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Effect of Channel Designs on Open-Cathode PEM Fuel Cell Performance: A Computational Study

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Abstract

This study presents the effect of cathode channel design with vary cross-sectional area and aspect ratio. Three dimensional, steady state, single phase and isothermal model is developed to investigate the effect of cross-sectional area and aspect ratio of cathode flow channel on the cell performance for open-cathode PEM fuel cell. The result shows that increasing of cross-sectional area lead to the decreasing of molar concentration of oxygen at the interface of gas diffusion layer and catalyst layer that then decrease cell performance. On the other hand, increasing aspect ratio lead to the increasing of the molar concentration of oxygen and cell performance.

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Keywords: PEMFC, open-cathode, cathode channel aspect ratio, cell performance, CFD

1. Introduction

Today social awareness about global warming caused by carbon dioxide due to the burning of carbon fuels is recognized. Therefore, finding new alternative to reduce carbon dioxide emission has got more attention. Hydrogen energy is one of alternatives since when hydrogen is burnt, it does not emit carbon dioxide. One of the engines using hydrogen to produce power efficiently is fuel cells.

A fuel cell is an energy conversion process that can convert chemical energy directly into electrical energy by electrochemical reaction. There are many types of fuel cells. Proton exchange membrane (PEM) fuel cell is one type that is widely used because it operates at low pressure and temperature. Reactants for PEM fuel cell are hydrogen and oxygen and its products are water and heat.

To operate a typical fuel cell system, there are a number of components, such as reactant feeding system, humidifier, cooling fan, air compressor and control components, connecting with each other to

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support the system. To reduce the number of components, an open-cathode PEM fuel cell is recently developed by inducing ambient air to the cathode as a reactant and cooling media. Its main disadvantage is that air feeding into cathode side is by natural convection causing lower cell performance than those by compressed air. However, the disadvantage of using compressed air is the non-uniform oxygen mass transport. According to the literatures, X.-D. Wang et al. [1] studied the effect of cathode channel size on performance of PEM fuel cell with serpentine flow field. They found that decreasing of the flow channel size increased the reactant inlet velocity, which enhanced liquid water removal from the porous layers and transported more oxygen to the cathode catalyst layer. Thus, the cell performance was improved. However, the smaller unit does not give the best performance because it will lost the power due to high pressure drop. A.P. Manso et al. [2] reported that for serpentine PEM fuel cell, models with high channel cross-section aspect ratio exhibited more uniform temperature distributions with gentler gradients, and higher water content in the membrane, which gave better performance. Sasmito et al. [3] showed that for open-cathode PEM fuel cell, the increasing of channel height increased the air flow rate and consequently increased current density.

One of the solutions to improve the system can be obtained by appropriate cathode flow field design. In this study, the effect of cross-sectional area and aspect ratio on the cell performance for open-cathode PEM fuel cell is investigated.

Nomenclature

a	effective catalyst area per unit volume (m^{-1})
A	reaction area (m^2)
C	molar concentration (mol/m^3)
D	diffusion coefficient ($m^2\ s^{-1}$)
E	activation energy ($J\ mol^{-1}$)
F	Faraday's constant (96485 $C\ mol^{-1}$)
i	local current density ($A\ m^{-3}$)
i_0	exchange current density ($A\ m^{-2}$)
I	current density ($A\ m^{-2}$)
M	molecular weight ($kg\ mol^{-1}$)
P	pressure (kPa)
R	gas constant (8.314 $J\ mol^{-1}\ K^{-1}$)
R_{cell}	total cell resistance ($\Omega\ cm^2$)
S	source term
T	temperature (K)
$\vec{v}$	velocity vector ($m\ s^{-1}$)
V_{cell}	cell voltage (V)
V_{OCV}	open circuit voltage (V)
V_{act}	activation overpotential (V)

