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Effect of the geometry and pattern of the flow channel on the performance of polymer electrolyte membrane fuel cell

Kronkanok Hongthong, Kejvalee Pruksathorn, Pornpote Piumsomboon† and Paiboon Sripakagorn*

Fuels Research Center, Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
*Department of Mechanical Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok 10330, Thailand
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Abstract−This research focuses on the effect of the geometry and patterns of the gas flow channel on the PEM fuel cell performance. Simulation was conducted and the results were verified by experiments. Three-dimensional, single phase, compressible and isothermal models of 5 cm^2 electrodes, anode and cathode, were developed and studied by utilizing a commercial Computational Fluid Dynamics (CFD) software, FLUENT 4.5. Two types of gas flow channel were investigated: conventional and interdigitated. The results showed that the flow channel pattern does not have a significant effect on the anode cell performance, whereas it has a strong effect/influence on the cathode cell performance. The interdigitated design provides a higher limiting current density and cell performance than the conventional design on the cathode side. Moreover, the cell performance does not depend on the inlet and outlet channel widths. On the contrary, for the interdigitated design, it was influenced by the shoulder width. Finally, experiments were conducted to validate the simulation results.

Key words: Flow Channel Pattern, PEM Fuel Cell, Modeling, FLUENT

INTRODUCTION

The Polymer Electrolyte Membrane Fuel Cell (PEMFC) is an energy conversion device which is a strong candidate for an alternative power generator due to its high-energy efficiency, pollution free, and low operating temperature. Hydrogen as fuel and oxygen or air as oxidant are used to generate electricity, while heat and water are typical byproducts. Anode and cathode are made of an electrically conductive porous material, typically carbon base. At the anode side, hydrogen is fed into the cell as fuel and oxidized at the surface of electrode releasing protons (H^+) and electrons. The H^+ ions are driven by electrical force field to migrate through the polymer electrolyte membrane, while electrons will flow to the cathode through an external circuit. At the cathode side, air or oxygen is fed and reduced with H^+ and electron to form water.

The results from many research works indicate that the cell performance is limited by the oxygen reduction reaction [1]. The cell performance can be improved by increasing the rate of O_2 transfer to the catalyst surface. With suitable gas flow channel pattern, the transfer rate can be increased. Its pattern has a strong effect on the mass transfer mechanisms - either diffusion or convection. This research focused on two types of the gas flow channel pattern: conventional and interdigitated flow field design. In the conventional flow field design, gas flows along the interface between the gas flow channel and the gas diffusion layer, thereby leading to gas transport controlled by molecular diffusion through the gas diffusion layer. This is in contrast to the interdigitated flow field design where the two flow channels around each shoulder are dead-end. The reactant gas is forced to flow through the gas diffusion layer in order to move out from the cell. This convection mechanism facilitates the transport of the reactant to, and the product from, the catalyst surface, thus increasing the current density.

The development of PEMFC is generally quite costly. Thus, the application of mathematical modeling and simulations has become an important tool in the fuel cell development. Over the last decades a number of fuel cell models have been developed. Several modeling attempts have been made to understand the effect of gas flow channel pattern, such as He et al. [2] who presented a two phase, two-dimensional, steady state, isothermal model to investigate the effect of interdigitated gas flow channel design on the cathode cell performance. The results show that the interdigitated design induces the reactant gas to flow through gas diffusion layer by convective mechanism, and the cell performance can be improved by using interdigitated design with large channel width/shoulder width ratio. Grujicic et al. [3] studied the optimization of air cathode PEMFC that used an interdigitated gas flow channel pattern as a gas distributor. The optimization of cathode cell performance arrived at a low value of gas flow channel width, but this research does not consider the effect of shoulder width. There are other research works that have studied the effect of gas flow channel geometry on the anode cell performance, such as Hontanon et al. [4] and Kumar and Reddy [5]. Because the anode over-potential is generally very small, it is very important to develop a model of the anode side. Berning et al. [6] developed a full cell model to study transport phenomena in PEMFC when the conventional gas flow channel design was used as a gas distributor. The smaller shoulder width of the conventional design induces higher cell performance since the mass transport limitation effect is minimized and the cell performance is controlled by the oxidation reaction and the diffusivity of oxygen. Lee and Yi [7] presented a two dimensional, isothermal and steady state model to analyze the physical phenomena occurring in PEMFC by using

