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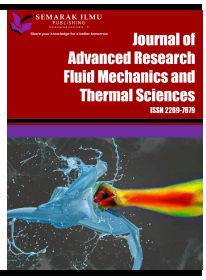

Optimizing Proton Exchange Membrane Fuel Cell Across Varied Inlet and Outlet Dimensions

C.T Aisyah Sarjuni [1], Bee Huah Lim[1,*], Edy Herianto Mailan[1], Masli Irwan Rosli[1,2]

[1] Fuel Cell Institute, Universiti Kebangsaan Malaysia, Bangi, Malaysia
[2] Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, Bangi, Malaysia

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ABSTRACT

A proton exchange membrane fuel cell (PEMFC) is a promising hydrogen energy converter to curb climate change and energy security through its application. The stability of PEMFC performance is related to the reactant uniformity along the flow field of the bipolar plate. An uneven distribution of reactants and products diminishes the overall electrochemical performance by obstructing ion and electron transport over the membrane electrode assembly region. A parallel flow field was employed to study the impact of different cathode inlet/outlet widths on the current density distribution in a PEMFC. Namely simulations A and B for the inlet/outlet width of 8 millimeters and 28 millimeters on the cathode side. Results showed that simulation B generated an even flow with a less drastic change in velocity and an 8078 Pascal lower pressure drop than simulation B. This significantly prevented partial flooding when having a larger inlet/outlet width, enhancing the reactant O2 crossflow across the cathode active area interface. Hence, simulation A attained a 24 % lower average current and power density than simulation B. The improvement in PEMFC performance when using large inlet/outlet width highlights the significance of performance improvement considering the inlet/outlet dimension to obtain the optimum design for future commercialisation.

1. Introduction

The increasing global energy demand has become increasingly concerning especially with the environmental consequences. In order to sustain energy supply for long-term, a multi-pathway strategy is progressively employed. Hydrogen power plays a pivotal role as one of the main energy sources within the planned global energy mix. Following the growth of this industry, PEMFC have been a pivotal alternative, especially for mobile and stationary systems. PEMFC's domination in the fuel cell market, especially in the Asian region, can be attributed to its high power density and relatively more straightforward mechanism, which only needs humidified hydrogen and oxygen to produce power, water, and heat [1–4]. In the process of PEMFC maturity and commercialization,

* *Corresponding author.*
E-mail address: beehuah@ukm.edu.my

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there are still several challenges to be tackled for long-term durability and cost that are economically feasible. The PEMFC is constructed with a membrane electrode assembly (MEA) consisting of a gas diffusion layer (GDL), catalyst layer (CL) and polymer electrolyte membrane (PEM), all of which are sandwiched in between two bipolar plates equipped with flow fields. Optimization of the bipolar plates and gas flow channels is essential to ensure efficient heat and reactant transport throughout the MEA. This will then improve the MEA durability and PEMFC reliability in the long run. Attaining maximum reactant and heat distribution while maintaining efficient water management and optimum power loading remains a critical challenge in PEMFC design. Multiple studies have shown that operating parameters such as the cathode reactant flowrate can improve cell performance by reducing cell starvation region and improve water management. Hassani et al. researched the impact of air flowrate towards the degradation rate of a PEMFC [5]. It was found that higher air flow rate increased water removal which gradually improved the PEMFC performance, allowing more active sites for oxygen reduction reaction. This result aligns with studies from Chen et al., Yang et al. and Nguyen et al. [6–8]. Chen et al. highlighted that as the gas starvation area reduced with increasing air flow rate, the cell power output becomes more stable. Similarly, Yang et al. showed enhanced gas diffusion rate with higher air flow rate. However, they stressed that a specific fuel cell design is limited to a certain flow rate. Exceeding this flowrate will only cause fuel wastage as there will be insignificant improvement in cell performance. Nguyen et al. also showed that the cathode reactant crossover through the PEM increases with higher flow rate. This raises the concentration of oxygen diffusing through the membrane towards the anode side. When operated in a multiple-cell stack, González et al. showed similar trend in performance increase with greater cathode flow rate especially at higher current densities [9]. Like Yang et al., they highlighted that oversupply of cathode flow rate may cause membrane dehydration with the increased water removal. Another way to enhance the reactant transport in a PEMFC is by optimizing the inlet/outlet configurations. Changes to this parameter may alter the pressure and velocity created by the moving fluid mass, which is the basis of the two-phase fluid homogeneity required to prevent dehydration, flooding and performance loss. Several works have proven the effect of having multiple inlet/outlets in a single flow field [10–13]. The drainage capability and pressure drop are easily manipulated depending on the location and number of inlet/outlets. These changes result in a higher reactant concentration at the CL- GDL interface due to the optimized humidity levels. For instance, Wang et al. proposed a combined serpentine and interdigitated flow field, which had three inlets and one outlet [11]. A single serpentine flow field with one inlet/outlet showed improved water drainage while reducing up to 87% of pressure drop, leading to a 13% higher peak power density. Zhang et al. investigated the impact of having additional outlet in different locations within a parallel flow field [12]. The additional outlet raised the oxygen concentration especially towards the outlet region. Water saturation was significantly reduced when the additional outlet was placed in the middle of the flow field. Nonetheless, these studies utilise the same inlet/outlet dimensions. The inlet/outlet dimensions also affect the mass transport throughout the flow field and eventually towards the MEA interfaces as well [14– 18]. Results generally showed that a smaller inlet/outlet or channel dimensions promote higher forced convection on the reactant gases, as a smaller area promotes higher fluid velocity. This increases the mass transfer rate and under-land cross flow, raising the performance through a higher reaction rate. Smaller channels contribute to a higher pressure, which could lessen the net power density. Liu et al. implemented micro-distributors of three different widths in between the distribution zone and channel inlets of a parallel flow field [15]. As the width of the micro-distributor inlet decreases, higher fluid velocity is generated, thus increasing water removal at the cathode GDL. Zhang et al. showed that smaller channel width

