The Model Development of Gas Diffusion Layer for PEM Fuel Cell

Dahiyah Mohd Fadzillah, Chin Lee Nee & Masli Irwan Rosli*
Fuel Cell Institute, Universiti Kebangsaan Malaysia, Bangi, Malaysia
Department of Chemical and Process Engineering, Universiti Kebangsaan Malaysia, Bangi, Malaysia

Abstract-- **Gas diffusion layer (GDL) is a crucial component of a proton-exchange membrane fuel cell (PEMFC) that participates in the transport of reactant gases and removes water from the system. In this research, a two dimensional (2D) model was developed and simulated to determine the effects of porosity and thickness of GDL on PEMFC performance by using MATLAB. The GDL model presented the contour profiles illustrating the distribution of oxygen mass fraction in the cathode GDL. The model also well agreed with experimental results available in literature. In the simulation of GDL model, higher-porosity GDL showed higher cell performance because of the numerous void spaces that enhanced the diffusion of oxygen to the catalyst layer. Simulation results further showed that a thicker GDL produced a lower-performance cell. All these factors contributed to the lower oxygen concentration near the catalyst layer and GDL interface and thus the lower cell performance. Through the GDL model, the optimum porosity and thickness of GDL were found to be 0.8 and 130 µm, respectively.**

Index Term-- **GDL; PEMFC; MATLAB; porosity; thickness**

I. INTRODUCTION

Proton-exchange membrane fuel cell (PEMFC), also known as polymer electrolyte membrane fuel cell, is an electrochemical device that converts the chemical energy of hydrogen and oxygen into electricity and heat with water as a byproduct. PEMFCs operate at low temperature and high current density [1]. PEMFCs are applied mainly in the automotive industry and occasionally in stationary power generators [2]. PEMFCs are a potential area for research because they are attractive alternative energy sources for electric-power generation, primarily for automotive applications. PEMFCs are unique compared with other fuel cells and have thus become research hotspots because of the increasing demand for PEMFC commercialization.

Gas diffusion layer (GDL) is a thin layer in a PEMFC that plays an important function in improving PEMFC performance. The most important function of GDL is to distribute hydrogen and oxygen to the catalyst layer and remove the water out of the fuel cell. In addition, GDL provides mechanical support to the membrane and a conductive path between the catalyst layer and the current collector [3]. Therefore, GDL characteristics such as thickness, porosity, and permeability that affect PEMFC performance must be examined. In recent years, researchers have worked to achieve progress in the development of cost-effective fuel cell technology. PEMFC operation is affected by GDL. Therefore, accurate prediction of the characteristics of an effective transportation is important in understanding fuel-cell performance. The experimental of PEMFC performance evaluation has been widely studied. Moreover, applying the modeling techniques for better understanding the effective parameters in designing and optimizing the fuel cell has advantages, for the purpose of improving fuel cell technology [4]. Many modeling studies have been done to investigate the transport phenomena in GDL.

Shokuhfar et al. [4] developed a model to study PEMFC performance by considering the opposite flow of hydrogen and air. The study confirmed that the change in the oxygen diffusivity by GDL porosity is less pronounced at cell voltage, $V_{cell} = 0.55$ V. Inamuddin et al. [5] simulated a 3D model by using computational fluid dynamics (CFD) commercial code-ACE + to study the effect of porosity and thickness of the GDL on PEMFC performance. The study showed that GDL porosity generates a high current density because the porosity provides more opportunities for reactants to reach the site of reaction. Lee et al. [6] conducted a study with a combination of semi-numerical experiments and model development. The study showed a decrease in oxygen concentration between the inlet and outlet because of an increase in the thickness of the GDL. A CFD 2D for PEMFC are developed by Sahraoui et al. [7] with regard to modeling the electrochemical, heat, and mass transport that occur in the entire fuel cell. The study showed a decrease in the oxygen concentration during the gas flow because of the gas usage in the reaction to produce water. The oxygen usage affects the GDL interface and catalyst layer because of the most significant concentration gradient. The highest concentration gradient occurs in the reaction zone in which the proton joins with an electron to produce water. The range of values for each parameter that has been used in other modeling studies obtained from literature review is updated in table form as shown in Table I. Based on this table, the range for both parameters that been used in modeling work is determined. For GDL, an optimum porosity should be high enough to provide enough space gas diffusion and to remove water between the reaction zone and gas distributor [8]. However, a too high porosity will cause water flooding due to lower capillary pressures [9] and also will lower the thermal conductivity due to higher contact resistance [10]. As for the thickness, an optimum value should efficiently facilitate the flow of reactants and water removal, as well as provide low electronic resistance. A very thick GDL will restrict gas distribution because of the lengthened path in the layer and poor gas diffusivity. Whereas, a very thin GDL gives high electronic resistance and causes voltage losses in the cell.