†To whom correspondence should be addressed.
E-mail: pornpote.p@chula.ac.th

Computational Fluid Dynamics (CFD) software, FLUENT. The model showed that the proton conductivity is a function of water content in MEA. The current calculated by this model was slightly lower than the experimental data from Ticianelli's paper. In this work, three-dimensional, single phase models of the anode and cathode cells were developed separately with commercial Computational Fluid Dynamics (CFD) software, FLUENT 4.5. The models were developed to study the effect of geometry and pattern of gas flow channel on the performance of PEMFC. Then the simulation results were validated by constructing flow field plates and testing them on the single cell test-station.

SIMULATION AND EXPERIMENTAL

1. Modeling

According to the fact that the current density generated in a fuel cell depends on the mass transfer mechanisms in the gas diffusion layer, the modeling domain includes only gas distributor, gas diffusion layer and catalyst layer as shown in Fig. 1.

With some limitations of the studied system and software, it is necessary to introduce a number of assumptions to achieve the objectives of this model.

- The cell was operated under steady state, isothermal condition.
- The liquid water generated during the oxygen reduction reaction on the cathodic catalyst layer was assumed to have a negligible volume (single phase model). It should be noted that this simplification is the limitation of FLUENT 4.5.
- All gases in the system behave as compressible ideal gases.
- The gas diffusion layer was considered as a homogeneous medium in which the porosity and permeability were distributed uniformly.
- The catalyst layer was considered as a thin layer and the electrochemical reactions were assumed to be surface reaction.

2. The Governing Equations

Although the commercial computational fluid dynamic software was used, basically, it solves conservation equations that describe transport phenomena inside the system such as the conservation equations of mass, species, energy, momentum, and Darcy's law (momentum conservation equation for porous medium). Moreover, some equations will be completely described by adding suitable source terms.

Species equation

$$\frac{\partial(c_i^g)}{\partial t} + \nabla \cdot (c_i^g \vec{v}^g) = \nabla \cdot (D_i^{eff} \nabla c_i) + S_i \quad (1)$$

Momentum equation

$$\frac{\partial(\rho^g \vec{v}^g)}{\partial t} + \nabla \cdot (\rho^g \vec{v}^g \vec{v}^g) = -\nabla P^g + \nabla \cdot (\mu^g \nabla \vec{v}^g) \quad (2)$$

On the catalyst surface, the electrochemical reactions are taking place as the surface reactions so the source terms for species conservation equations of H_2, O_2 and H_2O must be specified.

$$S_{H_2} = -\frac{i_0}{2F}\left[\frac{C_{H_2}(0,t)}{C_{ref}}\right]\exp\left[\frac{\alpha \eta_{act,anode} F}{RT}\right] \quad (3)$$

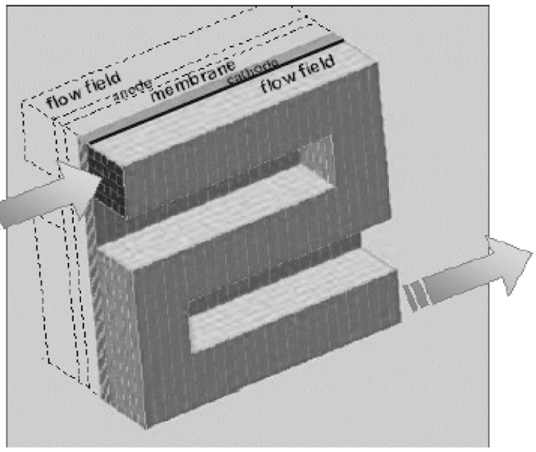

Fig. 1. Domain of the model.