increases the overall current density, but the cell reaches the concentration loss phase faster than a wider channel width [16]. Considering the fluid entrance and exit within different channel dimensions affect the mass transport, studies that consider the design of distribution zone within a flow field may reveal a different outcome. This is because fluid must be dispersed from the inlet/outlet towards the distribution zone before travelling through the flow channels; in contrast to conventional channels with direct access from inlet/outlet to the flow channels. The emergence of newer studies employing flow fields with distribution zones further emphasises the need to investigate the effects of inlet/outlet dimensions especially for flow fields with a distribution zone [19,20]. For example, Zhang et al. use a wider cathode inlet/outlet dimension than the anode side to cater for the heavier density of oxygen reactant gas [19].

Hence, this paper aims to fill the research gap by conducting a computational fluid dynamics (CFD) simulation for two single-stack PEMFCs with parallel flow fields. Both stacks differ only in terms of the cathode inlet/outlet dimensions, while the anode inlet/outlet dimensions remain the same. The performance of both stacks was compared through the fluid flow, mass transport and electrochemical characteristics via graphical and numerical data. This research will aid in the design engineering of flow field patterns for further optimisation of PEMFCs in future works. The results will also provide insight into the correlation between fluid flow rate and fuel cell design towards PEMFC performance.

2. Methods

2.1 Computational Domain

The three-dimensional (3-D) simulation study was conducted using the commercial software ANSYS Fluent R2 2022. To highlight the impact of inlet/outlet dimensions, a well-researched design like parallel flow field is used. The base model for the flow field was taken from a previous study [21], which was inspired by several research from Zhang et al. [19,20]. In contrast to Zhang et al., this research considers the distribution zone as a reaction area together with the parallel channels. Fig. 1 shows the computational domain of the single-cell PEMFC simulation models. Two configuration models with different cathode inlet/outlet dimensions were employed. The inlet width for the cathode flow field in simulation A is 8 millimeters, whereas in simulation B is 28 millimeters. For the anode side, a single inlet/outlet width of 8 millimeters is used for both simulations. The total active area is 27 square centimeters with a channel and rib cross-sectional area of 1 square millimeter. All anode and cathode flow fields are identical with 17 channels each.