Table I
The range of values for the porosity and thickness of GDL

Parameter Study	Porosity (%)	Thickness (µm)
Shokuhfar et al. [4]	40 – 60	
Inamuddin et al. [5]	40 – 70	
Zamel et al. [11]	40 – 90	
Jang et al. [12]	30 – 60	
Yan et al. [13]	30 – 60	
Inamuddin et al. [5]		400 – 600
Jang et al. [12]		200 – 600
Youssef et al. [14]		260 – 360
Chun et al. [15]		200 – 500
Final range	**40 – 90**	**200 – 600**

II. METODOLOGY

A two-dimensional (2D) GDL model was developed and subsequently used for simulation based on two parameters: porosity and thickness. The 2D model was built based on schematic by Benziger et al. [16] in Figure 1.

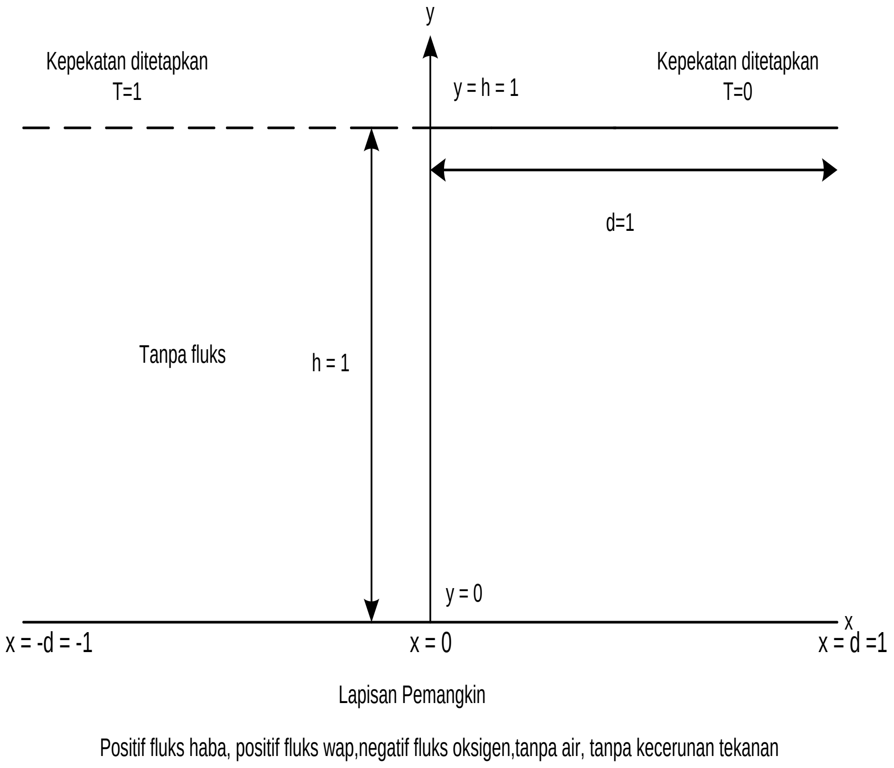

Fig. 1. The schematic diagram of 2D model [12]