Table 1. The values of parameters used in the model

Parameter	Value	Symbol	Unit
Inlet channel width	vary	CH_{in}	mm
Outlet channel width	vary	CH_{out}	mm
Shoulder width	vary	S	mm
MEA area	5.0E-04		m^2
Gas permeability of the electrode [2]	1.20E-12	K_0	m^2
Dry porosity of the electrode [2]	0.3	e	-
Inlet mole fraction of H_2	1	-	-
Inlet mole fraction of H_2O	0.00	-	-
Inlet mass flux	2.5 A/cm^2 equivalent	-	kg/m^2 sec
Outlet pressure	1	P_{out}	atm
Operating temperature	60	T	°C
Gas viscosity [2]	2.03E-05	μ^g	kg/(m·sec)
Transfer coefficient of H_2 oxidation reaction [8]	0.5	α_{anode}	-
Transfer coefficient of O_2 reduction reaction [2]	0.5	$\alpha_{cathode}$	-
Exchange current density for oxidation reaction [8]	5.0E06	$i_{0,\ anode}$	A/m^2
Exchange current density for reduction reaction [2]	100	$i_{0,\ cathode}$	A/m^2

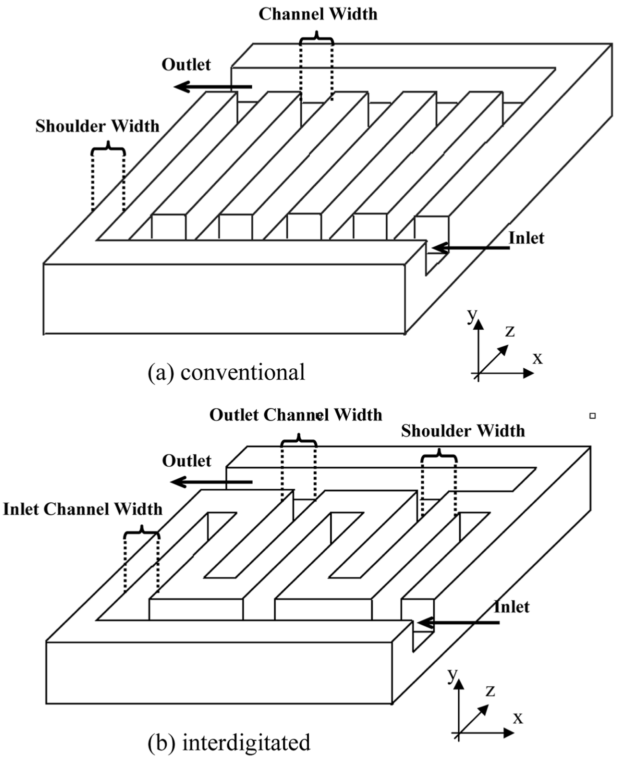

Fig. 2. Gas flow channel (a) conventional (b) interdigitated.

$$S_{O_2}=-\frac{i_0}{4F}\left[\frac{C_{O_2}(0,t)}{C_{ref}}\right]\exp\left[\frac{\alpha\eta_{act,cathode}F}{RT}\right] \tag{4}$$

$$S_{H_2O}=-\frac{i_0}{2F}\left[\frac{C_{O_2}(0,t)}{C_{ref}}\right]\exp\left[\frac{\alpha\eta_{act,cathode}F}{RT}\right] \tag{5}$$

Several species source terms were solved by utilizing the Butler-Volmer equation and Faraday's law. In the equations above, C(0, t) denotes the concentration of reactant on the catalyst surface, α are the so-called transfer coefficients and η are known as anode or cathode over-potential. The reference exchange current density (i_0) depends on various parameters such as operating temperature and catalyst loading. The values of parameters used in the model are shown in Table 1. To study the effect of the geometry, variations in both the gas flow channel patterns, and the channel and shoulder widths of conventional and interdigitated designs were investigated (Fig. 2).

3. Algorithm

The detail of the solving procedure is shown in Fig. 3. The first step was to specify the values of necessary data, parameters and boundary conditions of the cathode model such as inlet mass flux, feed composition, operating temperature and pressure, and fluid properties. Then, the model provides the average surface mass flux of O_2. The value of oxygen mass flux obtained from the model was then used to predict the average current density at a given over-potential value by Faraday's law. Finally, the average current density was used to calculate the anode over-potential using Tafel's equation.

