEMFC shown in Fig. 1 are:

- The gas channel (GC) is machined in the collector plate and serves as a conduit for the reacting gas species.
- The gas diffusion layer (GDL) is made of a porous material such as carbon cloth or carbon paper. The porous nature of the GDL facilitates reactant distribution across the catalyst layer while being a good electrical conductor, providing a low electrical resistance connection between the

catalyst layer and the collector. Also the GDL layer with the hydrophobic coating facilitates the removal of liquid water produced at the cathode.

- The catalyst layer (CL) main role is to accelerate the electrochemical reaction. It is a porous structure made up of the three different components, namely membrane polymer, GDL, and catalyst particles supported by the porous carbon structure. Platinum is the typical catalyst used in PEMFC applications.

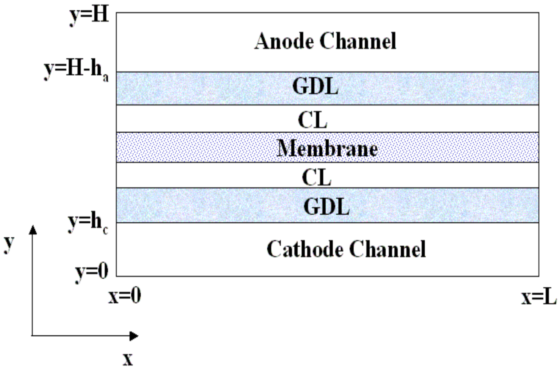

Figure 1: Two-dimensional representation of a PEMFC.

Previous studies on the performance of PEMFC have mainly focused on models that only consider water vapor in the model. Um and Wang [1] investigated water vapor transport in PEMFC using a 3D model. In the MEA they assumed that water exists only in the vapor phase and in the polymer they used a fictive gaseous phase assumed to be in equilibrium with the water content. Their model allowed the study of the performance of the fuel cell for the effect of humidity ratio of inlet mixtures for different values of membrane thickness, and for co-flow and counter flow conditions. Their results show with the counter flow design and at low humidity ratio, the current density produced is comparable to that of the co-flow condition with fully humidified inlet mixtures. Kamarajugadda and Mazumder [2] using a two-dimensional single phase model to investigate different models for membrane conductivity and they found that the choice of the membrane model can affect the current density results significantly. Nguyen et al. [3] and Sivertsen and Djilali [4] have also used a three-dimensional model for the study of PEMFC. In both models they only considered that only water vapor is present. Siegel et al. [5] developed a two-dimensional model for PEMFC with water vapor only. Siegel et al. [6] extended the previous work to include the effect of liquid water and have improved further the electrochemical model. Their results show that the agglomerate geometry and liquid water influence significantly the efficiency of the fuel cell. Sahraoui et al. [7] presented a two-dimensional model for PEMFC which does not include the transport of liquid water. The model was used to investigate many parameters on the efficiency of the fuel cell. These include humidity ratio, porosity, membrane thickness, etc…..

In this study, the previous model presented in our study [7] is extended in order to include the effects of liquid water transport. We use a two-dimensional numerical model to examine the mass and heat transfer occurring in all regions of the fuel cell and the electrochemical chemical reactions occurring in the catalyst layers. In this model the liquid water transport in the CL and GDL layers is included in addition to the mass transfer of the different gaseous species (H_2O, O_2, H_2), the proton transfer and dissolved water in the polymer. The water liquid phase is solved for by using the saturation equation obtained through the liquid phase continuity equation and the Darcy model for flow in porous media. All the transport equations are solved for using the finite volume method.

2. MODEL

The two-dimensional model used for this study is depicted in Figure 1 showing all regions of the PEMFC.

The model assumptions are:

- Steady state;
- Compressible and laminar flow;
- Newtonian fluid;
- Ohmic losses due to electrons transfer are neglected in the GDL and CL;
- Dispersion in the porous media is neglected;
- Each region is isotropic and homogeneous;
- Local thermal equilibrium between the fluid and solid (GDL,CL, and PEM);
- Water produced through chemical reactions is in the liquid phase if the local water vapor pressure exceeds the local saturation pressure;
- H_2 is present in the anode only, O_2 and N_2 are present in the cathode only, and H_2O vapor and liquid are present in the entire computational domain except in the membrane where it is modeled as dissolved water (liquid form).