A complete set of algorithms was developed by using relevant equations for GDL modeling and simulation. The physical parameters and the dimensions of the domain were obtained through literature study. The model was based on Fickian equation in Equation 1. To relate the porosity and GDL thickness, the equation below [17] was used:

$$\nabla \cdot (D_u(\theta)\nabla\tilde{u} - \tilde{u}\check{V}_g = 0 \qquad (1)$$

Where,

$\tilde{V}_g$ = Velocity of gas phase

$\tilde{u}$ = Oxygen concentration

D_u = Oxygen diffusion coefficient

θ = Volume fraction of water

Effective oxygen diffusivity coefficient $D_{O_2}^{eff}$ is associated with porosity, and ε is through Bruggeman correlation [5].

$$D_{O_2}^{eff} = D_u \varepsilon^{1.5} \tag{2}$$

To relate the porosity and GDL thickness, the equation below [17] was used:

$$\varepsilon = 1 - \frac{W_A}{\rho_{real} t} \tag{3}$$

Where,

W_A = Actual weight (g/cm^2),

ρ_{real} = Density of gas phase (g/cm^3),

t = Thickness of GDL (cm^2)

Subsequently, a 2D model of GDL for PEMFC was developed using MATLAB software. Through this model, oxygen concentration and power in each case were obtained. Figure 1 shows a schematic of the cross-section of the cathode GDL as presented by Benziger et al. [16]. The dotted line illustrates the gas line, and the bottom layer of the GDL is the catalyst layer. At the top of the channel, gas is fed into the system; at the bottom, the gas outlet is channeled to the catalyst layer where the reaction occurs. Given that the half of the upper boundary of GDL is a solid cathode material and the other half is an open channel, the boundary conditions are mixed. Benziger suggested that Neumann boundary conditions should be used in a cathode without flux, whereas Dirichlet boundary conditions should be used in a cathode without liquid water.

To simplify the model equations and reduce the complexity of writing GDL algorithm, four assumptions were made: (1) without liquid state, (2) without convection, (3) steady flux, and (4) steady pressure. The modeling process using MATLAB is execute by grid meshing, determination of boundary condition and calculation of interior domain.

I. RESULT AND DISCUSSION

Model Validation

Figure 2 displays the results of the comparison curve obtained from these studies with the experimental model of Lee et al. [6]. This comparison is conducted at a voltage of 0.7 V and a surface area of 25 cm^2 GDL.

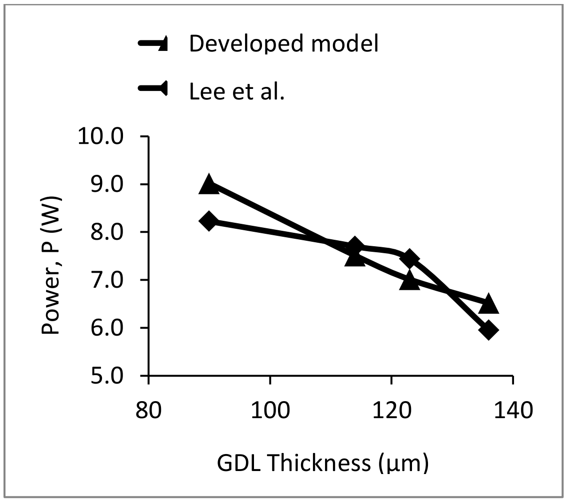

Fig. 2. Comparison curve for model validation based on GDL thickness

Through comparison data from the model study with the experimental data, the data generated from GDL model shows a similar curve patterns. With increased GDL thickness, current density and fuel-cell power decrease. At thicknesses of 114 and 123 m, model results well agree with experimental data. However, at thicknesses of 90 and 136 m, the data from the model show little difference from experimental data, with an error of 8.7%. For GDL with 90 m thickness, the model result for power is higher that experimental data; the opposite is observed for 136 m thickness.