4. The Validation of the Simulation by Experiments

To validate simulation results, the experiments were conducted with the conditions suggested by the simulation results. Flow field plates, both conventional and interdigitated designs, were prepared

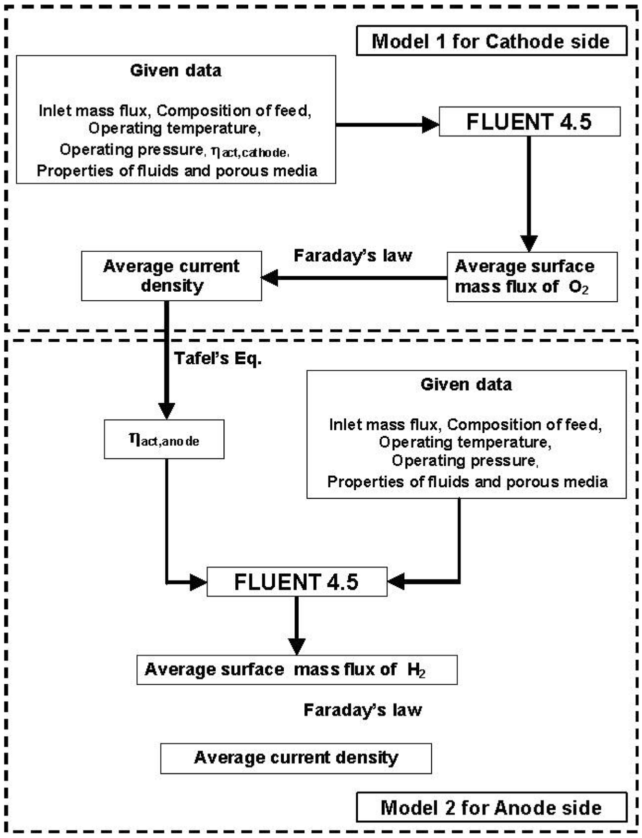

Fig. 3. Problem solving procedure of the model.

by using the results obtained from the simulation. A conventional design plate was prepared with the channel and shoulder widths of 1 mm. However, for the interdigitated design, the channel width was fixed at 1 mm., but the shoulder widths were varied with the size of 1, 2 and 20.5 mm., respectively. 5 cm^2 MEAs from Electrochem Company were used for assembling the test cells. The cells were operated at 60 °C and 1 atm with 207 sccm of humidified air and 87 sccm (equivalent with 2.5 A/cm^2) of hydrogen flow rate. Current drawn from the test cell was measured at different potentials by potentiostat/Galvanostat model PGSTAT 30 Autolab with a 10 A current booster.

RESULTS AND DISCUSSION

1. Simulation Results

The model was developed as a three-dimensional, single-phase steady-state model. Air was the oxidant at cathodic electrode with porosity of 0.3 and height of 0.25 mm. which is in contact with a gas distributor, which has 1 mm. of inlet and outlet flow channel widths. A pressure drop of 0.007 atm. was applied between the inlet and outlet ports and a cathode over-potential of 0.5 V was set. Other conditions and parameters used in the study are shown in Table 1. The result from this model was compared with the results reported by He et al. [2]. He's model employed an interdigitated design and his model was developed as a two-phase, two-dimensional model at steady state condition, whereas in this study, the model was three-dimensional and single phase. Fig. 4 shows the domain of cathodic model with an area of 4.9 mm^2 in three dimensions.

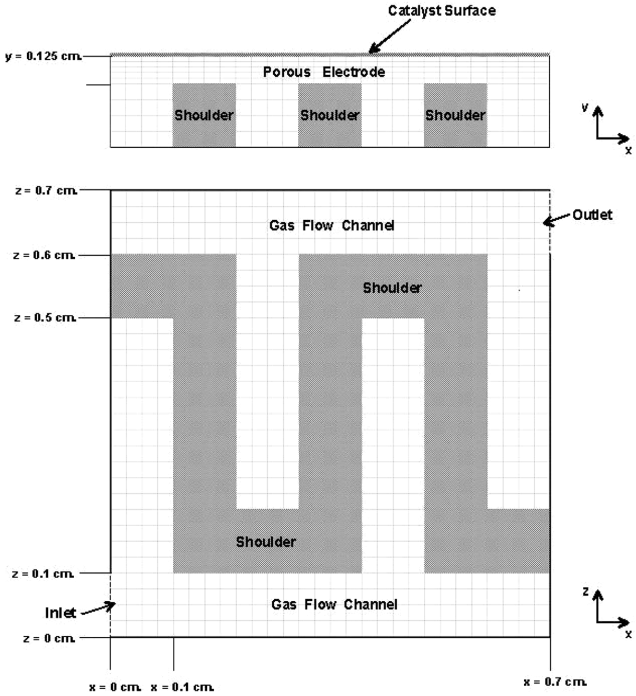

Fig. 4. The domain of the base-case model.