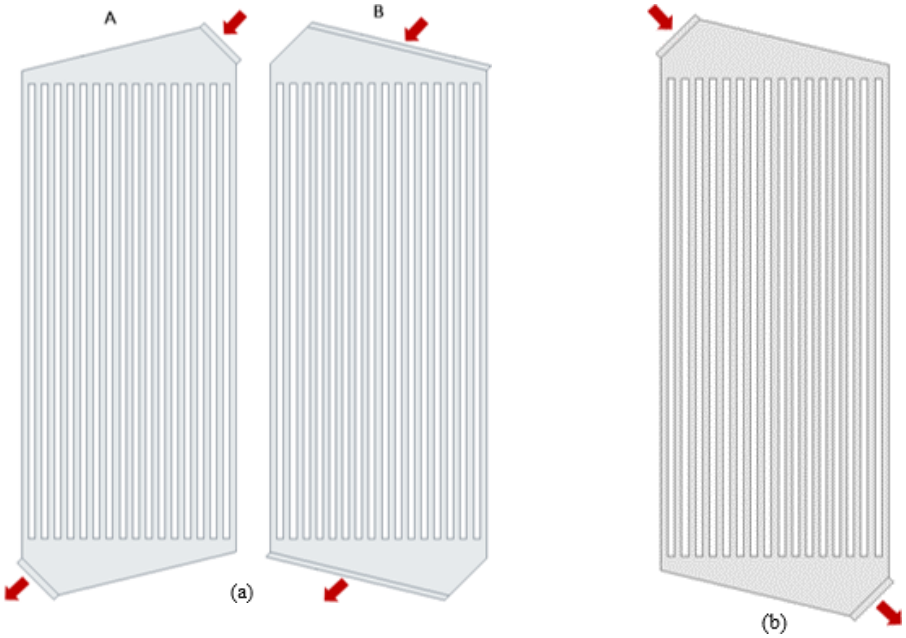

Fig. 1. Flow field used for simulation A and B of (a) cathode side, (b) anode side

The construction of model geometry is followed by defining the boundary conditions for each model domain to prepare for the computational fluid dynamics (CFD) simulation. The model parameters are defined in Table 1. The simulation model was solved using the Semi-Implicit Method for Pressure-linked Linked Equations (SIMPLE) algorithm for velocity-pressure coupling with convergence criteria of 10-6 for all residuals. The overall Fluent setup was carried out based on the assumptions listed below:

- Two-phase flow model with laminar flow.
- Steady-state reaction.
- Gravity effect is neglected.
- All porous media are isotropic materials.

Table 1
Model Parameters

Parameter	Value
Temperature (K)	343
Pressure (atm)	1
Operating Voltage (V)	0.6
Anode Stoichiometric Ratio	5
Cathode Stoichiometric Ratio	10
GDL Thickness (µm)	35
CL Thickness (µm)	1
PEM Thickness (µm)	5

2.2 Governing Equations

Based on the assumption above, the governing equations to model this simulation research can be simplified according to the equations below:

Mass conservation equation:

$$\nabla.(\varepsilon\rho\vec{u}) = S_m \tag{1}$$

Where ε is porosity, ρ is the density, $\vec{u}$ is the fluid velocity and S_m is the quality source term.

Momentum conservation equation:

$$\frac{1}{\varepsilon^2}\nabla.(\rho\vec{u}\mu) = -\nabla p + \frac{1}{\varepsilon}\nabla\cdot(\mu\nabla\vec{u}) + S_u \tag{2}$$

Where p is pressure and μ is the fluid viscosity. S_u is the momentum source term which describes the physical characteristics of a porous media. This source term is also related to permeability in the equation:

$$S_u = -\mu_{eff}\varepsilon^2\, u/_k \tag{3}$$

Energy equation:

$$\nabla\cdot\left(\rho C_p\varepsilon\vec{u}T = \nabla\cdot(k^{eff}\nabla T) + S_T\right) \tag{4}$$

Where T, C_p and S_T represents temperature, specific heat capacity and energy source term respectively. Meanwhile, k^{eff} is the effective thermal conductivity which can be expressed further in equation (5), noting that k^f and k^s are the thermal conductivity of fluid and solid respectively.

$$k^{eff} = \varepsilon k^f + (1-\varepsilon)k^s \tag{5}$$

2.2 Grid Independence Test & Model Validation

A grid independence test (GIT) ensures that the simulation run is independent of the mesh size with maximum result accuracy. It is also critical to identify the optimum mesh size for time-efficient simulation. The test was done using the design of simulation A at three different mesh sizes, where the number of divisions was increased from 4, 6, and 8 at the channel, CL and PEM layers. Fig. 2 shows that employing layer division of 6 is sufficient for the model to generate minimal error of 0.35%. As for model validation, the result from simulation B is compared with the reference study by Zhang et al which was operated at similar operating conditions and flow field dimensions [20]. It was found that the current density at 0.65V differs by 5%, thus validating the accuracy of the simulation model.