Figure 3 shows the results of comparison curves for the developed model and model of Sahraoui et al. based on GDL porosity. This comparison is conducted at a voltage of 0.7 V and a surface area of 25 cm^2 GDL.

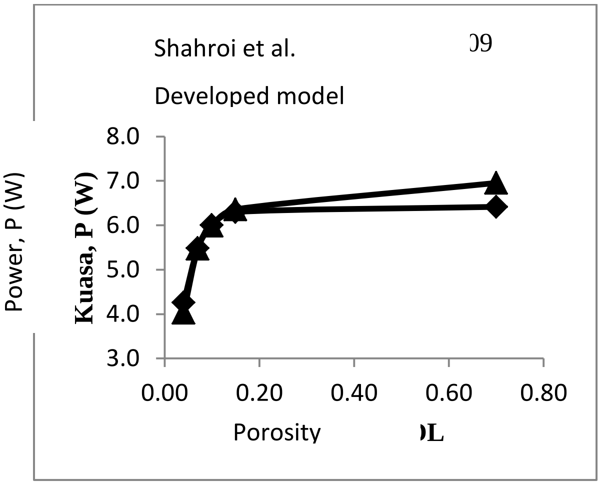

Fig. 3. Comparison curve for model validation based on GDL porosity

Through comparison data for the both models, both of these data have similar pattern of curves that shows increasing fuel-cell power with increased GDL porosity. The porosity of GDL is 0.04–0.15. The developed model contains an error of less than 1%.Therefore, the model results are consistent with data from the Sahraoui model. However, at a higher porosity such as 0.7, data from the model study demonstrate an error of 7.7%. Although the developed model does not show 100% consent with the literature review, but it managed to generate data that are close and similar to the study of Lee et al. and Sahraoui et al.. Thus, the model in this study can be considered as a model that could be used for further research. .

Result of GDL Modelling for Porosity

The values of porosity (ε) of the simulated GDL are 0.05, 0.1, 0.2, 0.4, 0.6, and 0.8. These values are based on the range of porosity values obtained in the study that are listed in Table 1. Figure 4 shows the curve of power against the porosity of GDL at a voltage of 0.7 V. The simulation results show that the increasing porosity contributes to the higher PEMFC performance. This result is due to the fact that GDL with higher porosity contains more empty spaces that facilitate the absorption of oxygen or air by the catalyst layer, resulting in more reaction sites and thus improving PEMFC performance [18]. Therefore, PEMFC performance is highest at a porosity of 0.8 and lowest at 0.05.

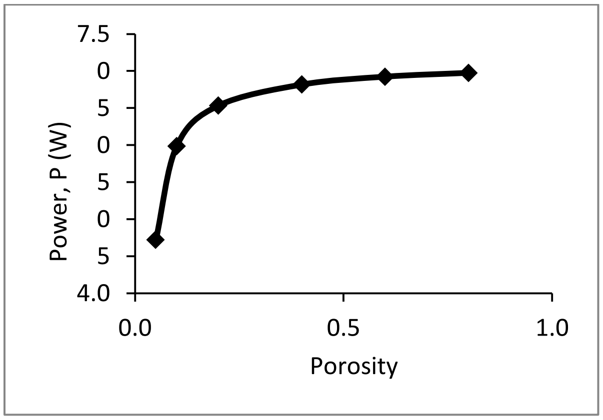

Fig. 4. Power versus porosity of GDL AT 0.7 V

Contour of Oxygen Mass Fraction Distribution at Different Porosity

Figure 5 shows a contour of oxygen mass fraction distribution in the cathode GDL that is based on different GDL porosity values. With regard to the contour, in the $-1 \leq x \leq 0$ GDL, the distribution of the mass fraction of oxygen is higher, which is in the range of 0.5–1.0. Whereas in the $0 \leq x \leq 1$ GDL, the distribution of the mass fraction of oxygen is lower, which is 0–0.7. Such contours is due to the part of $-1 \leq x \leq 0$ GDL which is an open channel in which oxygen or air is diffused into the GDL, whereas at the GDL $0 \leq x \leq 1$, it is a solid cathode material. Different colors in the contour illustrate the differences in oxygen concentration gradients in the GDL. The results show that the mass flux of oxygen decreases as porosity of the GDL increases. Therefore, diffusion of oxygen into the GDL increases as the porosity increases.