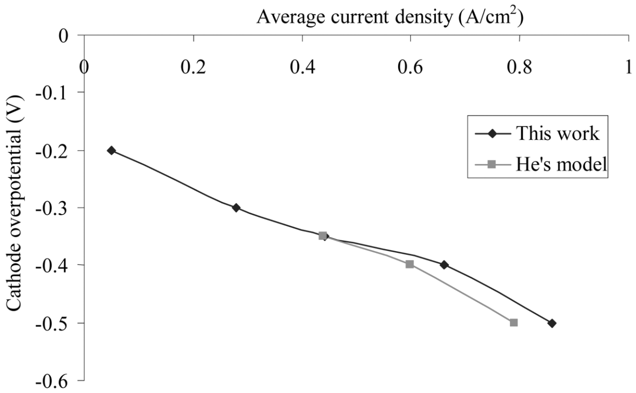

Fig. 5. Comparison of the polarization curve from this work with He's model.

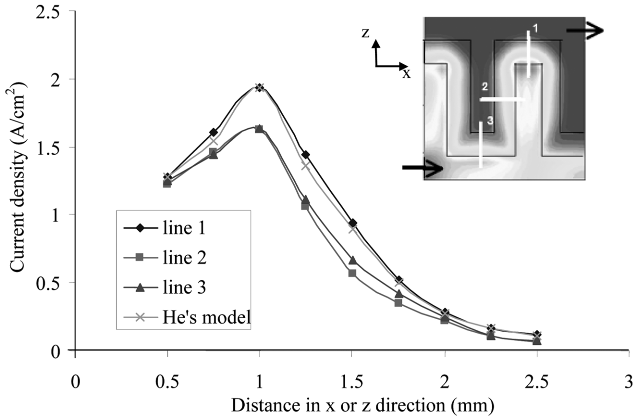

Fig. 6. Current density profiles along the electrode width.

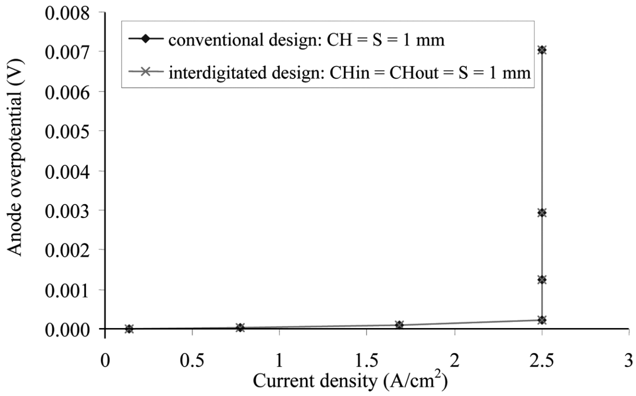

Fig. 7. Anodic polarization curves for different flow channel patterns.

The polarization curve in Fig. 5 showed that the developed model conforms with He's model at small values of cathode over-potential (−0.2 V. to −0.35 V.) whereas the deviation became obvious at the higher cathode over-potential. The difference is due to the difference in the level of simulation details. Not only were the third dimension along inlet and outlet gas flow channel length included in the model, the inlet and outlet gas flow channel header were also added. The developed three-dimensional model seems to predict the local current density profile more accurately than a two-dimensional model. This statement was suggested by observing Fig. 6. In this figure, several local current density profiles at different locations are reported between half of the inlet gas flow channel and the outlet gas flow channel. The profile at the area pointed out by line 1 agreed well with He's model, but those profiles along line 2 and line 3 provided lower predictions compared with He's model. The reason is that with a three-dimensional model, the pressure drop along the channel, which was excluded in He's model, was also calculated leading to a lower pressure along the channel. Thus, the mass-flux of the air through the gas diffusion layer will be less when using the three-dimensional model. This reason can be confirmed by the oxygen concentration profile in Fig. 6. It showed that line 1 had more concentration than line 2 and 3. Thus, more reaction could be taking place in the area of line 1 than that of line 3. Therefore, the current density in the vicinity of line 2 and line 3 was lower.