V_{conc}	concentration overpotential (V)
V_{ohm}	ohmic overpotential (V)
V_c	volume of catalyst layer (m^3)
x	mass fraction
Greek symbols	
α	charge transfer coefficient
β	permeability (m^2)
ρ	density (kg m^{-3})
μ	viscosity (kg m^{-1} s^{-1})
ε	porosity
Subscripts and superscript	
ave	average
$bulk$	in channels
c	cathode
eff	effective
H_2O	water vapor
i	species i
mom	momentum
O_2	oxygen
ref	reference
s	species
sur	interface between gas diffusion layer and catalyst layer

2. Numerical Model

In this study, the three-dimensional, single phase and isothermal model is developed for open-cathode PEM fuel cell. The governing equations including mass, momentum, and species conservations are solved. The assumptions for this model are as follows:

- The fuel cell operates at steady state.
- The inlet reactants are ideal gas.
- The gas diffusion layer and catalyst layer are isotropic porous layers.

2.1 Model equations

2.1.1 Continuity equation

$$\nabla \cdot \left(\varepsilon \rho \vec{v}\right) = 0 \tag{1}$$

2.1.2 Momentum conservation equation

$$\nabla \cdot (\varepsilon \rho \vec{v} \vec{v}) = -\varepsilon \nabla P + \nabla \cdot (\varepsilon \mu \nabla \vec{v}) + S_{mom} \tag{2}$$

The momentum source term is only applied to porous medium by adding Darcy's law term into equation. This source term expressed as:

$$S_{mom} = -\frac{\mu \vec{v}}{\beta} \tag{3}$$

In the flow channels, momentum source term is zero.

2.1.3 Species conservation equation

$$\nabla \cdot (\varepsilon \rho \vec{v}_i x_i) = \nabla \cdot (\varepsilon \rho D_i^{eff} \nabla x_i) + S_{s,i} \tag{4}$$

The effective diffusion coefficient of species in porous medium is expressed as:

$$D_i^{eff} = \varepsilon^{1.5} D_i^{ref} \left(\frac{P^{ref}}{P}\right)\left(\frac{T}{T^{ref}}\right)^{1.5} \tag{5}$$

The species source term is only applied to the catalyst layer and expressed as:

$$S_{s,O_2} = -\frac{M_{O_2}}{4F} i_c \tag{6}$$

$$S_{s,H_2O} = -\frac{M_{H_2O}}{2F} i_c \tag{7}$$

2.1.4 Electrochemical equations

The local current density at catalyst layer is calculated by using Butler-Volmer equation

$$i_c = a i_{c,0} \left(\frac{C_{O_2}}{C_{O_2}^{ref}}\right) \exp\left(\frac{\alpha_c F}{RT} V_{act,c}\right) \tag{8}$$

The exchange current density depends on temperature and express as:

$$i_{c,0} = i_{c,o}^{ref} \exp\left[-\frac{E_c}{RT}\left(1-\frac{T}{T^{ref}}\right)\right] \quad (9)$$

2.1.5 Fuel cell voltage

Fuel cell voltage is expressed by:

$$V_{cell} = V_{OCV} - V_{act} - V_{ohm} - V_{conc} \quad (10)$$

Ohmic overpotential is expressed by Ohm's law:

$$V_{ohm} = R_{cell} \cdot I_{ave} \quad (11)$$

Concentration overpotential is expressed as: [4]

$$V_{conc} = \frac{RT}{4F}\ln\left(\frac{C_{O_2}^{bulk}}{C_{O_2}^{sur}}\right) \quad (12)$$

Average current density is expressed as:

$$I_{ave} = \frac{1}{A}\int_{V_c} i_c dV \quad (13)$$

The boundary conditions for cathode flow channel are that the inlet mass flow rate is constant, the inlet gas compositions are constant and the flow is fully developed at cathode flow channel outlet. The solid walls are no slip with zero flux boundary conditions. At the interfaces between the gas channel, gas diffusion layer and the catalyst layer, the velocity, mass fractions, momentum fluxes and mass fluxes are assumed to be equal.

