Journal of Renewable Energy and Sustainable Development (RESD) Volume 8, Issue 2, December 2022 - ISSN 2356-8569
http://dx.doi.org/10.21622/RESD.2021.07.2.045

Received on, 07 September 2022 Accepted on, 07 October 2022 Published on, 26 October 2022

Three-dimensional CFD Analysis of PEMFC with Different Membrane Thicknesses

Mahmut Kaplan

Department of Machine and Metal Technology, Naci Topcuoglu Vocational High School, Gaziantep University, Gaziantep, Turkey

mahmutkaplan@gantep.edu.tr

ABSTRACT

PEM fuel cell (PEMFC) is a potential candidate for future source of power used in different applications such as transportations, stationary and portable power. PEMFC consists of different parts including membrane, bipolar plate, flow channel, gas diffusion and catalyst layers. Membrane is one of the most important components of a PEMFC and its physical and geometrical features significantly affect PEMFC efficiency. In this paper, a three-dimensional, single-phase computational model has been improved to scrutinize membrane thickness effect on the PEM fuel cell performance using the ANSYS PEM Fuel Cell Module.

Membrane thicknesses are in the range of 0.0127 to 0.189 mm. The results reveal that a decrease in membrane thickness augments the current density at 0.4 and 0.6 V. The peak current density of 3.12 A/cm^2 is achieved with 0.027 mm membrane thickness compared with the model current density of 1.26 A/cm^2 obtained by the model with 0.128 mm membrane thickness at 0.4 V. Oxygen consumption. Water production is also enhanced with reducing membrane thickness to 0.4 and 0.6 V. However, the changed thickness of the membrane has a negligible impact on impact pressure drop in the flow channel. It is found that optimization of membrane thickness is necessary for attaining high efficiency.

Index-words: *PEMFC, Membrane thickness, CFD, Cell performance, Pressure drop, Optimization.*

I. INTRODUCTION

The use of fossil fuels for power has resulted in many adverse impacts including climate change and air pollution. The interest in proton exchange membrane fuel cell (PEMFC) has grown noticeably because of the requirement for clean energy. The potential applications of the PEMFC are transportation (cars, trains, boats, planes and drones), stationary and portable power sectors (Wu, 2016).

Basic components of PEMFC are gas diffusion layer (GDL), catalyst layer (CL), membrane and flow channel (Xing et al., 2019). In a PEMFC, hydrogen as a fuel is converted electrochemically into electricity. During the PEMFC operation, molecular hydrogen (H_2) from anode gas flow channel is oxidized on the anode CL ($H_2 \rightarrow 2H^+ + 2e^-$) and hydrogen ions pass through the membrane. Meanwhile the electrons flow through GDL to the anode current collector and arrive by means of the cathode current collector. Oxygen is reduced by reaction between the electrons, the hydrogen ions, and oxygen supplied from cathode gas flow channel ($O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$).

In order to operate PEMFC efficiently, membrane must satisfy the needs such as high proton conductivity, an adequate barrier to the reactants chemically and mechanically stable (Barbir, 2013). Improving computational model of PEMFC helps to investigate the efficiency of membrane for different operating and geometrical parameters. Compared to experimental studies, computational models provide detailed information and save time and cost. Recently, several studies have been conducted to evaluate impacts of membrane geometry and materials property on PEMFC efficiency (Iranzo et al. 2014; Nishimura et al., 2021; Luo et al., 2021; Kienitz, 2021).

Iranzo et al. (2014) developed a three-dimensional numerical model to scrutinize the impact of the membrane thermal conductivity on cell performance using ANSYS Fluent. It was found that an increase in the membrane thermal conductivity leads to decreasing membrane temperature and augmenting protonic conductivity and cell electric power.

Nishimura et al. (2021) studied impacts of various thicknesses of membrane on the power generation

http://dx.doi.org/10.21622/RESD.2021.07.2.045

performance of PEMFC using the commercial software Comsol Multiphysics. Their results showed the thinner membrane promoted the current density because of enhancing water flux and conductivity of membrane. Luo et al. (2021) conducted experimental work to determine the impacts of membranes within thicknesses ranging from 5 μm to 70 μm on the structure and characteristics of membrane. Their findings revealed that below a certain thickness (<10 μm), membranes exhibited considerable change in their structure and features associated with increasing anisotropy and swelling.

