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Numerical Investigation of Anisotropic Electrical Conductivity Effects in Proton Exchange Membrane Fuel Cell

Gülşah Elden^{1*}, Mert TAŞ²

¹ Corresponding author: Erciyes University, Faculty of Engineering, Department of Energy Systems Engineering, Melikgazi, 38039, Kayseri, Turkey, gulsah@erciyes.edu.tr

² Erciyes University, Faculty of Engineering, Department of Energy Systems Engineering, Melikgazi, 38039, Kayseri, Turkey, merttas@erciyes.edu.tr

Abstract

The purpose of this study is to investigate numerically the effects of anisotropic electrical conductivity of gas diffusion layers on charge transport in Proton Exchange Membrane (PEM) fuel cell. To achieve this purpose, a single phase, three dimensional and anisotropic model is developed by using COMSOL Multiphysics 4.2a software. The numerical model is validated in experimental data which is obtained at the cell temperature of 343 K for the PEM fuel cell having $5x5 \text{ cm}^2$ active surface area. To find out numerically the effects of anisotropic electrical conductivity of gas diffusion layers on charge transport, two cases are examined. In the first case, the in-plane electrical conductivity of its is increased gradually as the through plane electrical conductivity is kept constant. In the second case, while the value of in-plane electrical conductivity is a constant, the through plane electrical conductivity is increased. When the both electrical conductivities are compared for all cases, the through plane conductivity has a greater effect on charge transport in PEM fuel cell than the in-plane plane electrical conductivity.

Keywords: PEM fuel cell, anisotropic electrical conductivity, numerical model.

^{*} Corresponding author : Erciyes University, Engineering Faculty, Melikgazi, Kayseri, Turkey, gulsah@erciyes.edu.tr, phone: +90 352 207 6666

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) are considered as a promising energy conversion technology because of their scalability, rapid start up and zero emission. Their electrochemical, mass and heat transfer phenomena have been tried to understand by computational simulations and experimental studies over the last decades. Modelling of fuel cell is used to analyse profoundly their performance and transfer phenomena. There are a wide range of PEM fuel cell numerical models in literature [Bernardi and Verbrugge (1990)-Haghayegh et al (2017)]. But anisotropic 3-D model studies are less than the others. Bapat and Thynell (2008) conducted two phase two dimensional PEMFC model operated at 353 K. The researchers tried to investigate that the effect of anisotropic electrical conductivity on current density and temperature distributions. The results of this study bring out that through plane electrical conductivity is more effective than in-plane electrical conductivity on the current density and temperature distributions. Zhou and Liu (2006) developed a 3D PEMFC model operated at 343 K. The purpose of their study is to investigate the effect of anisotropic electrical conductivity on cell performance. It is observed that increasing in-plane conductivity affects to fuel cell performance slightly. Ismail et al (2012) modelled a single phase, 3D, PEMFC model with serpentine and straight channel type. Furthermore, several cases which have different anisotropic electrical conductivities. It is shown that anisotropic electrical conductivity of gas diffusion layer influences to significantly fuel cell performance.

The main objective of this study is to investigate the effects of anisotropic electrical conductivity on electrochemical phenomena in detail. In order to achieve this objective, a single phase, three dimensional, having constant operating temperature and anisotropic PEM fuel cell model is developed and two cases are examined. In the first case [Case Group A], the in-plane electrical conductivities of gas diffusion layers are increased gradually (100 S/m, 200 S/m and 400 S/m) as the through plane electrical conductivity is kept constant (400 S/m). In the second case [Case Group B], when the value of in-plane electrical conductivity of gas diffusion layers is a constant (400 S/m), the through plane electrical conductivity is increased step by step (100 S/m, 200 S/m and 400 S/m).

2. Mathematical Modeling

The 3D PEM fuel cell model consists of seven layers which are anode channel, anode gas diffusion layer, anode catalyst layer, membrane, cathode catalyst layer, cathode gas diffusion layer and cathode channel as is shown in Figure 1.



Figure 1. Schematic illustration of PEM fuel cell (a) PEM fuel cell components (b) Mesh of 3D domain.

2.1 Model Assumptions and Equations

In the presented study, to better understand the effects of anisotropic electrical conductivity on electrochemical phenomena, PEM fuel cell is modelled numerically which solves mass, momentum, species and charge conservation equations under the certain assumptions. Table 1 depicts the using conservation equations in the mathematical model. Source terms using equations and boundary conditions are given in Table 2. The following assumptions are made to reduce complexity of the model.

- Model operated at steady-state conditions.
- The porous layers are considered as homogeneous pore structure.
- ▶ In all interface, contact resistances are neglected.
- ➤ All gases are ideal gas.