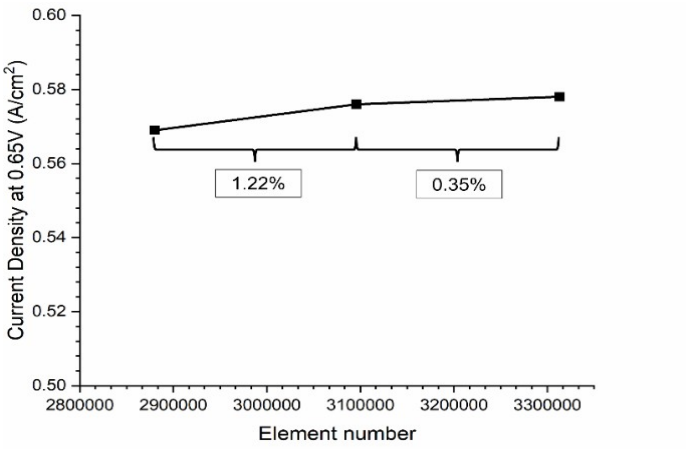

Fig. 2. Current density generation with different element number for grid independence test at 0.65V

3. Results

The simulated data were assessed through the simulation contours and numerical values taken at the appropriate interfaces according to the parameter assessed. The effects of varying cathode inlet dimensions and maintaining the anode inlet dimension at the same flow rate toward cell performance were observed and discussed below.

Fig. 3 shows the velocity magnitude of simulations A and B in between the interface of the channel and GDL. The fluid velocity range in Fig. 3(a) of the anode flow field in both simulations was similar at below 0.5 meters per second, due to the same inlet/outlet area. In contrast, the difference in fluid flow rate shown in Fig. 3(b) was drastically different for the cathode side, where simulation A produced 86% higher peak fluid velocity than simulation B. There is a 50% decrease in cathode fluid velocity from 38 meters per second to 19 meters per second for simulation A. As a result, the cathode pressure drop reached 8773 pascal and 695 pascal for simulations A and B, respectively. This can be easily justified through Bernoulli's principle, where a change in velocity has an inverse effect on pressure [22]. Therefore, the higher velocity gradient acquired by simulation A generated a more considerable pressure drop than simulation B. Kinetic energy increases because of the higher fluid velocity, thus causing pressure to drop to balance the energy change for mass conservation. Moreover, a streamline of high-velocity fluid was formed through the smaller inlet area and was forced to disperse through the multiple-channel inlets. Instead of dispersing evenly, a dead- end area was produced in the last channel due to the minimal presence of fluid flow. The impact of this phenomenon can be discussed further by relating them with the reactant molar concentrations and resulting electrochemical output.

