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Effect of Hexagon Land Size in Honeycomb Flow Channel of a Polymer Electrolyte Fuel Cell

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Abstract

According to our previous work, honeycomb design was shown as a promising flow field configuration for a PEFC that could provide the power as high as that of the single channel serpentine flow field, but could achieve significantly lower pressure drop. However, the uniformity of the distributions in the previously designed honeycomb was not good enough. Thus, the study on the proper design must be carried out in order to obtain the honeycomb flow field with uniform distributions. The new honeycomb design geometry on a 5 cm^2 was generated in ANSYS WORKBENCH. It was designed to have smaller hexagon land size and gas flow channel width, and thus the higher total hexagon cells. In this work, an investigation on the effects of the hexagon land size on distributions and performance in honeycomb flow field, was carried out numerically via ANSYS FLUENT software. At a practical operating condition of 0.6 V, the simulation revealed that the new honeycomb design outperformed the previous honeycomb design, resulting in an enhancement of the net power output approximately by 3.51% and more uniform distributions of current density, hydrogen mass fraction, oxygen mass fraction and temperature which would consequently lead to the longer cell lifetime. Although the new honeycomb design provided higher power density and more uniform distributions, the pressure drop was also found to be three-time higher than that of the previous honeycomb design, but it still maintained relatively low pressure drop as compared to that of the single channel serpentine, which was approximately 540% lower.

Keywords*:* PEFC, Simulation, Honeycomb, Hexagon land size

1. Introduction

Due to the increasing environmental pollution and the depletion of fossil fuel at the present, the power generation from clean energy technology is being focused on the global scale. The polymer electrolyte fuel cell is an energy conversion device that is considered promising to be developed for transportation and stationary applications. Due to its high energy conversion efficiency and its environmentally friendly by-product, i.e., water, PEFC has become a very attractive device for future power generation. To operate a PEFC, hydrogen and oxygen are fed into the anode and the cathode gas flow channels as shown in Fig. 1, respectively, for generating electrical energy. The reactant gases diffused through the gas diffusion layer to reach the catalyst layer which contains a noble metal, typically platinum, to catalyze the electrochemical reactions. Hydrogen gas catalytically splits into protons and electrons at the anode electrode. Then, the protons permeate through the polymer electrolyte membrane to the cathode side while the electrons travel through the external circuit to the cathode side for generating the electricity. To form up water, the oxygen, the protons and the electrons have to reach the triple-phase boundary and catalytically react together at the cathode electrode.

There were many researchers working on the effects of conventional flow field designs of PEFC [1] since it has been widely considered one of the main factors affecting on polymer electrolyte fuel cell (PEFC) performance and lifetime [1]. However, a good flow field design, which has a high quality of competing in the global energy market, has to satisfy the ideal roles of the flow fields proposed by Arvay et al [2] which are to 1) distribute the reactants uniformly all over the cell to prevent hot spots, (excessive heat can dry and damage the cell), and cold spots (representing inefficiencies in the cell), 2) transport the by-products out of the reaction site and the cell which allow the reactants to reach the triple phase boundary easier and more efficient, 3) transport the electrons as freely as possible to the external circuit with large contact area between the bipolar plate and the GDL, and 4) have a low pressure drop which does not necessarily required the external blower to compensate, hence higher overall cell performance.

However, the conventional flow fields such as the single channel serpentine and the parallel cannot satisfy 4 critical conditions of the flow fields. Thus, the study of transport behaviors inside PEFC with new flow field designs that could satisfy the criteria should be further studied and developed so that they can become useful information for the future flow field design. Nature inspired flow field designs are currently an interest in PEFC technological development [3, 4] since these designs shows the promising potential in PEFC performance enhancement.