Mohanty et al. (2021) analyzed the influences of membranes having different thicknesses (2, 3.5 and 5 mil) on PEMFC performance using COMSOL Multiphysics software. It was concluded that membranes with 2 mm thickness developed the cell performance by 17%, thanks to decreasing internal resistance compared to other thicknesses. Kienitz (2021) improved a new numerical model to optimize membrane thickness for automotive hydrogen PEMFC systems. The results showed that the model was capable of estimating optimal membrane thickness but this thickness is dependent on operating conditions.

The objective of this investigation is to study the interrelationship between membrane thickness and the PEMFC efficiency using a single-phase computational fluid dynamics (CFD) model improved in the previous work (Kaplan, 2021). The outcomes of the work can help geometry optimization in PEMFC design. Besides, the suggested model can be used to improve reactants utilization in PEMFC.

II. COMPUTATIONAL METHOD

SOLIDWORKS is used to produce the geometry of PEMFC. Then the geometry is imported the Fluid Flow Analysis System in ANSYS Workbench Platform (ANSYS, 2018). The structured mesh is generated in Meshing. As shown in Figure 1, the mesh must consist of nine elements including anode and cathode GDL, CL, flow channel and membrane in order to identify the properties of these elements in the ANSYS FLUENT Fuel Cell Module.

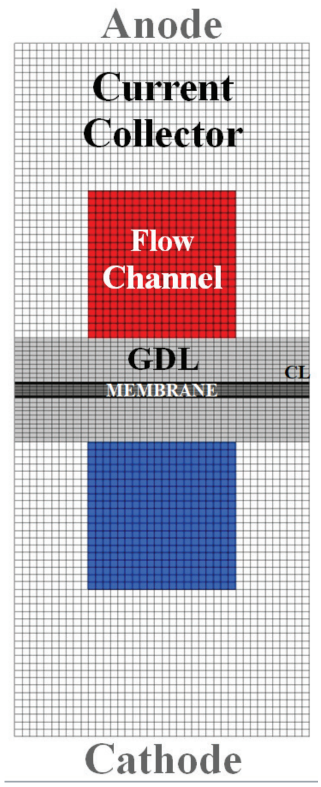

Fig. 1. Meshing of PEMFC model

Model geometrical parameters based on Wang et al.'s experimental study are presented in Table I.

TABLE I. GEOMETRICAL PARAMETERS FOR THE MODEL (Wang et al., 2003)

Parameter	Value
Cell width	2 mm
Cell length	70 mm
Channel width and	1 mm
GDL thickness	0.3 mm
CL thickness	0.0129 mm
Membrane thickness	0.108 mm

http://dx.doi.org/10.21622/RESD.2021.07.2.045

In the present study, the mass, momentum, species and energy equations are employed in the PEMFC model. Mass equation:

$$\nabla(\rho \boldsymbol{u}) = S_m \quad (1)$$

Here, ρ is gas density, u is velocity vector and Sm is mass source term. Momentum equation:

$$\frac{1}{\left(\varepsilon^{eff}\right)^2}\nabla(\rho \boldsymbol{u}\boldsymbol{u}) = \nabla(\mu\nabla \boldsymbol{u}) - \nabla P + S_{mom} \quad (2)$$

Here, ε^{eff} is effective porosity. μ is gas dynamic viscosity. S_{mom} is momentum source term. *P* is pressure. Species equation:

$$\nabla(\vec{u}C_k) = \nabla(D_k^{eff}\nabla C_k) + S_k \quad (3)$$

Here, C_i and D_i^{eff} are molar concentration and effective diffusivity of species *i*, respectively. Si is source term for species *i*. Charge conservation:

$$R_m + \nabla\left(\sigma_m \nabla \phi_m\right) = 0,\ R_s + \nabla\left(\sigma_s \nabla \phi_s\right) = 0 \quad (4)$$

R_m, σ_m , $\emptyset_m$ and R_s, σ_s , $\emptyset_S$, volumetric transfer current, electrical conductivity, electric potential of membrane and solid (current collector), respectively. The anode and cathode overpotentials are calculated by,

$$\eta_{anode} = \phi_s - \phi_m,\ \eta_{cathode} = \phi_s - \phi_m - V_{oc} \quad (5)$$

Here η_{anode} and $\eta_{cathode}$ are overpotential of anode and cathode. V_{oc} is open-circuit voltage. V_{oc} is 0.94 V, in this work. The operational parameters employed in the model are summarized in Table II. The boundary conditions for the model are given in Table III.