The coupled set of equation is solved iteratively; with the solution consider to be converged when the relative error in each field between two consecutive iterations is less than 10^{-6}. [1]

3. Flow field design and operating condition

In this study, only cathode side is simulated. The computational domain contains flow channel, gas diffusion layer and catalyst layer. Cathode channels are designed by varying channel aspect ratio (Width/Depth) and cross-sectional area (Width*Depth) with 6 different configurations as shown in Table 1 and Figure 1. All configurations have the same reaction area of 100 mm^2 and the same gas diffusion layer and catalyst layer thickness of 0.41 mm and 0.01 mm, respectively. In addition, the fuel cell modeling parameters and operating conditions are shown in Tables 2 and Table 3, respectively.

Table 1. Detail of cathode channel designs.

Design No.	Cross-sectional area (mm^2)	Aspect ratio	Width (mm)	Depth (mm)	Rib (mm)	No. of channels
1	2.0	0.80	1.26	1.58	1.26	40
2		1.25	1.58	1.26	0.94	40
3	5.0	0.80	2.00	2.50	2.00	25
4		1.25	2.50	2.00	1.50	25
5	8.0	0.80	2.53	3.16	2.53	20
6		1.25	3.16	2.53	1.90	20

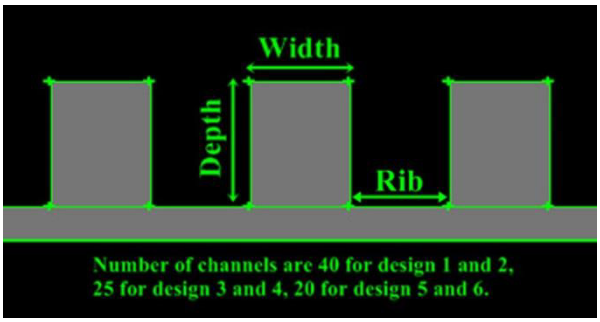

Fig. 1. Cathode channels.

Table 2. The fuel cell modeling parameters.

Parameter	Symbol	Value	Unit
Gas diffusion layer porosity	ε_{GDL}	0.5	
Catalyst layer porosity	ε_{CL}	0.5	
Gas diffusion layer permeability	β_{GDL}	1.76E-10	m^2
Catalyst layer permeability	β_{CL}	1.76E-11	m^2
Oxygen diffusion coefficient at reference condition	$D_{O_2,0}$	2.20E-05	$m^2\ s^{-1}$
Water diffusion coefficient at reference condition	$D_{H_2O,0}$	2.56E-05	$m^2\ s^{-1}$
Effective catalyst area per unit volume	a	4.50E+07	m^{-1}
Reference exchange current density	$i_{c,0}^{ref}$	2.80E-03	$A\ m^{-2}$
Activation energy	E_c	6.60E+04	$J\ mol^{-1}$
Oxygen reference concentration	$C_{O_2}^{ref}$	25.629	$mol\ m^{-3}$
Cathode charge transfer coefficient	α_c	1	
Faraday's constant	F	96485	$C\ mol^{-1}$
Gas constant	R	8.314	$J\ mol^{-1}\ K^{-1}$
Open circuit voltage	V_{OCV}	0.95	V
Total cell resistance	R_{cell}	0.9	$\Omega \cdot cm^2$

Table 3. The fuel cell operating conditions.

Parameter	Value	Unit
Gas inlet temperature	298	K
Operating temperature	348	K
Operating Pressure	101325	Pa
Relative humidity of gas inlet	70%	-
Mass flow inlet for 2 mm^2 cross-sectional area	2.47E-04	kg s^{-1}
Mass flow inlet for 5 mm^2 cross-sectional area	3.20E-04	kg s^{-1}
Mass flow inlet for 8 mm^2 cross-sectional area	3.03E-04	kg s^{-1}

4. Results and discussion

4.1 Model validation

In this study numerical results are validated by comparing with experimental results. [4] Figure 2-7 show the polarization curves of numerical result and experimental result for each configuration. The polarization curves show simulation results are close to experimental results at low and medium current density for all configurations but at high current density, some design simulation result does not fit to experimental result. The reason is that at high current density, water vapor is produced with high rate. Water vapor may condense into liquid water which does not include in the model.