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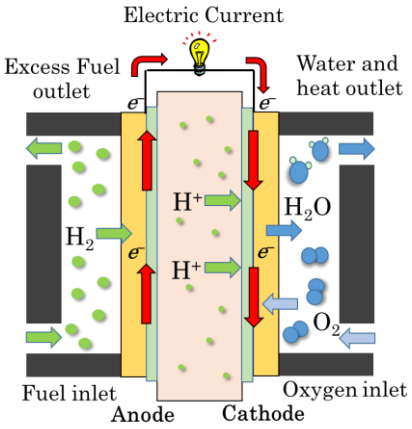

Fig. 1 The schematic shows how polymer electrolyte fuel cell works [3]

According to our previous work [3], the flow field design which was based on the pattern of the natural honeycomb structure (see Fig. 2b) seemed to be very promising flow field configuration for the PEFC since its structure has been well known as the geometry that divides a surface into equal areas with the least total perimeter. This characteristic provides a relatively large area to facilitate electrons and short total channel length, resulting in the lower friction and hence the pressure drop. Moreover, the results from previous honeycomb design revealed that, it could provide a power as high as the single channel serpentine, which is often used as a reference design of PEFC gas flow channel because of its high performance and simplicity. The honeycomb could also offer significantly lower pressure drop at the practical cell voltage of 0.6 V which is a typical operating condition for using PEFC to supply electricity to recharge a battery in an automotive application [5]. However, the uniformity of the distributions in the previous honeycomb design was found to be not good enough.

To obtain honeycomb flow field with uniform distributions, a new honeycomb design, presented in Fig. 2a, was designed to have the smaller hexagon land size and gas flow channel width to help the reactants to reach the reaction sites more efficiently, especially the areas under the hexagon land area (so-called under rib area for the conventional designs), and consequently

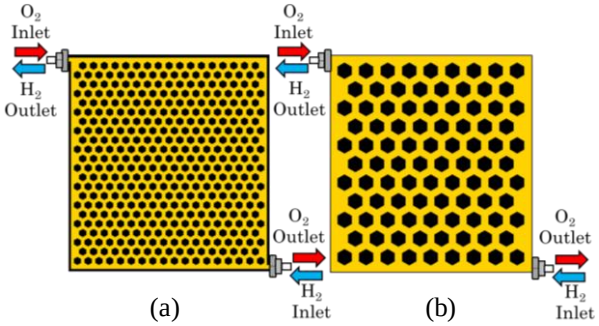

Fig. 2 The schematic illustration of the flow fields simulated in this work a) new honeycomb and b) previous honeycomb (→) Anode and (→) Cathode flow directions

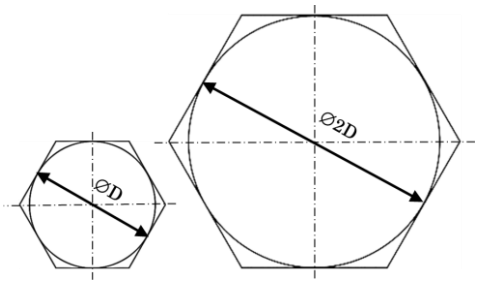

Fig. 3 Hexagon land size a) new honeycomb and b) previous honeycomb design

higher total hexagon cells. The investigation on the effects of the hexagon land size in honeycomb, including distributions, performance and transport characteristics of the 5 cm^2 PEFC flow fields with two different honeycomb designs at a practical condition had been carried out via numerical simulation in ANSYS FLUENT.

2. Model Development

The new honeycomb was designed to have a smaller hexagon land size. The hexagon was inscribed in a circle with a half diameter of the previous hexagon as shown in Fig. 3, and a narrower channel width of 0.4 mm while maintained the same channel height of 0.8 mm to result in a higher total number hexagons cell. In addition, rectangular land areas with the thickness of 0.3 and the channel height of 0.8 mm were also generated along the border of the cell, except the inlet and the outlet, to provide larger contact area between the bipolar plate and the GDL. Similar to the previous work, the regular hexagons with all internal angles are 120° was also used in this new design. To control the cell active area of the honeycomb to be 5 cm^2, the geometric parameters of each hexagon for the new honeycomb and the previous honeycomb were given in Table 1.

The new honeycomb and the previous honeycomb design 3D geometries on a 5 cm^2 PEFC were generated in ANSYS WORKBENCH based on the real geometries. The geometric parameters of each component of the simulated PEFC were given in Table 2. Note that, in this work, the geometries were discretized based on our previous study [3] which suggested that the computational cells in the through plane direction (i.e., number of cell layers) should be 5, 5, and 5 in anode catalyst layer, membrane, and

Table. 1 The geometric parameters of each hexagon

Parameter	New Value	Previous Value	Unit
Hexagon height	0.8	0.8	mm
Diameter of a circle (D)	0.8	1.6	mm
Hexagon area	0.554	2.217	mm^2
Total number of hexagons	385	94	cell

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Table. 2 Model geometries dimension

Parameter	Value	Unit
Membrane thickness	0.050	mm
Catalyst layer thickness	0.015	mm
Gas diffusion layer thickness	0.190	mm
Bipolar plate thickness	0.800	mm
Channel height and width	0.800	mm

cathode catalyst layer, respectively, so that the solution would be independent to the number of cells. For discretizing the geometries of both honeycombs into small computational cells, ANSYS ICEMCFD was used, resulting in a total of 647,472 and 739,189 cells, respectively.