TABLE II. OPERATING PARAMETERS FOR THE MODEL

Parameter	Value
H_2 and H_2O diffusivity	7.33 x 10^{-5} m^2/s (Biyikoglu and Alpat, 2011)
O_2 diffusivity	2.13 x 10^{-5} m^2/s (Biyikoglu and Alpat, 2011)
Other species diffusivity	4.9 x 10^{-5} (Biyikoglu and Alpat, 2011)
GDL and CL porosity	0.5 (Kahveci and Taymaz, 2018)
GDL and CL viscous resistance	1 x 10^{12} 1/m^2 (Kahveci and Taymaz, 2018)
CL surface/volume ratio	200000 1/m
Anodic reference exchange current density	4000 A/m^2
Cathodic Reference exchange current density	0.1 A/m^2

TABLE III. THE BOUNDARY CONDITIONS FOR THE MODEL

Parameter	Value
Anode and cathode inlet mass flow rates	5.398 x 10^{-6} and 3.294 x 10^{-5}kg/s
Mass fraction of H_2 and H_2O at the inlet (anode)	0.2 and 0.8
Mass fraction of O_2 and H_2O at the inlet (cathode)	0.2 and 0.1
Outlet pressure	101.325 kPa
Inlet, outlet and wall temperature at anode and cathode	343 K
Wall anode terminal (upper current collector face)	0 V
Wall cathode terminal (lower current collector face)	0-0.94 V

Volume 8, Issue 2, December 2022 - ISSN 2356-8569
http://dx.doi.org/10.21622/RESD.2021.07.2.045

The assumptions of the present computational model are: isotropic and homogenous solid (membrane, CL and GDL) materials and steady state, single phase and laminar flow.

III. RESULTS AND DISCUSSIONS

A. Validation

The numerical model used in this work was validated with experimental results from Wang et al. (2003) who used the same geometry and materials as shown in Figure 2. It is found that the developed model is reliable at lower and medium current densities since the model predictions give good agreement to the experimental data. However, at higher current densities, the overestimation of the current density is observed as a result of assuming that CL and GDL do not contain liquid water. It is found that the model used in the present work is reliable at lower and medium current densities since the model predictions demonstrate good agreement with experimental data. However, at higher current densities, the overestimation of the current density is observed as a result of assuming that CL and GDL not containing liquid water.