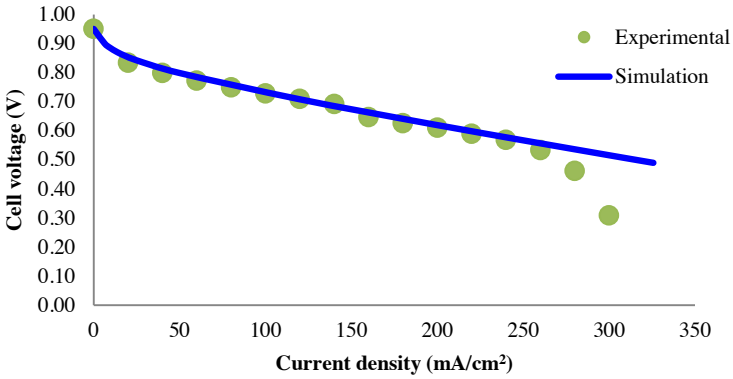

Fig. 2. Comparison of simulation result with experimental result of design 1.

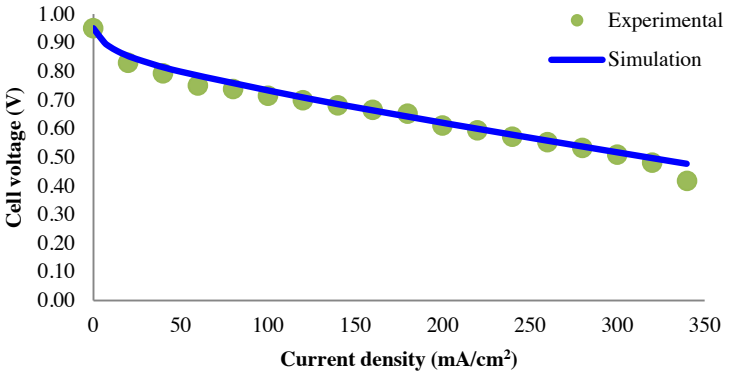

Fig. 3. Comparison of simulation result with experimental result of design 2.

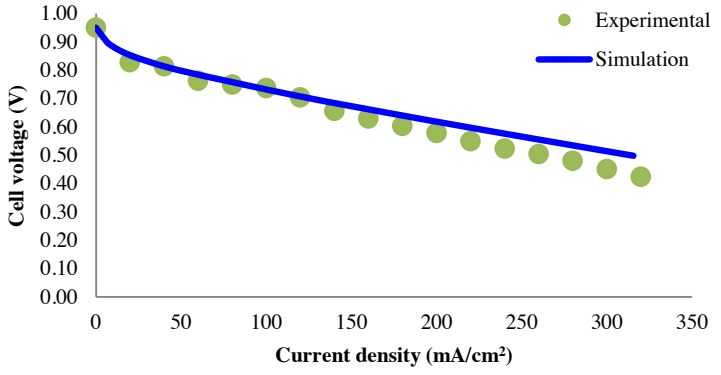

Fig. 4. Comparison of simulation result with experimental result of design 3.

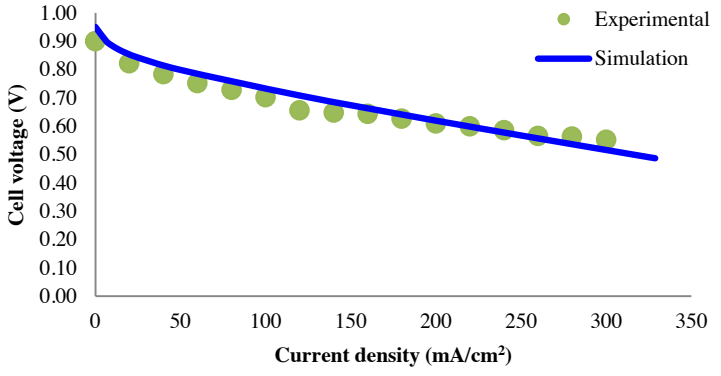

Fig. 5. Comparison of simulation result with experimental result of design 4.