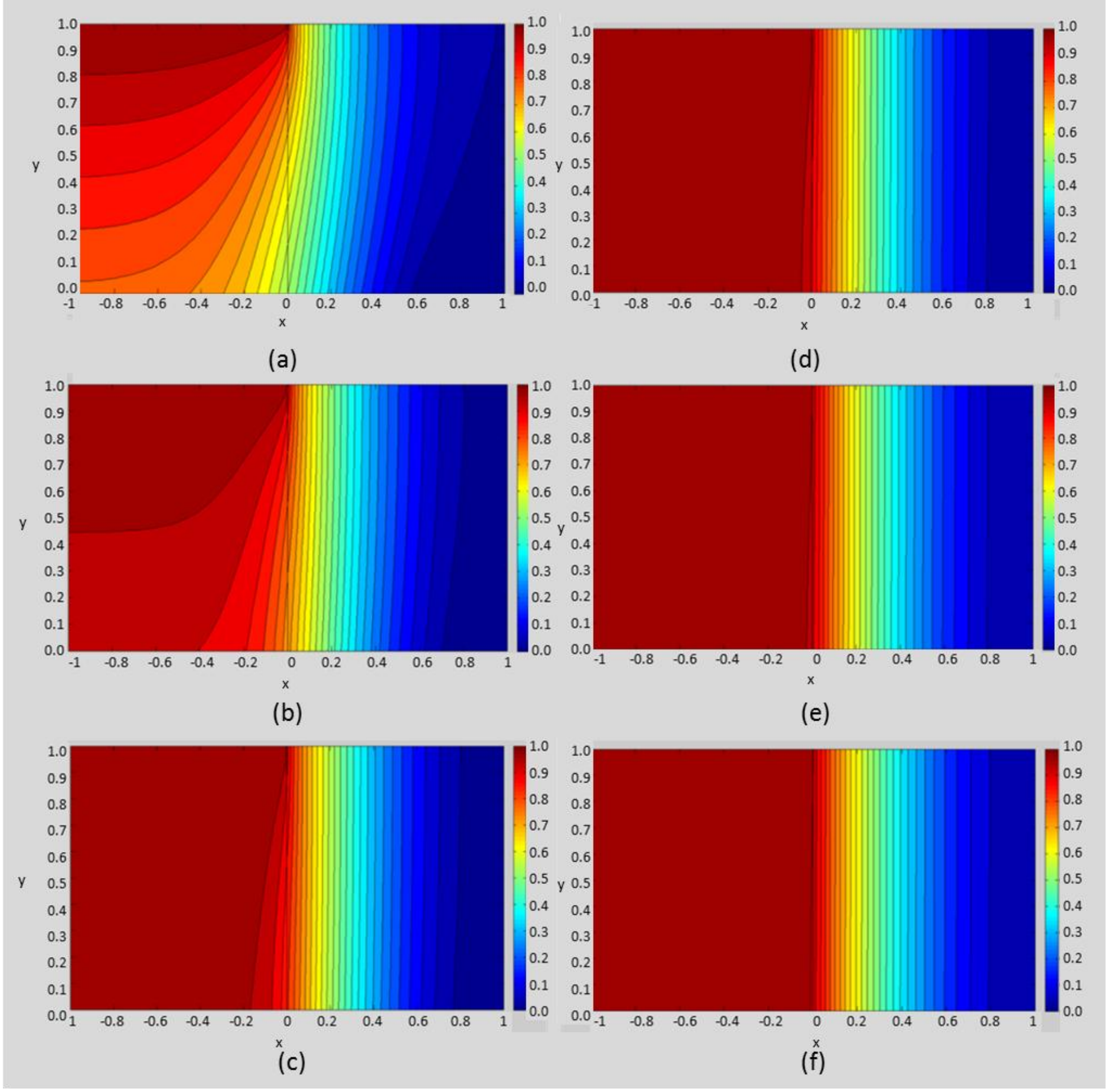

Fig. 5. Contour of oxygen mass fraction for porosity, ε = (a) 0.05 (b) 0.1 (c) 0.2 (d) 0.4 (e) 0.6 (f) 0.8