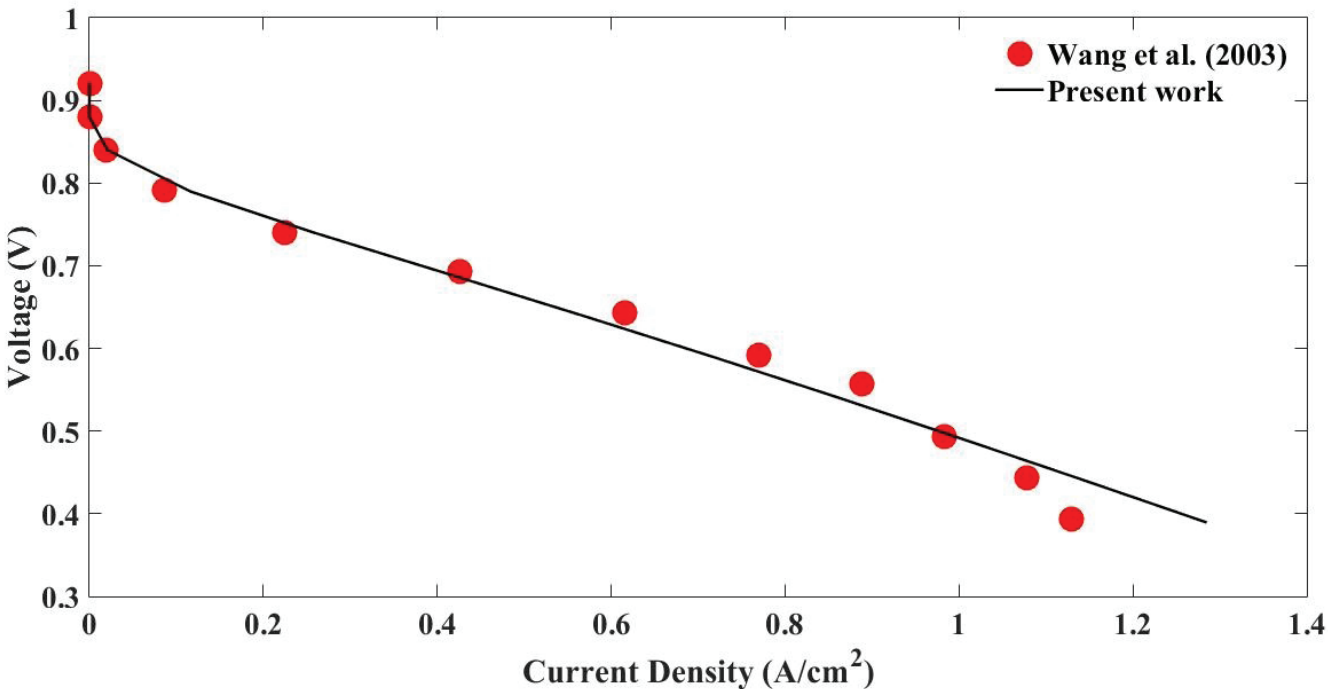

Fig. 2. Validation of the model with experimental data (Wang et al., 2003)

B. Influences of Membrane Thickness on Current Density

Figure 3 illustrates the predicted current densities for the different thicknesses of membrane varying between 0.027 and 0.189 mm at 0.4, 0.6 and 0.8 V. As displayed in Figure 3 that the current density increases nearly linearly with a decrease in the membrane thickness until 0.081 mm whereas a fast rise in the current density is examined for lower membrane thickness (<0.054 mm) at 0.4 and 0.6 V. On the other hand, almost no change in current density is observed at 0.8 V. The peak current density of 3.12 A/cm^2 is achieved with the membrane thickness of 0.027 mm. The results display that determining an optimal membrane thickness required to augment the cell efficiency.

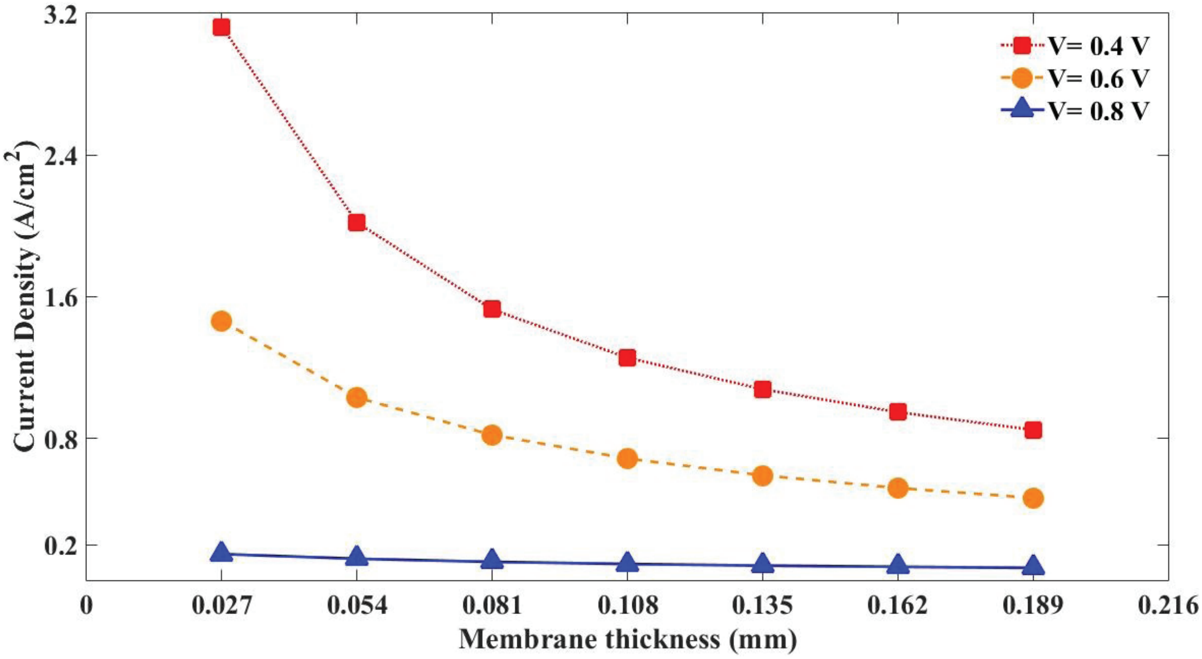

Fig. 3. Variation of current density for different membrane thicknesses at 0.4, 0.6 and 0.8 V