Table 3 presents the summary of the boundary conditions used in the simulation. The PEFC model simulated in this study was operated under the atmospheric pressure and at the temperature of 60 °C. To achieve the cell temperature of 60°C, the temperature of the external boundary of the bipolar plates and the temperature of the reactant gases were set constant at 60°C. The reactant gases consisted of hydrogen and air, used as the oxidant, which were fed into the anode and cathode gas flow channels, respectively. The mass flow boundary condition was applied at the inlet on each side. Those mass flow rate and mass fraction required to be input were calculated based on the stoichiometric flow rate of 1.1 at 90% RH. The galvanostatic boundary condition was applied to obtain the cell voltage for completing the polarization curve.

The models developed in this study were governed by the mass conservation, and the Navier-Stokes equation which are coupled and expressed in a general form in Eq. (1).

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\phi\vec{V}) = \nabla\cdot(\Gamma_\phi\nabla\phi) + S_\phi \qquad (1)$$

where ϕ is the transported quantity, ρ is the density of the mixture, t is the time, $\vec{V}$ is the velocity vector, Γ_ϕ is the transported quantity diffusivity, and S_ϕ is the source term. The conservation of energy, the species transport equations and a set of several theoretically and experimentally derived equations which their details were already given elsewhere [1].

Table. 3 Boundary conditions

	Value	Unit
Anode reactant		
Stoichiometric number	1.1	-
Inlet Temperature	60	°C
Relative Humidity	90	%
Cathode reactant		
Stoichiometric number	1.1	-
Inlet Temperature	60	°C
Relative Humidity	90	%
Operating conditions		
Cell temperature	60	°C
Outlet pressure	101,325	Pa

The SIMPLE (Semi-Implicit Method for Pressure Linked Equation) algorithm which is a numerical iterative procedure was applied to solve these equations. However, the oscillation of the solution may occur due to too-coarse grids and the high value of the conventional term. Therefore, a second-order upwind discretization scheme was applied. The double precision calculation and the algebraic multigrid (AMG) method were used for achieving accurate results and improving the convergence rate, respectively.

3. Results and Discussion

In Fig. 4, the numerical polarization and power curves of two different flow field designs are presented. In the view of the overall performance of PEFC, at the same current density, the new honeycomb flow field design provided a higher cell voltage which also brought the power density to be higher as compared to those of the previous design in the current density range of 0 – 1.2 A cm^{-2}. The difference in the IV performance and the power curves of both flow field designs could be caused by the better uniformity of hydrogen and the oxygen mass fraction distribution provided by the new honeycomb design. The new honeycomb design's higher total number of hexagon cells and smaller hexagon land size allowed the reactant gases reached the shortage area, eliminating the cold and the hot spot areas. The following simulations were conducted to confirm this hypothesis.

Generally, the practical operating voltage is approximately at 0.6 V (around 0.8 A cm^{-2} in this study), which is used to supply and recharge the battery [5] for PEFC stacks. An investigation on the transport behaviors on how the new honeycomb flow field design could be able to outperform the previous design in a better uniformity of the distributions was also conducted and discussed below when current density was 0.8 A cm^{-2}.

The current density distributions on the cathode catalyst and the gas diffusion layer interface of those two flow fields are shown in Fig. 5a and b. To avoid the existence of hot and cold spots which consequently

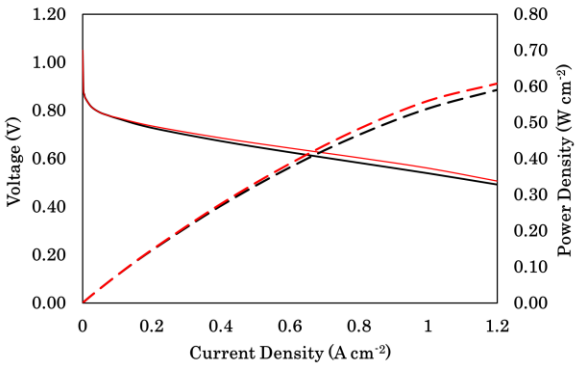

Fig. 4 The IV performance (solid lines) and power curves (dashed lines) of two different flow fields designs. (▬) New honeycomb and (▬) previous honeycomb design.