2. Effect of the Flow Field Channel on the Performance of the Fuel Cell at the Anode Side

The effect of the flow field channel on the performance of the fuel cell at the anode side was studied by using different flow channel patterns (conventional and interdigitated) and designs (channel and shoulder width). The electrode area used in the study was 5 cm^2. The hydrogen flow rate was kept constant at 6.4E-05 mole/s, which is equivalent to 2.5 A/cm^2. The outlet pressure for the test cell was set at 1 atm. The model predicted the average current as a function of over-potential at the anode side. The result showed that flow channel patterns and designs have no effect on the cell performance on the anode side (Fig. 7). The polarization curves at all conditions were identical. It can be explained by the fact that the diffusion coefficient of hydrogen on the porous electrode is high (1.89E-05 m^2/s). Therefore, the hydrogen is able to diffuse through electrode and dissociate with ease. Although the flow channel patterns are different, the effect on the rate of mass transfer cannot be observed.

3. Effect of the Flow Field Channel on the Performance of the Fuel Cell at the Cathode Side

The conventional and interdigitated flow channel patterns were also used to study their influence on the cell performance at the cathode side. The electrode area for this study was also 5 cm^2. The oxygen flow rate was kept constant at 3.2E-05 mole/s, equivalent to 2.5 A/cm^2. The outlet pressure for the test cell was atmospheric pressure. The results from simulation show that the channel and shoulder widths of conventional design have an effect on the cathodic performance as shown in Fig. 8. The effect becomes more pronounced at high current density. Should the channel width be increased, the current density is increased. On the other hand, should the shoulder width be increased, the current density is decreased. The performance of the cathode cell can be improved by decreasing the shoulder width. Moreover, the figure also shows that a fuel cell with interdigitated flow channel performed far better than the conventional one. The current density attained was 120-150% higher. The changes in channel and shoulder widths also affect the cathodic performance at high absolute over-potentials when the interdigitated design is adopted as shown in Fig. 9. The results also exhibit the mass transfer effect on the reduction reaction. It can be explained that the diffusion coefficient of oxygen on porous electrode (3.28E-06 m^2/s) is much lower than that of hydrogen (1.89E-05 m^2/s). Therefore, the quantity of oxygen diffused through the porous electrode was not enough for the reaction requirement. The interdigitated design can force the gas to diffuse through the porous electrode before flowing out of the cell. At high current density, high oxygen quantity was required for the reaction, which led to a higher pressure drop in the electrodes. In this case study, when the shoulder width was 1 mm, the inlet pressure of 1.012 atm or 2.5 A/cm^2 equivalent of air was required, while the pressure of 2.409 atm was required for 20.5 mm. shoulder width. For the interdigitated design, the mass transfer effect was more pronounced when the absolute over-potential becomes larger than 0.5 V (Fig. 9). The design with large shoulder width will give higher current density because more gas is being forced through the porous electrode than small shoulder width. According to Fick's law, the large shoulder width requires higher inlet pressure to force the same amount of gas through the gas diffusion layer. The higher inlet pressure induces a higher convective mass transfer in the gas diffusion layer leading to the higher mass transfer rate and higher reaction rate at several cathodes over potential.

The performance at the cathode side can be improved by using larger interdigitated's shoulder width as the gas distributor at the cathode side as shown in Figs. 10 and 11. That is because the mass transport mechanism was more convective and the direct contact

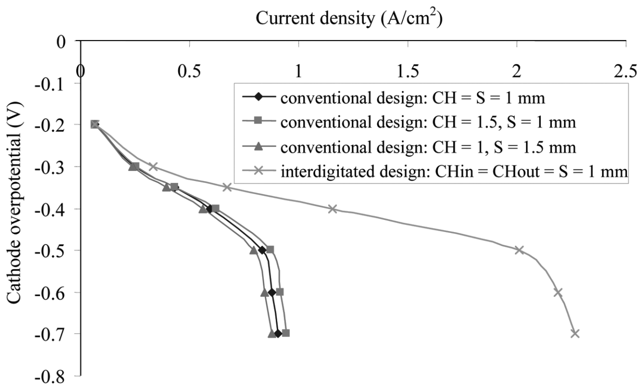

Fig. 8. Cathodic polarization curves at different flow channel patterns.