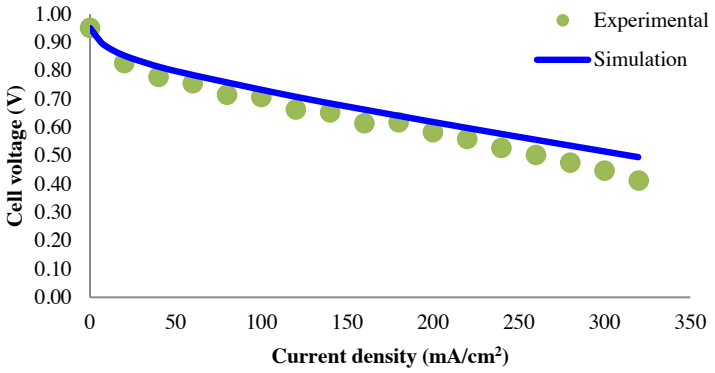

Fig. 6. Comparison of simulation result with experimental result of design 5.

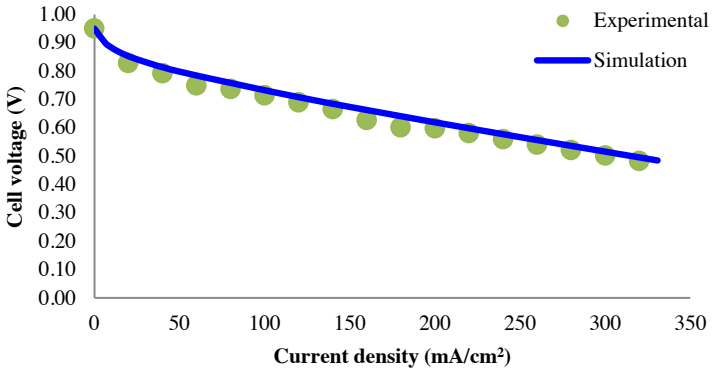

Fig. 7. Comparison of simulation result with experimental result of design 6.

4.2 Effect of cross-sectional area

Figure 8 shows polarization curves of design 1, 3 and 5 that have different cross-sectional areas with same aspect ratio of 0.8 and figure 9 shows polarization curves of design 2, 4 and 6 that have aspect ratio of 1.25.

From figures 8 and 9 that show the decrease of cross-sectional area does not have significant effect on the cell performance. However, when the aspect ratio is increased, one can observe slight effect on the performance. With higher aspect ratio, the smallest cross-sectional area shows better performance than the bigger one at high current density zone. The reason was that the decrease of cross-sectional area would increase the oxygen concentration at the interface between gas diffusion layer and catalyst layer, leading to the higher rate of reaction. For open cathode PEM fuel cell, cathode flow channels are straight. Pressure distribution along the flow channels is uniform for all channels as shown in figure 10.

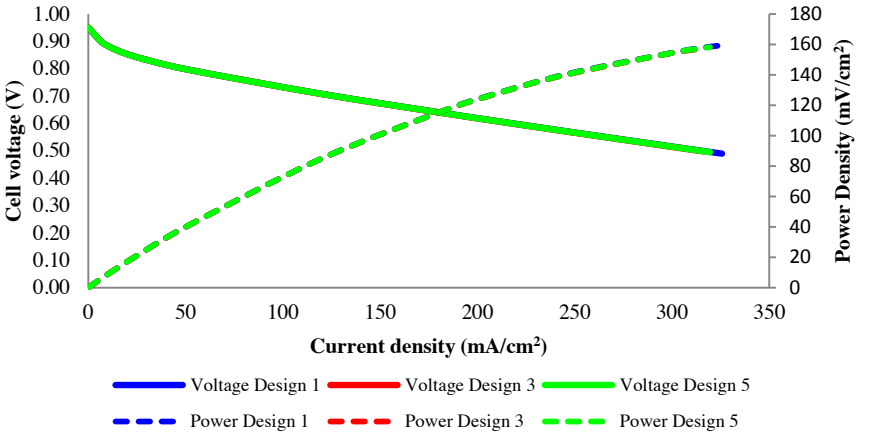

Fig. 8. Polarization curves of design 1, 3 and 5.