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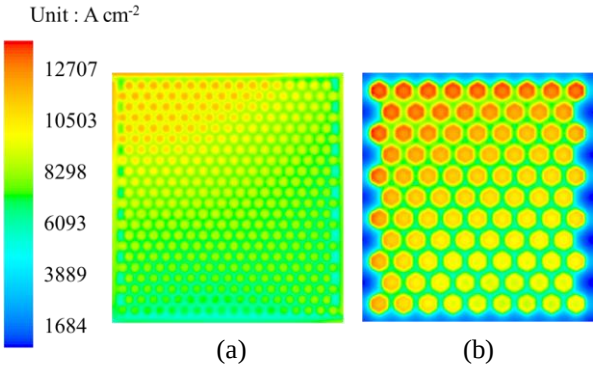


Fig. 5 Current density distribution on the cathode catalyst and the gas diffusion layer interface of a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}

reduce the PEFC life time, a proper flow field design should utilize the cell active area effectively by spreading the electrochemical reactions all over the cell active area and facilitating the reactants to reach the triple-phase boundary easier. In this study, the result revealed that the current density distribution of the new honeycomb design was found to be clearly more uniform as compared with that of the previous design, especially around the border of the cell and the O_2 inlet area. This indicated that the new honeycomb design had an enough potential to minimize cold and hot spots more efficiently. This could imply that, with a smaller hexagon land size and consequently the higher total number hexagon cell, the hydrogen and the oxygen mass fraction distribution of the new honeycomb design should also be more uniform since the current density was evenly produced in every region of the cell. Nevertheless, it should be noted that the rectangular land areas mentioned earlier might aid minimizing the cold spot areas which was a major problem of the previous design.

The hydrogen mass fraction distributions on the anode catalyst and the gas diffusion layer interface are displayed in Fig. 6a and b. As expected, the hydrogen mass fraction distribution of the new honeycomb design was found to be more uniform, with hexagon land size reduction, the new honeycomb design could provide a high efficiency of spreading the reactant gases all over the cell active area so that it could be

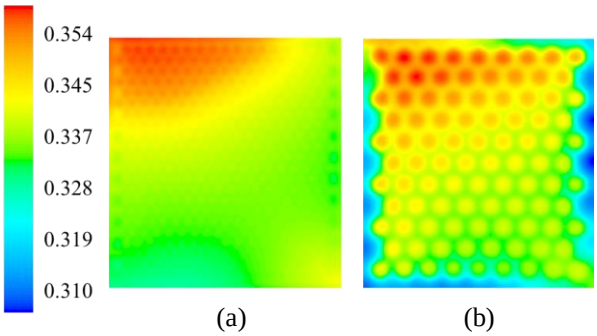


Fig. 6 Hydrogen mass fraction distribution on the anode catalyst and the gas diffusion layer interface of a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}

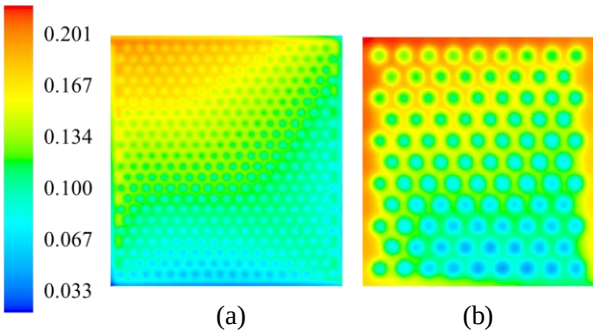
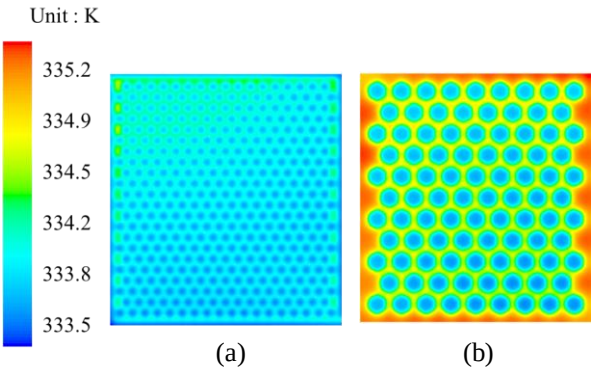