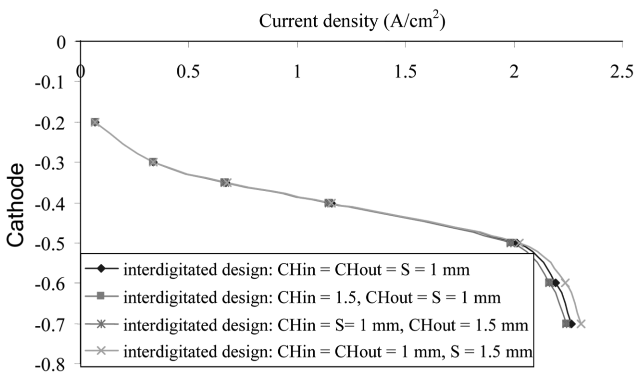

Fig. 9. Cathodic polarization curves at different channel and shoulder widths for the interdigitated flow channel design.

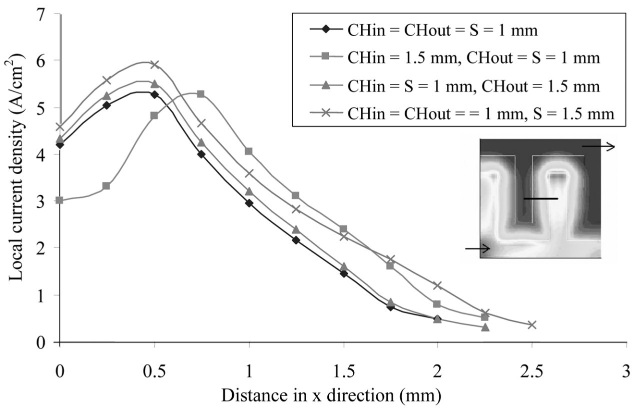

Fig. 10. Effect of the channel and shoulder widths for the interdigitated design on the current density at the cathodic over-potential of 0.7 V.

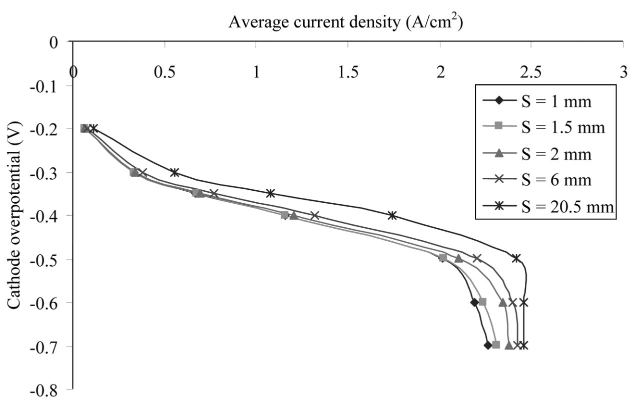

Fig. 11. Effect of the shoulder widths for the interdigitated design on the cathodic polarization.

area between reactant and catalyst was increased when the shoulder width was increased. However, it should be noted that the better performance came with a higher inlet pressure since it is necessary to force the gas to flow through porous electrode under the shoulder area. This will provide higher oxygen concentration to active surface of the electrode and increase the reaction rate. This will also lead to the increase in the parasitic loss in the system. On the contrary, in case of interdigitated design, the effects of inlet and outlet channel widths on the cathode cell performance were not observed.

4. Validation of Simulation Results by Experiments

As mentioned earlier, the channel and shoulder widths of flow field plates, in case of the conventional design, were 1 mm. However, in the case of the interdigitated design, the channel width was 1 mm, but three values of shoulder width that are 1, 2 and 20.5 mm were used. The graphite flow field plates were prepared with the specified dimensions. Their effects were tested in a test station with 5 cm^2 of MEA from Electrochem Co. Ltd. with the flow rates of 207 sccm of humidified air and 87 sccm (equivalent with 2.5 A/cm^2) of hydrogen flow. The cell was operated at 60 °C and 1 atm.