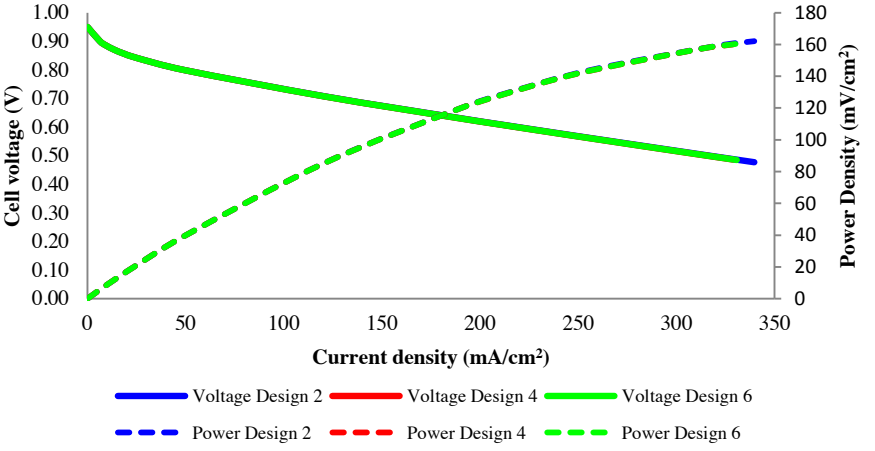

Fig. 9. Polarization curves of design 2, 4 and 6.

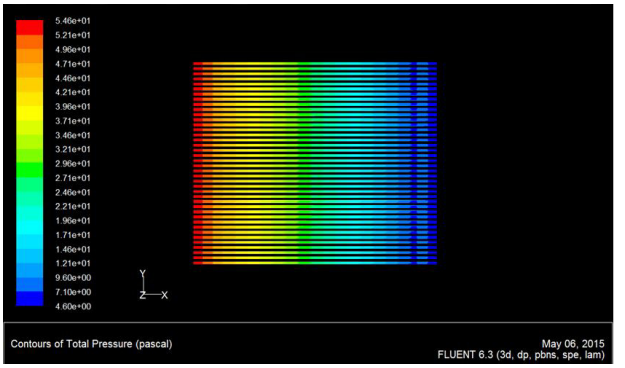

Fig. 10. Total pressure distribution in cathode flow channel.

If the pressure difference between two adjacent channels does not occur, the under-rib convection will not observe. Decreasing of cross-sectional area decreases rib area which will give higher oxygen concentration at interface between gas diffusion layer and catalyst layer as shown in Figure 11.