The models for momentum and electrochemistry are treated in detail in our previous work [7]. Here we only present the equations that are added in order to include the effect of liquid water. The liquid phase velocities in the x- and y-directions are governed by the continuity equation

$$\frac{\partial u_l}{\partial x}+\frac{\partial v_l}{\partial y}=0 \tag{1}$$

and the velocities of the liquid for two phase flow in a porous structure is given by

$$u_l=-\frac{KK_{rl}}{\mu_l}\frac{\partial p_l}{\partial x} \qquad v_l=-\frac{KK_{rl}}{\mu_l}\frac{\partial p_l}{\partial y} \tag{2}$$

where K is absolute permeability for single phase flow, K_{rl} and K_{rg} are the relative permeabilities of the liquid and gas phases, respectively and they are given by [8]

$$K_{rl}=s^3 \qquad K_{rg}=(1-s)^3 \tag{3}$$

where s is the saturation representing the volume fraction of the liquid phase. The liquid and gas pressures are linked through the capillary pressure given by

$$p_c=p_l-p_g=\frac{\sigma\cos(\theta_c)}{\left(K/\varepsilon\right)^{1/2}}J(s) \tag{4}$$

where σ is the surface tension coefficient , θ_c is the contact angle, and ε is the porosity. Le Leverett J-function is given by

$$J(s)=1.417s-2.120s^2+1.263s^3 \tag{5}$$

In this model we assume that the liquid water motion is governed by the capillary pressure (i.e., $p_l \approx p_c$ and combining equations (1) and (2) we obtain

$$\frac{\partial}{\partial x}\left(K_{rl}\frac{dp_c}{ds}\frac{\partial s}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{rl}\frac{dp_c}{ds}\frac{\partial s}{\partial y}\right)=0 \tag{6}$$

The effect of saturation on the Butler Volmer equation and species diffusion equation is included by introducing the factor $(1-s)$. This takes into account the presence of the liquid water inhibiting species diffusion to the reaction sites.

The model equations are discretized using the finite volume method for a non-uniform staggered grid. The SIMPLE algorithm is used to solve for pressure and the velocity fields. Some results for the current density for different inlet temperature and gas relative humidity are discussed below.

3. RESULTS AND DISCUSSIONS

The dimensions used for this study are shown in table 1 [6]. The model results with liquid water shown in Fig. 2 are in good agreement with the experimental measurements performed by Siegel et al. [6]. The results show that when liquid water is not taken into account in modeling PEMFC, current density can be over predicted and in this case the difference in current density is about 15%. This difference will be larger as the PEMFC channel length, along the flow direction, increases since more water accumulates as the channel length is increased.

In subsequent discussions the conditions for the nominal case used are reported in Table 2. Figure 3 shows the liquid water content of the cathode side represented here by the saturation. These results show that water content in the catalyst layer is somewhat uniform in the catalyst layer but it tends to cumulate more on the exhaust side of the cathode. In this region, the current density is expected to be the lowest since the reactant concentration is lower than at the inlet region due to consumption by the chemical reaction.

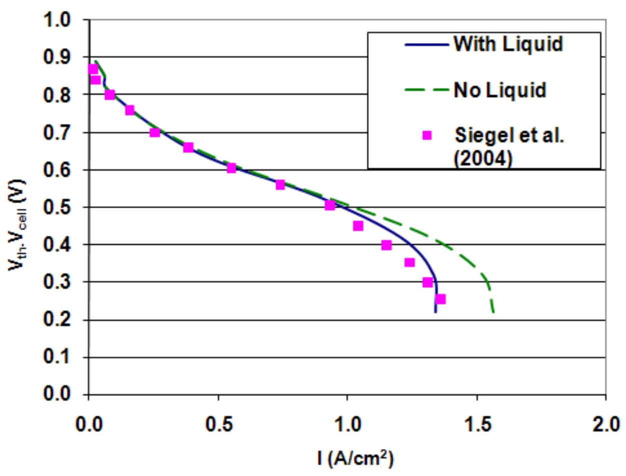

Figure 2: Comparison of predicted current density (with and without liquid water) to experimental results of Siegel et al. [6] .