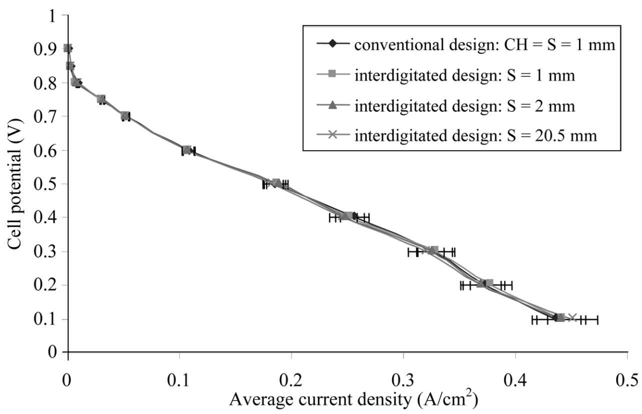

Fig. 12. Polarization curves of the test cells when the cathode used an interdigitated design with 1 mm of channel and shoulder widths, while the anode used both conventional and interdigitated designs with various shoulder widths.

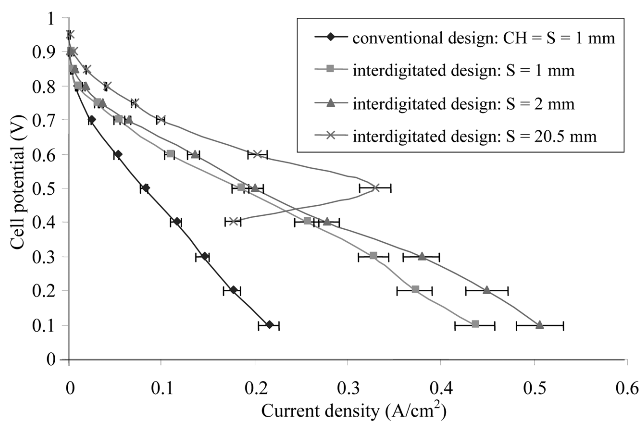

Fig. 13. Polarization curves of the test cells when the anode used a conventional design with 1 mm of channel and shoulder widths, while the cathode used both conventional and interdigitated designs with various shoulder widths.

The experimental results corresponding to the conditions from the simulation models are shown in Fig. 12. The results show that the design of flow field plate at the anode side has no effect on the cell performance. On the other hand, it has a significant effect on the cell performance when different designs are used at the cathode side (Fig. 13). The conventional design flow field plate showed a lower cell performance than the interdigitated design. The interdigitated flow field plate with larger shoulder width can also improve the cell performance. The cell performance could be improved up to 93% and 124% compared to the conventional design when the interdigitated design was employed at the shoulder widths of 1 and 2 mm, respectively. These results corresponded very well with the simulation results as shown in Fig. 11. The experimental data corresponding to the case of 20.5 mm of shoulder width also gives high performance when the cell potential is higher than 0.5 volt. Nevertheless, beyond this potential, the current density dropped rapidly from 0.31 A/cm^2. The reason was that the cell was under flooding phenomenon. The water removal from the cell with the air outlet was much less than the amount of water produced in the cell due to the very large shoulder width. This phenomenon was not found in the simulation result because the model is only a one-phase model. The water produced in the model was in gas phase and could be removed at the air outlet.

CONCLUSIONS

Three-dimensional, single phase, compressible and isothermal models of 5c m^2 electrodes, anode and cathode, were developed and studied by employing a commercial Computational Fluid Dynamics (CFD) software, FLUENT 4.5. The results show that the gas flow channel pattern does not have a significant effect on the anode cell performance, whereas it plays a prominent role in the cathode cell performance. On the cathode side, interdigitated design can promote the cathode cell performance by 120-150% over the conventional design, should a larger shoulder width be used. On the contrary, the effect of inlet and outlet channel widths of the interdigitated design on the cathode cell performance was not observed. In comparison to the simulation results, experiments show similar trends regarding the effect of various parameters on the fuel cell performance.

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