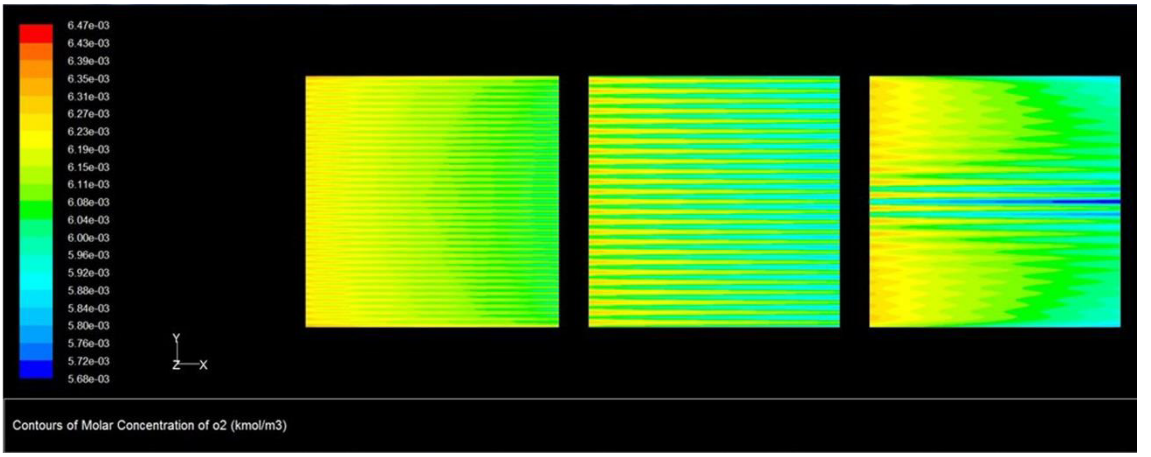

Fig. 11. Oxygen concentration distributions of design 1, 3 and 5, respectively

4.3 Effect of channel aspect ratio

Figures 12 to 14 show polarization curves of cross-sectional area of 2, 5 and 8 mm^2 with difference aspect ratio, respectively.

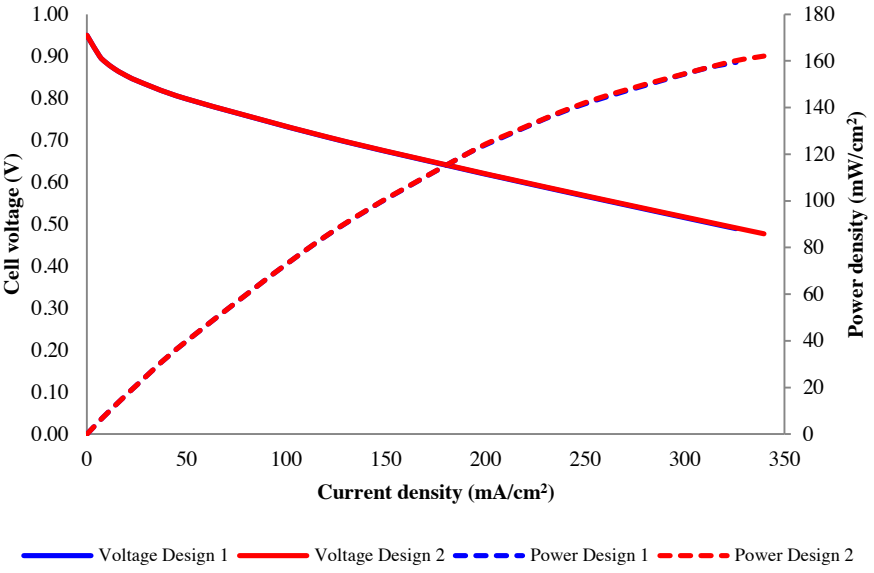

Fig. 12. Polarization curves of design 1 and 2.

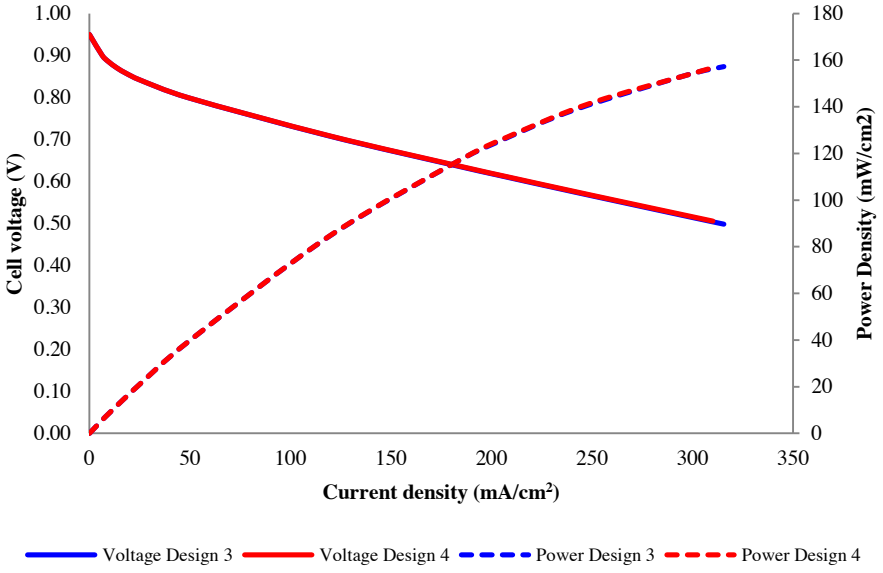

Fig. 13. Polarization curves of design 3 and 4.