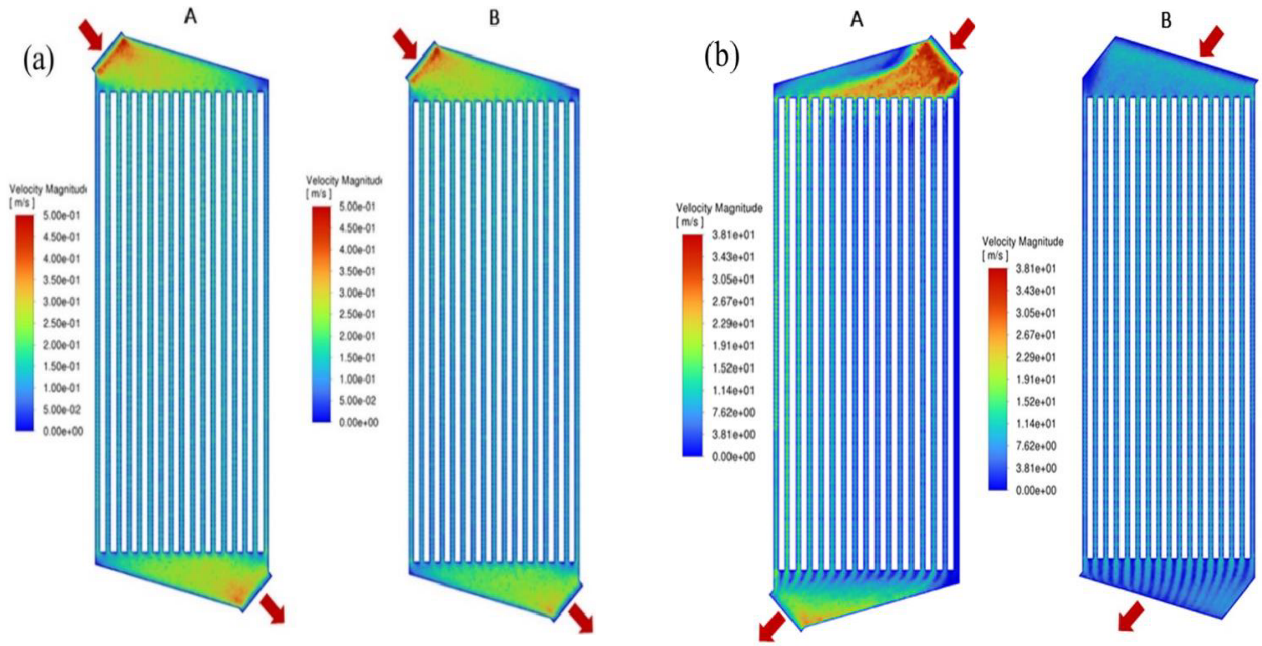

Fig. 3. Velocity distribution contour of simulation A and B at the channel-GDL layer (a) cathode side, (b) anode side

Since both simulations' anode inlet/outlet had the same dimensions, the hydrogen reactant and water product in Fig. 4 (a) and (b) had similar distribution patterns. The hydrogen consumption was noticeably faster in simulation B compared to simulation A, resulting in more water concentration in the channels of simulation B. Similar results were recorded at the cathode side in Fig. 5, whereby simulation B showed greater oxygen consumption than simulation A in Fig. 5(a). The minimal change in concentration gradient may indicate an oversupply of oxygen reactant at the cathode side, particularly in simulation A. Since the oxygen concentration is lower in simulation B, the high entrance velocity initiated by the smaller inlet width of simulation A could contribute to the excessive reactant surplus. The slower fluid velocity in simulation B allowed more oxygen flow control. Thus, the uniform fluid flow generated an even dispersion of oxygen reactant throughout the flow field. Meanwhile, partial flooding occurred in the last channel of simulation A, which is the same dead-end region seen in Fig. 5(b). The accumulation of excess water is detrimental to the performance of PEMFC as the water molecules may reduce the MEA layers' porosity, decreasing the permeability of reactants. The reduction in the available active surface area for reactant dissociation at the CL diminishes the overall cell performance due to concentration loss [23–25]. This is proven through the lower current density distribution recorded by simulation A in comparison to simulation B as seen in Fig. 6. This occurrence proves the impact of exceeding flow rate limitation for a specific PEMFC design [5–9]. The nature of design A may require a lower air stoichiometric ratio for optimised performance. The resulting power density at 0.6 volts came around to 0.34 watts per square centimeter and 0.44 watts per square centimeter for simulations A and B respectively. Moreover, the high-pressure drop generated by simulation A contributes to parasitic power, further reducing the net power output.