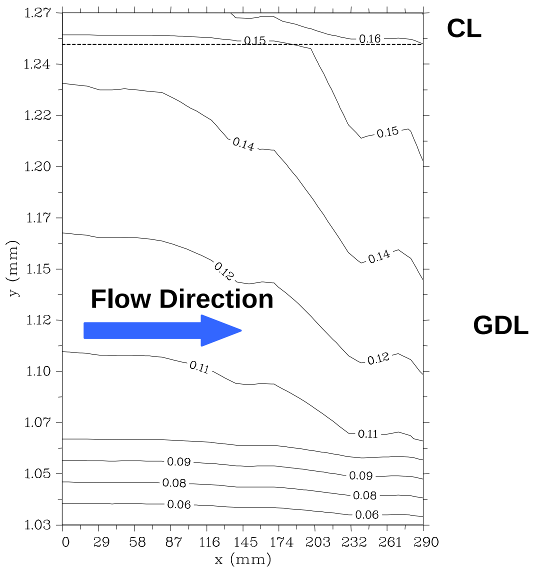

Figure 3: Water saturation in the cathode (GDL and CL).

The effect of temperature on the performance of a PEMFC is shown in Fig.4 for 100% RH for both the anode and cathode sides. As expected, the higher temperature case gives higher current density. This is due to that fact that the equilibrium water content within the polymer decreases as the temperature decreases hence increasing the voltage losses for the protons crossing from the anode to the cathode.

Figure 5 shows the effect of relative humidity on current density. For a fully humidified anode gas, the maximum current density is obtained for a 60 % cathode RH. This is due to the fact that as the cathode RH is increased more liquid water is formed hindering diffusion and reaction. On the other hand, if the cathode RH is reduced below the optimum value, the lower water content starts to affect proton conductivity, thereby, increasing resistance and reducing the current density.

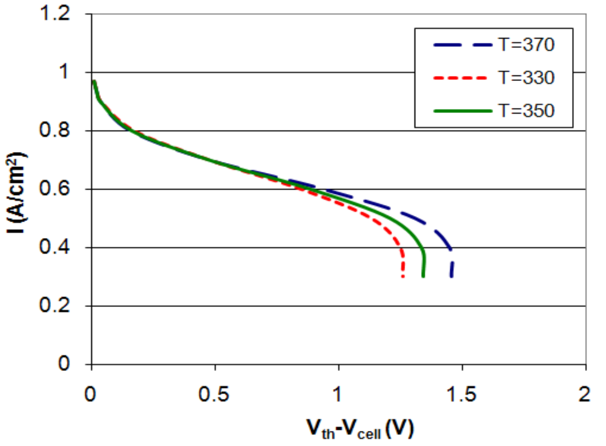

Figure 4: Effect of Temperature on current density.

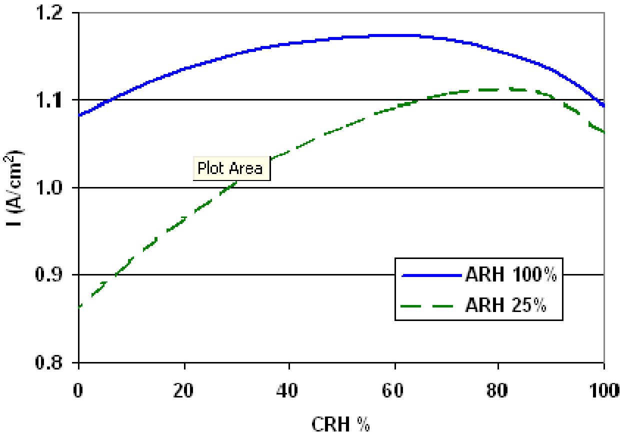

Figure 5: Effect of cathode relative humidity on current density

4. CONCLUSIONS

In this work, a two dimensional CFD model for a PEMFC is presented in order to study the effect of liquid water on the performance of the fuel cell. Water transport is modeled using liquid phase saturation and capillary pressure. The current density results presented are in good agreement with experimental data. The model is then used to investigate the effect of relative humidity on the current density and the results show that for an optimum performance with a fully humidified anode inlet gas, the cathode relative humidity needs to be about 60%.

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Table 1: Dimensions of the fuel cell used in the present study.

Property	**Value**
Gas channel length (L)	300 mm
Gas channel depth	1 mm
Gas channel height (h_a and h_c)	1 mm
Anode GDL thickness	0.290 mm
Cathode GDL thickness	0.254 mm
Catalyst layer thickness	0.0165 mm
Membrane thickness	0.0508 mm

Table 2: Nominal condition for the present numerical study.

Anode		Cathode	
H2	90 mol/m3	O2	18.98 mol/m3
		N2	71 mol/m3
%RH	100	%RH	100
T	353 K	T	353 K
Velocity	1.55 m/s	Velocity	3.75 m/s