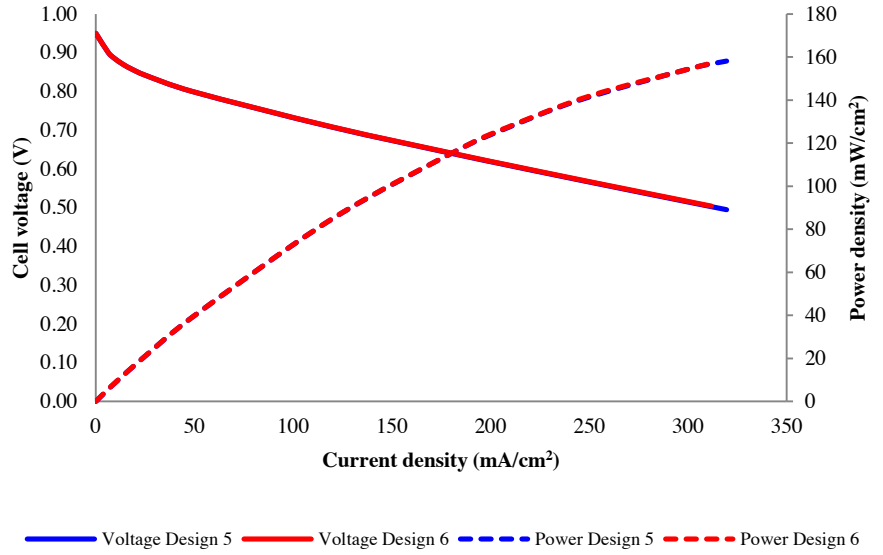

Fig. 14. Polarization curves of design 5 and 6.

From Figures 12 to 14, increasing of channel aspect ratio slightly improve the cell performance. Similar to the effect of cross-section area, increasing channel aspect ratio decreased rib area that caused increasing of oxygen concentration at interface between gas diffusion layer and catalyst layer as illustrated in Figure 15.

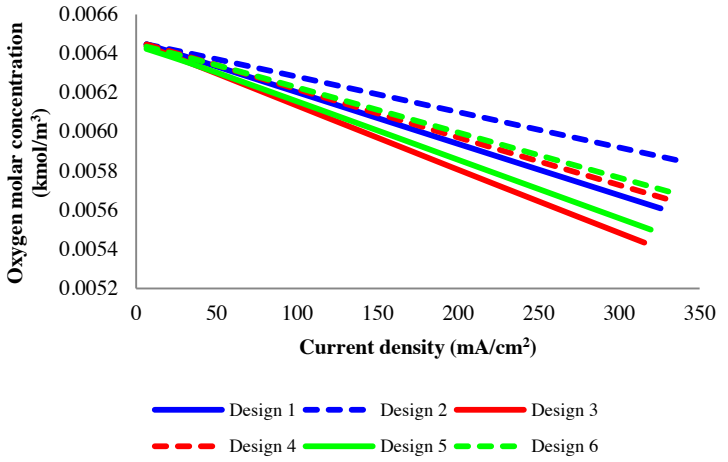

Fig. 15. Oxygen concentration at interface between gas diffusion layer and catalyst layer.

5. Conclusion

This work had developed a three-dimensional, single phase and isothermal model of an open-cathode PEM fuel cell. The model was focused on the cathode side. It was employed to investigate the design of cathode flow channels. The effects of cross-sectional area and aspect ratio on the cell performance of open-cathode PEM fuel cell were studied. Six configurations of cathode flow channels with a reaction area of 100 cm^2 were studied. The results showed that, designing of cathode flow channel by varying channel aspect ratio and cross-sectional area has a very small effect on performance of open-cathode PEM fuel cell. Increasing of channel aspect ratio and decreasing of cross-sectional area led to the reduction of rib area. Without under-rib convection, decreasing of rib area may lead to increasing of oxygen concentration between gas diffusion layer and catalyst layer which increases the rate of reaction and improves the cell performance.

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