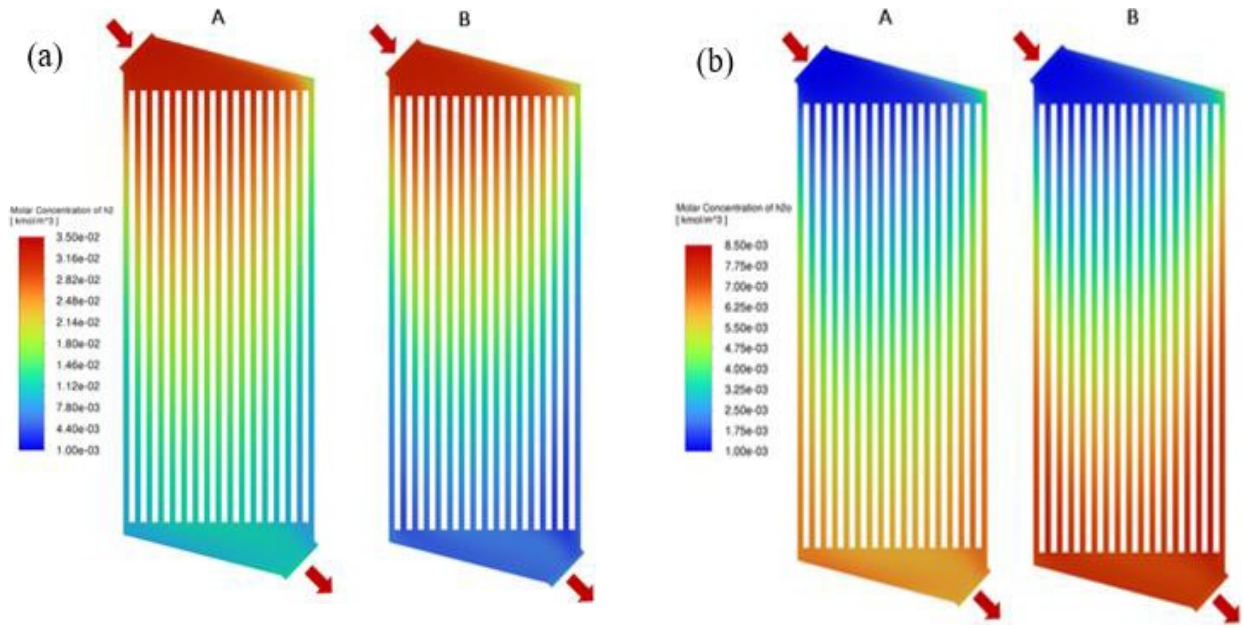

Fig. 4. Molar concentration at the channel-GDL interface for anode of simulation A and B (a) Hydrogen, (b) Water

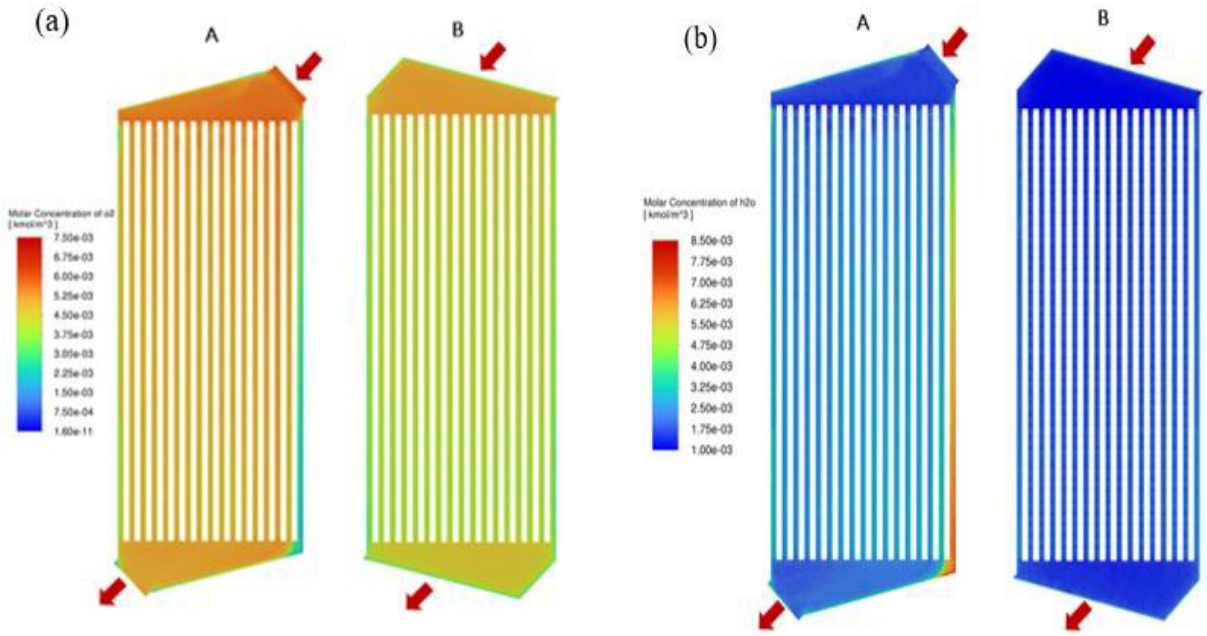

Fig. 5. Molar concentration at the channel-GDL interface for cathode of simulation A and B (a) Oxygen, (b) Water