C. Influences of Membrane Thickness on Oxygen and Water Mass Fraction in the Cathode

In this section, since higher current density values are obtained at 4 V, the influences of membrane thicknesses on cathode oxygen and water mass fractions are examined at this cell voltage. Figures 4 illustrates the oxygen mass fraction in the plane including the membrane and cathode CL, GDL and flow channel at mid length of the cell for 0.027, 0.108 and 0.189 mm membrane thicknesses at 0.4 V.

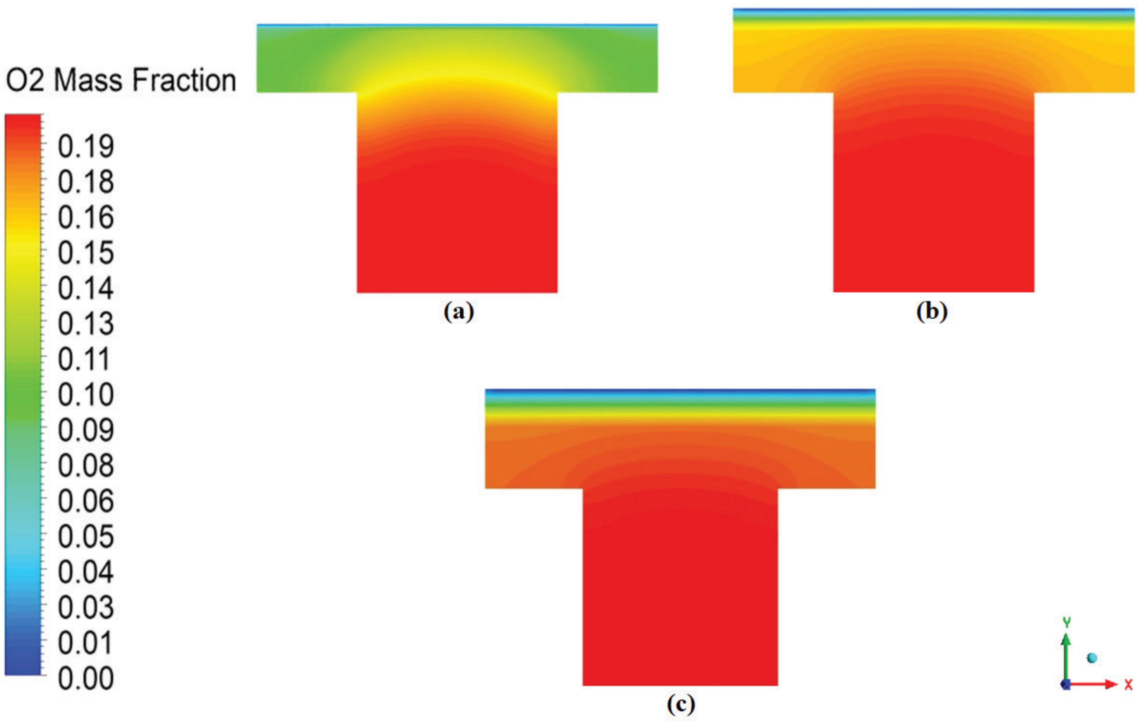

Fig. 4. Contours of O_2 mass fraction in the plane (membrane and cathode CL, GDL and flow channel) at mid length of the cell for different membrane thicknesses: (a) 0.027 mm, (b) 0.108 mm and (c) 0.189 mm (base case) at 0.4 V

 Volume 8, Issue 2, December 2022 - ISSN 2356-8569
http://dx.doi.org/10.21622/RESD.2021.07.2.045

It is clearly seen in Figure 4 that oxygen mass fraction in cathode GDL and CL diminishes with a decrease in membrane thickness at 0.4 V. The result proves that the cell with 0.027 mm membrane thickness generating the highest current density in Figure 3 consumes more oxygen on the cathode catalyst surface compared to other membrane thicknesses.