Result of GDL Modelling for Thickness

Based on the range of thickness in Table 1, the values of GDL thickness (t) for the simulation are 130 m, 200, 300, 400, 500, and 600 µm. Figure 6 shows the curve of power against the thickness of GDL at a voltage of 0.7 V. The simulation results show that PEMFC performance decreases when the GDL thickness decreases. This result is due to the higher resistant of the gas diffusion in thicker GDL, and to seep into the reaction zone takes longer time [15]. Hence, oxygen concentration on the surface of the catalyst layer decreases and contributes to power reduction and follows by a decline in the PEMFC performance. Therefore, fuel-cell performance is highest at a thickness of 130 µm and lowest at 600 µm.

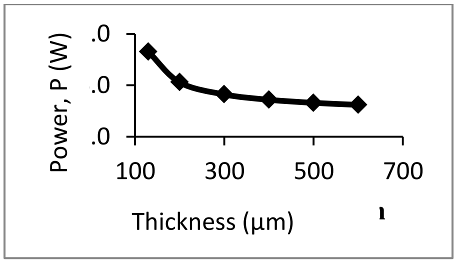

Fig. 6. Power versus thickness of GDL

Contour of Oxygen Mass Fraction Distribution at Different Thickness

Contour of the mass fraction distribution of oxygen in the cathode GDL based on the GDL thickness is shown in Figure 7. With regard to the results of the current study, the contour differences at the different thickness values are more pronounced in the GDL $-1 \leq x \leq 0$ where it is an open channel for the oxygen diffusion. At lower thickness, the oxygen mass flux increases leading to the increase of oxygen mass fraction. This phenomenon can be observed in the increased contour profile for the mass fraction of 0.9–1.0 which is represented by the red color, and the reduction of the mass fraction contour profile of 0–0.1 is represented in blue in Figure7.