Fig. 7 Oxygen mass fraction distribution on the cathode catalyst and the gas diffusion layer interface of a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}

able to compensate the hydrogen shortages at around the border of the cell founded in the previous design as seen in Fig. 6b. For a small PEFC of 5 cm^2 cell active area, the result was in concurrence with the conventional flow field designs which also revealed that the hydrogen concentration at the inlet was generally lower than that at the outlet [6]. Since the current density and the hydrogen mass fraction concentration for both flow field designs were found to be intense at around the O_2 inlet and the H_2 outlet areas, due to an intense electrochemical reaction, the oxygen mass fraction should also be intense at the same area. This phenomenon was confirmed by the result of oxygen mass fraction distribution presented in Fig. 7 in which high oxygen mass concentration was at around the O_2 inlet area and gradually reduced across the cell area toward the O_2 outlet.

The oxygen mass fraction distributions are displayed in Fig. 7a and b on the cathode catalyst and the gas diffusion layer. With a higher total number hexagon cell by duplicating a smaller hexagon cell, the gas flow channel width was narrower by 0.4 mm which is a half of the previous design. The new design provided not only a uniform distribution of the current density and the hydrogen mass fraction by eliminating the drawbacks of the previous design, but also a uniform oxygen mass fraction distribution, as seen in the contour of Fig. 7a. For both designs, as expected, the oxygen mass fraction concentration was found to be high at around the O_2 inlet area and gradually reduced along the flow channel until the O_2 outlet area. Although the previous honeycomb design showed a higher oxygen mass fraction concentration at around the inlet area and the border of the cell, (see Fig. 6b), the hydrogen was hardly distributed into the same area on the anode side. This made the areas around the inlet area and the border of the cell of the previous honeycomb design inactive areas, also called the stagnant flow areas, which led to the non-uniform current density distribution, as shown in Fig. 5b. On the contrary, the new honeycomb design could be able to eliminate this major problem by providing more

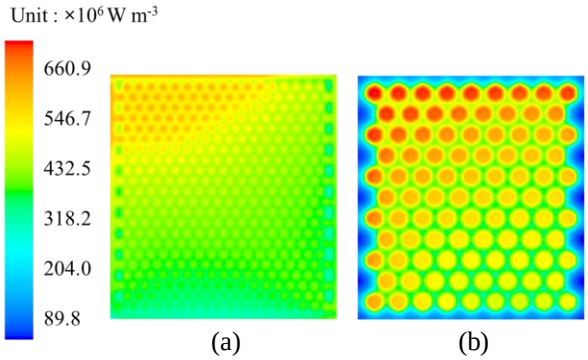


(a) (b)

Fig. 8 Temperature distribution on the cathode membrane and the catalyst interface of a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}

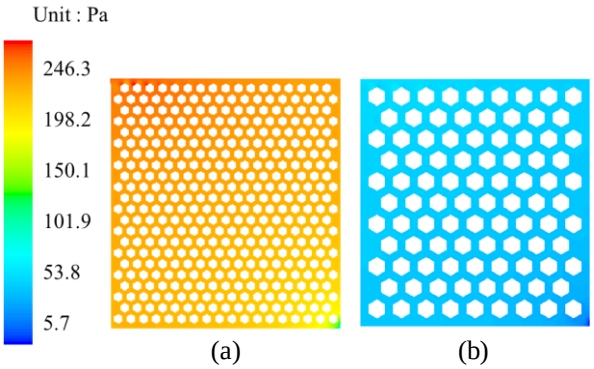
uniform distributions of the current density, the hydrogen and oxygen mass fraction, and hence higher the overall cell voltage and longer cell lifetime.