Figure 5 illustrates the water mass fraction in the plane including the membrane and cathode CL, GDL and flow channel at mid length of the cell for 0.027, 0.108 and 0.189 mm membrane thicknesses at 0.4 V. It is obvious in Figure 5 that decreasing membrane thickness enhances production of water during the electrochemical reaction at cathode side. Therefore, water mass fraction in cathode GDL and flow channel increases with decreasing membrane thickness as displayed in Figure 5.

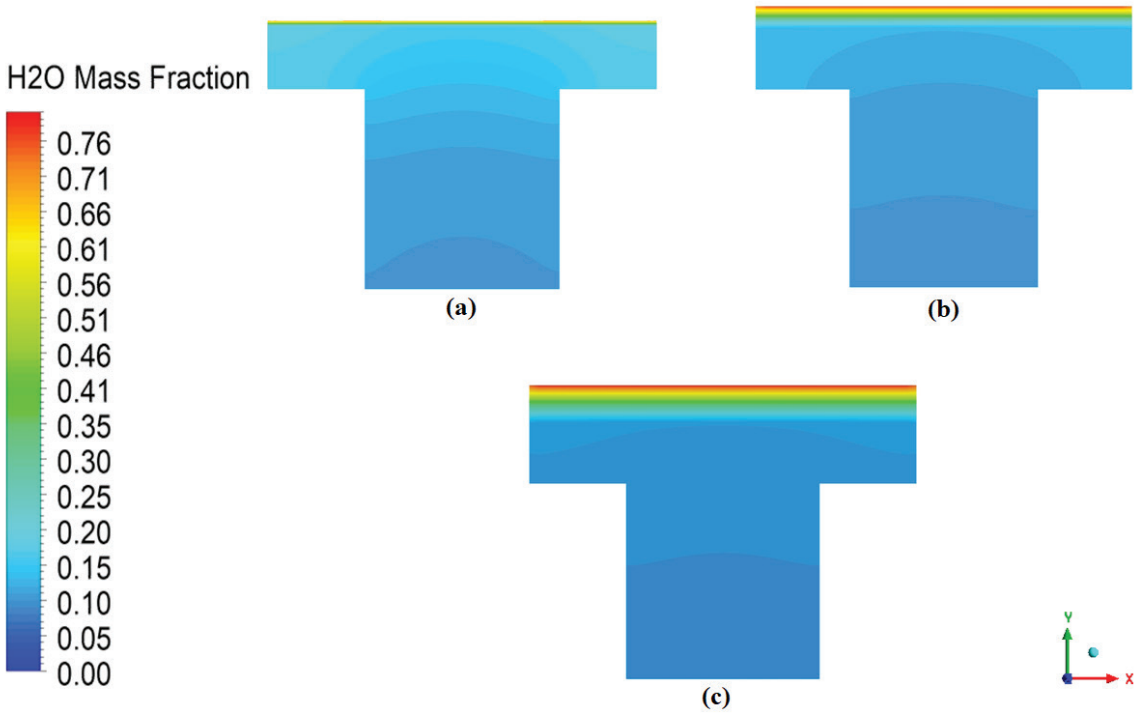

Fig. 5. Contours of H2O mass fraction in the plane (membrane and cathode CL, GDL and flow channel) at mid length of the cell for different membrane thicknesses: (a) 0.027 mm, (b) 0.108 mm and (c) 0.189 mm (base case) at 0.4 V

It is found that reducing the membrane thickness results in enhancing the cell current density associated with a higher oxygen consumption and water production and thus improves the cell performance.

D. Influences of Membrane Thickness on Pressure Drop in Anode and Cathode Channels

Table IV indicates the effects of variation of membrane thickness on pressure drop in the channels at 0.4 V.

TABLE IV. VARIATION OF PRESSURE DROP FOR DIFFERENT MEMBRANE THICKNESS

	Membrane thicknesses (mm)						
	0.027	**0.054**	**0.081**	**0.108**	**0.135**	**0.168**	**0.189**
Pressure drop (anode channel) (kPa)	0.617	0.618	0.644	0.662	0.687	0.682	0.683
Pressure drop (cathode channel) (kPa)	2.071	2.090	2.191	2.232	2.363	2.355	2.356

A large pressure drop in the flow channels leads to generate higher parasitic energy losses and increase pumping work. As shown in Table IV, pressure drop in the channels is not significantly affected by the decrease of the membrane thickness at 0.4 V. It is concluded that 0.027 mm membrane thickness provides better cell performance concerning current density and pressure drop in the channels.