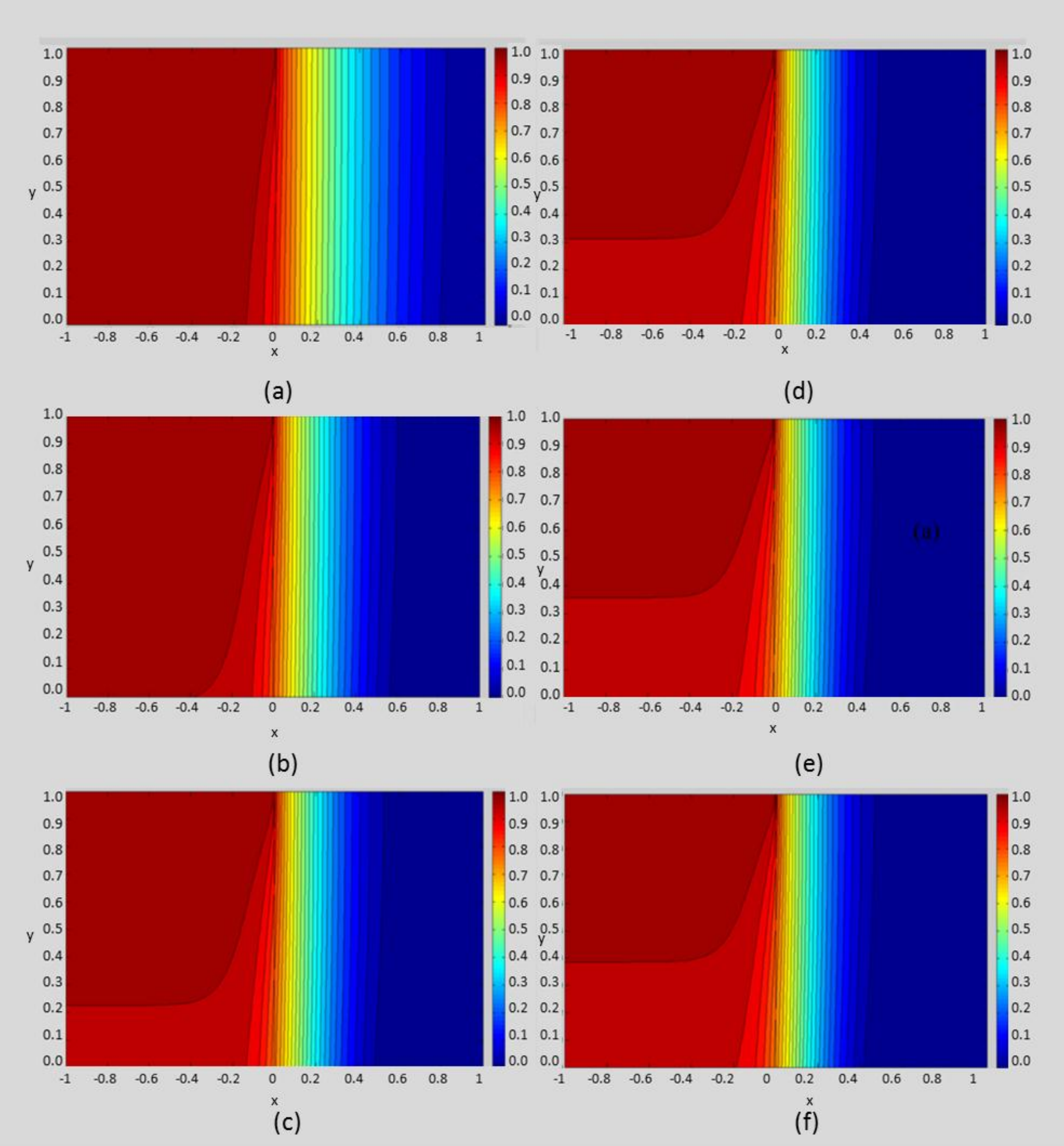

Fig. 7. Contour of oxygen mass fraction for thickness, t = a) 130 (b) 200 (c) 300 (d) 400 (e) 500 (f) 600

II. CONCLUSION

The developed 2D model of GDL cathode can generate a contour distribution of the mass fraction of oxygen. The model was validated, and results well agreed with experimental data. In a simulation study of GDL porosity, the studied porosity values were 0.05, 0.1, 0.2, 0.4, 0.6, and 0.8. Simulation results showed that increasing the porosity of GDL improved PEMFC performance, and that fuel-cell power was highest at a porosity value of 0.8. Moreover, in a simulation study of GDL thickness, the studied values were 130, 200, 300, 400, 500, and 600 µm. Results showed that increasing the GDL thickness decreased PEMFC performance. Therefore, PEMFC performance was highest at a thickness of 130 µm.

III. ACKNOWLEDGEMENT

This work was supported by the financial support provided by UNIVERSITI KEBANGSAAN MALAYSIA under Grant Number FRGS/1/2013/TK07/UKM/02/3

REFFERENCES

[1] Wang, Y., Chen, K. S., Mishler, J., Cho, S. C. & Adroher, X. C. 2011. A Review of Polymer Electrolyte Membrane Fuel Cells: Technology, Applications, and Needs on Fundamental Research. *Applied Energy* 88(4): 981-1007.

[2] Wee, J. H. 2007. Applications of Proton Exchange Membrane Fuel Cell Systems. *Renewable and Sustainable Energy Reviews* 11(8): 1720-1738.