Fig. 8a and b show the temperature distributions on the cathode membrane and the catalyst interface which indicated that the new honeycomb design provided a clearly more uniform temperature distribution. In addition, the temperature in the region under the land area was lower as compared with that in the region under the gas flow channel for both flow field designs since the heat transferred more efficiently through the land area (graphite) than the void. In a previous study, the result also revealed that there was a higher accumulated heat as compared to the new design since the land areas are not connected and the wider gas flow channel width means more areas of the void, resulting in an accumulated heat throughout the cell area as shown in Fig. 8b. It should be noted that a safety limit, ensuring that the temperature differences throughout the cell area would not affect the MEA durability is approximately 5 K in general [7]. The maximum temperature difference of the new honeycomb design was only 1 K which lower than that of the previous design by 0.5 K. Although, the PEFC with both flow field designs can be operated under the given operating conditions, but it can be concluded that the temperature distribution of the new



(a) (b)

Fig. 9 Reaction heat source distribution on the cathode membrane and the catalyst interface of a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}



(a) (b)

Fig. 10 Pressure drop distribution on the cathode gas diffusion layer and the gas flow channel interface a) new honeycomb and b) previous honeycomb design at 0.8 A cm^{-2}

honeycomb design was more uniform than that of the previous design.

The reaction heat source distributions on the cathode membrane and the catalyst interface are displayed in Fig. 9a and b, to indicate the area at which the electrochemical reaction occurred. The result revealed that the reaction activity generally occurred more under the land areas than that the gas flow channel which was in concurrence with the current density and temperature distributions presented in Fig. 5 and Fig. 8, respectively. The reaction activity of the new honeycomb design was found to be evenly occurred, and therefore provided a more uniform distribution of the temperature throughout the cell active area as compared to the previous design.

The pressure drop distribution of the new honeycomb design was found to be higher than that of the previous design, as shown in Fig. 10a and b. The average pressure drop of the new design was approximately 246 Pa, while it was around 68 Pa in the previous design which is three-time higher due to its narrower gas flow channel width, causing higher the reactant gases friction, and hence the pressure drop.

The overall power production of the new honeycomb design which was calculated and compared to that of the previous honeycomb design, as displayed in Fig. 11. Considering all aspects, the

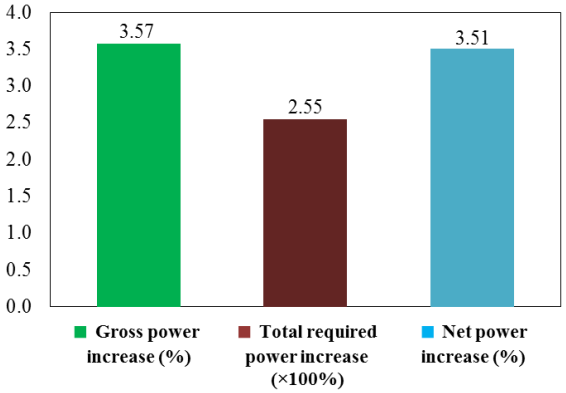


Fig. 11 The overall power production of the new honeycomb design compared to that of the previous honeycomb design.

proposed honeycomb flow field with a smaller hexagon land size seemed to be very promising due to its high performance by providing a higher cell voltage and more uniform distributions as compared to the previous design. It can be observed that the new honeycomb design could be able to provide a significantly higher gross power about 3.57%, even though the required power to compensate the pressure drop was around 255% higher due to its larger pressure drop. Nevertheless the net power obtained from the new honeycomb design was still significantly higher by 3.51%.

However, it should be noted that a proper flow field design should not only satisfy all the uniform distributions, but also be simple so that it would be easy for manufacturing. Therefore, a newer version of the honeycomb flow field design should be further studied for the simplicity of the gas flow channel design while still maintained all of the uniform distribution and also provided a high performance.

4. Conclusion

In this study, the numerical investigation of the new honeycomb design with a smaller hexagon land size and the previous honeycomb design in a 5 cm^2 PEFC MEA was successfully carried out via ANSYS FLUENT software. The results revealed that although the required power which need to compensate the pressure drop in the new honeycomb design was found to be higher by approximately 255% than that of the previous design, but the new honeycomb design still significantly outperformed the previous honeycomb design by providing an enhancement of the net power output approximately by 3.51% and more uniform distributions which consequently led to the longer cell lifetime. This brought the new honeycomb design to be considered as one of the promising flow fields inspired by nature.

5. Acknowledgement

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