IV. CONCLUSIONS

In the current study, the numerical simulation of 3-dimensional single-phase PEM fuel cell model was performed to observe the impact of different membrane thickness on the cell efficiency using the commercial ANSYS Fluent. The following are the main conclusions of the study:

1. The better PEMFC performance is achieved with the lower membrane thickness at 0.4 and 0.6 V.

2. The highest current density of 3.12 A/cm^2 is obtained with 0.027 mm membrane thickness compared with the model current density of 1.26 A/cm^2 at 0.4 V

3. A decrease in the membrane thickness results in increase oxygen consumption and water production in the cathode at 0.4 and 0.6 V.

4. No significant change in the current density is found with all membrane thicknesses at 0.8 V.

5. Variation of the membrane thickness does not have a significant impact on pressure drop in the anode and cathode channels.

6. Determining an optimal membrane thickness is needed to improve the cell efficiency.

References

[1] ANSYS Inc., ANSYS Workbench User's Guide, Release 19.2. Canonsburg, Pennsylvania: ANSYS Inc., 2018.

[2] F. Barbir, PEM fuel cells: Theory and practice. 2012. doi: 10.1016/C2011-0-06706-6.

[3] C. Spiegel, PEM Fuel Cell Modeling and Simulation Using Matlab. 2008. doi: 10.1016/B978-0-12-374259-9.X5001-0.

[4] A. Biyikoğlu and C. Ö. Alpat, "Parametric study of a single cell proton exchange membrane fuel cell for A bundle of straight gas channels," Gazi University Journal of Science, vol. 24, no. 4, 2011.

[5] A. Iranzo, A. Salva, E. Tapia, and F. Rosa, "Effect of the membrane thermal conductivity on the performance of a polymer electrolyte membrane fuel cell," J Fuel Cell Sci Technol, vol. 11, no. 3, 2014, doi: 10.1115/1.4026522.

[6] E. E. Kahveci and I. Taymaz, "Assessment of single-serpentine PEM fuel cell model developed by computational fluid dynamics," Fuel, vol. 217, 2018, doi: 10.1016/j.fuel.2017.12.073.

[7] M. Kaplan, "Numerical investigation of influence of cross-sectional dimensions of flow channels on pem fuel cell performance," Journal of Energy Systems, vol. 5, no. 2, 2021, doi: 10.30521/jes.871018.

[8] B. Kienitz, "Optimizing polymer electrolyte membrane thickness to maximize fuel cell vehicle range," Int J Hydrogen Energy, vol. 46, no. 19, 2021, doi: 10.1016/j.ijhydene.2020.03.126.

[9] X. Luo et al., "Thickness Dependence of Proton-Exchange-Membrane Properties," J Electrochem Soc, vol. 168, no. 10, 2021, doi: 10.1149/1945-7111/ac2973.

[10] S. Mohanty, A. N. Desai, S. Singh, V. Ramadesigan, and S. M, "Effects of the membrane thickness and ionomer volume fraction on the performance of PEMFC with U-shaped serpentine channel," Int J Hydrogen Energy, vol. 46, no. 39, 2021, doi: 10.1016/j.ijhydene.2021.03.252.

[11] A. Nishimura, K. Toyoda, Y. Kojima, S. Ito, and E. Hu, "Numerical simulation on impacts of thickness of nafion series membranes and relative humidity on pemfc operated at 363 k and 373 k," Energies (Basel), vol. 14, no. 24, 2021, doi: 10.3390/en14248256.

[12] L. Xing et al., "Membrane electrode assemblies for PEM fuel cells: A review of functional graded design and optimization," Energy, vol. 177. 2019. doi: 10.1016/j.energy.2019.04.084.

[13] L. Wang, A. Husar, T. Zhou, and H. Liu, "A parametric study of PEM fuel cell performances," Int J Hydrogen Energy, vol. 28, no. 11, 2003, doi: 10.1016/S0360-3199(02)00284-7.

[14] H. W. Wu, "A review of recent development: Transport and performance modeling of PEM fuel cells," Applied Energy, vol. 165. 2016. doi: 10.1016/j.apenergy.2015.12.075.