[3] Spiegel, C. 2008. Chapter 8 - Modeling the Gas Diffusion Layers. Dlm. Spiegel, C. (pnyt.). *Pem Fuel Cell Modeling and Simulation Using Matlab,* hlm. 197-241. Burlington: Academic Press.

[4] Shokuhfar, A., Nejadseyfi, O. & Zolriasatein, A. 2013. A Numerical Study of the Influence of Gas Diffusion Layer Porosity on Cell Performance of Counter Flow Proton Exchange Membrane Fuel Cells. *Iranica Journal of Energy and Environment (IJEE)* 4(2): 126-129.

[5] Inamuddin, Cheema, T. A., Zaidi, S. M. J. & Rahman, S. U. 2011. Three Dimensional Numerical Investigations for the Effects of Gas Diffusion Layer on Pem Fuel Cell Performance. *Renewable Energy* 36(2): 529-535.

[6] Lee, H. K., Park, J. H., Kim, D. Y. & Lee, T. H. 2004. A Study on the Characteristics of the Diffusion Layer Thickness and Porosity of the Pemfc. *Journal of Power Sources* 131(1–2): 200-206.

[7] Sahraoui, M., Kharrat, C. & Halouani, K. 2009. Two-Dimensional Modeling of Electrochemical and Transport Phenomena in the Porous Structures of a Pemfc. *International Journal of Hydrogen Energy* 34(7): 3091-3103.

[8] Walter, L. 2008. Towards a Model Concept for Coupling Porous Gas Diffusion Layer and Gas Distributor in Pem Fuel Cells. nstitut f□ur Wasserbau, Universit□at Stuttgart.

[9] Bazylak, J. H. a. A. 2011. Pem Fuel Cell Gas Diffusion Layer Modelling of Pore Structure and Predicted Liquid Water Saturation *ASME 2011 9th Fuel Cell Science, Engineering and Technology Conference*, hlm.

[10] Larbi, B., Alimi, W., Chouikh, R. & Guizani, A. 2013. Effect of Porosity and Pressure on the Pem Fuel Cell Performance. *International Journal of Hydrogen Energy* 38(20): 8542-8549.

[11] Zamel, N. 2011. Transport Properties of the Gas Diffusion Layer of Pem Fuel Cells. Tesis Doctor of Philosophy in Mechanical Engineering, University of Waterloo.

[12] Jang, J. H., Yan, W. M. & Shih, C. C. 2006. Effects of the Gas Diffusion-Layer Parameters on Cell Performance of Pem Fuel Cells. *Journal of Power Sources* 161(1): 323-332.

[13] Yan, W. M., Soong, C. Y., Chen, F. & Chu, H. S. 2004. Effects of Flow Distributor Geometry and Diffusion Layer Porosity on Reactant Gas Transport and Performance of Proton Exchange Membrane Fuel Cells. *Journal of Power Sources* 125(1): 27-39.

[14] Youssef, M. S., Khalil, M. H. & Al-Nadi, K. E. 2010. Neural Network Modeling for Proton Exchange Membrane Fuel Cell (Pemfc). *Advances in Information Sciences and Service Sciences* 3(2): 61-66.

15] Chun, J. H., Park, K. T., Jo, D. H., Kim, S. G. & Kim, S. H. 2011. Numerical Modeling and Experimental Study of the Influence of Gdl Properties on Performance in a Pemfc. *International Journal of Hydrogen Energy* 36(2): 1837-1845.

[16] Benziger, J., Chia, E., Karnas, E., Moxley, J., Teuscher, C. & Kevrekidis, I. G. 2004. The Stirred Tank Reactor Polymer Electrolyte Membrane Fuel Cell. *AIChE Journal* 50(8): 1889-1900.

[17] Zhang, J. 2008. *Pem Fuel Cell Electrocatalysts and Catalyst Layers*. 1. Springer.

[18] Chang, S. M. & Chu, H. S. 2006. Transient Behavior of a Pemfc. *Journal of Power Sources* 161(2): 1161-1168.