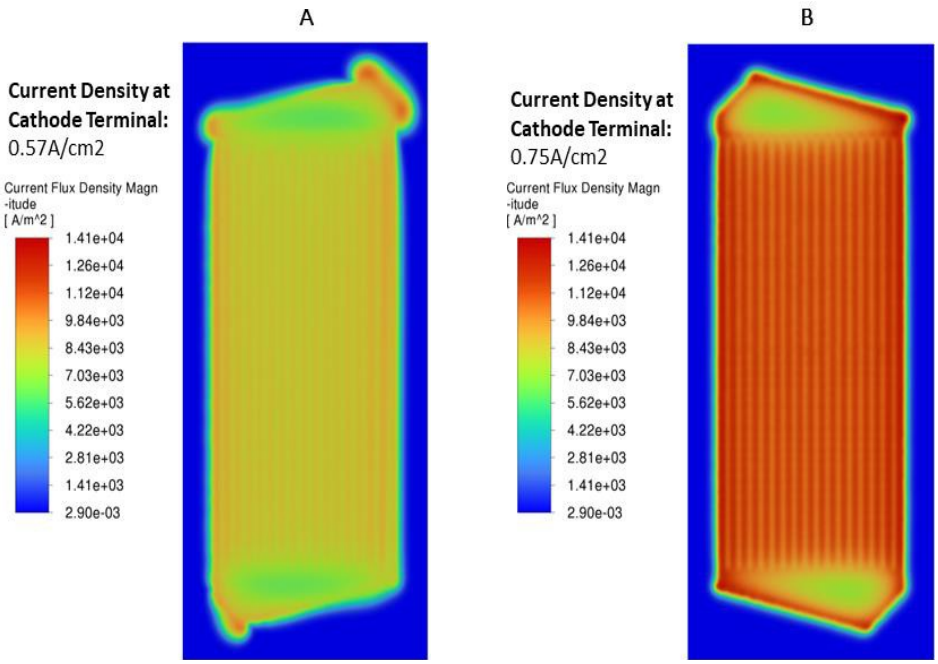

Fig. 6. Current distribution contour of simulations A and B at the CL-PEM interface

The industrial operation of PEMFC often calls for multiple cell stacks to achieve higher power generation. The mass transport of reactants is much more complicated due to the more significant number of layers that reactants must diffuse. Thus, the effect of partial flooding and lower current density generated by simulation A may be more apparent when constructed in a stack [26]. Therefore, the simulation results showed that employing an optimal flow field design is crucial as it can manipulate the fluid flow characteristics. It also proved the importance of considering the inlet/outlet dimension when designing a flow field, especially when used with higher flow rate. Uneven and uncontrolled fluid flow may trigger adverse effects such as flooding or dehydration that can diminish the electrochemical properties of the MEA layers.

4. Conclusion

This paper investigated the performance of two single-cell PEMFC with different inlet widths under the same operating conditions. Results show that although the anode side of simulations A and B had similar fluid velocity ranges, the resulting pressure difference generated varying hydrogen and water concentrations at the channel-GDL interface. Hydrogen reactant was consumed faster in simulation B than in simulation A, which naturally caused the excess water vapor to fill the consumed spaces downwards the channel. Water condensation can be mitigated by increasing the hydrogen supply rate to raise its dispersion area throughout the anode flow field. Meanwhile, simulation A on the cathode side exhibited poorer fluid flow homogeneity compared to simulation B, which formed partial flooding at the last channel. The higher water concentration in Simulation A ultimately led to a 24 percent lower average current and power density than in simulation B. The high-pressure drop generated by simulation A will also reduce the net power output, further reducing cell efficiency. In conclusion, the study showed the importance of considering the inlet/outlet conditions to acquire an optimum flow field simulation to maximize the active contact surface area and mass transport

efficiency. Its effect will be much more evident in multiple-stacked PEMFCs, which will be an exciting research prospect on the impact of inlet/outlet dimensions.

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