Table 1.	Governing	Equations
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Continuity equation	$ abla(\epsilon hoec u)=0$	
Navier Stokes Equation	$\nabla(\epsilon\rho u u) = -\epsilon \nabla P + \nabla^* (\epsilon \mu^{eff} \nabla u) + S_u$	
Darcy Law	$u=-\frac{k_p}{\mu}$	
Stephan-Maxwell equation	$\mu \nabla m = \nabla \left[\rho \varepsilon m \sum_{j=i}^{N} D_{ij} \left\{ \frac{M}{M_{i}} (\nabla m_{i} + m \frac{\nabla M}{M}) \right\} \right]$	
Species conservation equation	$\nabla(\epsilon u c_k) = \nabla(D_k^{eff} \nabla c_k) + S_k$	
Charge conservation equation	$\nabla . (k_e^{e_f} \nabla \Phi_e) + S_{\Phi} = 0$	

Table 2. Source terms using equations and boundary conditions

Equations	Flow Channels	GDL	Catalyst Layer	Membrane	
Momentum	Su=0	S _u =-⊽P ^{<u>k</u>_p}	u=0	u=0	
Species	S _k =0	S _k =0		S _k =-⊽n _d Fl _e	
Charge	S₀=0	S _Φ =0	S₀=j	S _Φ =0	
Boundary Conditions					
U _{in,anode} = U _{a,in} , U _{in,cathode} = U _{c,in}					
CH2,anode=CH2,a; CO2,cathode=CO2,c; CH2O,anode=CH2O,a; CH2O,cathode=CH2O,c					

3. Results

3.1 Validation of the numerical model

The computational model solved for reference conditions and polarization curve validated with Ismail et al's (2012) experimental and computational results. As shown in Figure 2, model values and reference values fitted each other.



Figure 2. Validation of model with reference experimental and model values.

3.2 Results of case studies

For two different case groups (as shown in Table 3), the effects of anisotropic electrical conductivity on electrochemical phenomena in PEM fuel cell are analyzed separately. Figure 3 illustrates the interface that measuring of potentials and current densities values of fuel cell.

Case Group A				
Case Number	In-plane conductivity [S/m]	Through-plane conductivity [S/m]		
1	100	400		
2	200	400		
3	400	400		
Case Group B				
1	400	100		
2	400	200		
3	400	400		

Table 3. Case Study Parameters

Polarization curves of the two different case groups are demonstrated in Figure 4. As it is seen in the figure, for the Case Group A, when the in-plane electrical conductivities of gas diffusion layers increase gradually, fuel cell performance decreases dramatically at constant through plane electrical conductivity. Furthermore, there is an increment in fuel cell performance by increasing through plane electrical conductivities of gas diffusion layers at constant in-plane electrical conductivity.



Figure 3. Interface that measuring potentials and current densities.



Figure 4. The variations of polarization curves for cases (a) Case Group A (b) Case Group B.

The variations of electrolyte potential depending on anisotropic electrical conductivities are shown in Figure 5. As the electrolyte potential increases by increasing through plane electrical conductivity at constant in-plane electrical conductivity, the increment of in-plane electrical conductivity leads to decreases in electrolyte potential. The reason of the increasing in the electrolyte potential is that charged particles go towards rapidly triple phase boundary in through plane.

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(b)

(a)

Figure 5. The variation of electrolyte potential depending on anisotropic electrical conductivities, Vcell=0.45 V [I. at in plane a) $\sigma IP = 100 \text{ S/m}$, b) $\sigma IP = 200 \text{ S/m}$, c) $\sigma IP = 400 \text{ S/m}$, constant $\sigma TP = 400 \text{ S/m}$ II. a) $\sigma TP = 100 \text{ S/m}$, b) $\sigma TP = 200 \text{ S/m}$, c) σTP = 400 S/m, constant $\sigma IP = 400 \text{ S/m}$].

Figure 6 illustrates the variation of electrode potentials depending on anisotropic electrical conductivities. As shown this figure, when the electrode potential increases approximately from 0.03V to 0.46 V in the Case Group A, the electrode potential increases from 0.03V to 0.48 V in the Case Group B.

Figure 6. The variation of electrode potential depending on anisotropic electrical conductivities, Vcell=0.45 V [I. at inplane a) $\sigma IP = 100 S/m$, b) $\sigma IP = 200 S/m$, c) $\sigma IP = 400 S/m$, constant $\sigma TP = 400 S/m II. a$) $\sigma TP = 100 S/m$, b) $\sigma TP = 200 S/m$, c) $\sigma TP = 400 S/m$, constant $\sigma IP = 400 S/m$].

The variations of electrolyte current density depending on anisotropic electrical conductivities are indicated in Figure 7. It is shown that electrolyte current density has uniform distributions on membrane electrode assembly in Case Group B.

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Figure 7. The variation of electrolyte current density depending on anisotropic electrical conductivities, Vcell=0.45 V [I. at in plane a) $\sigma IP = 100 \text{ S/m}$, b) $\sigma IP = 200 \text{ S/m}$, c) $\sigma IP = 400 \text{ S/m}$, constant $\sigma TP = 400 \text{ S/m}$ II. a) $\sigma TP = 100 \text{ S/m}$, b) $\sigma TP = 200 \text{ S/m}$, c) $\sigma TP = 400 \text{ S/m}$, constant $\sigma IP = 400 \text{ S/m}$].

4. Conclusion

The effects of anisotropic electrical conductivity of gas diffusion layers on charge transport in PEM are investigated in this paper. Conclusions of the study are listed briefly as follows:

Through plane conductivity has more important influence impact on fuel cell performance and electrochemical phenomena than in-plane electrical conductivity.

The electrolyte current density on membrane electrode assembly is distributed uniformly by increasing through plane electrical conductivity at constant in-plane electrical conductivity. Thus, membrane electrode assembly can have better mechanic stability and durability.

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