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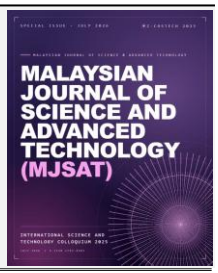

Effect of Different Shapes and Sizes of Planar Cell on the Performance of Proton Ceramic Fuel Cell: A Preliminary Study Via Computational Fluid Dynamics

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ABSTRACT

Proton ceramic fuel cell (PCFC) that operates at intermediate temperature (400°C – 700°C) has been introduced as an alternative to conventional solid oxide fuel cell (SOFC). There are numerous theoretical studies using computational fluid dynamics (CFD) have been done for studying the performance of PCFC. However, the study is limited to only single-channel rectangular PCFC and tubular PCFC with limited literature that covers the effects of cell geometry and size on the performance of PCFC. Thus, this study presents a novel comparative CFD simulation that compare the performance of single channel rectangular PCFC (A_{R1} = 5 mm x 27 mm and A_{R2} = 5 mm x 100 mm) and planar button PCFC with two different sizes in diameter which are 13 mm (A_{B1} = 133mm^2) and 25 mm (A_{B2} = 491 mm^2) in terms of fuel utilisation efficiency and power density operating at 700°C under 60% hydrogen fuel . Both models are designed with nearly identical active areas of 135 mm^2 and 500 mm^2 for a fair performance comparison by using Ansys CFD software. The larger size of single-channel rectangular cell (A_{R2} = 500 mm^2) demonstrates the highest fuel utilisation efficiency of 71.2% while planar button cell (A_{B2} = 491 mm^2) achieve 41.2% efficiency. The highest value of peak power density demonstrates by smaller size of single-channel rectangular cell (A_{R1} = 135 mm^2) with 0.54 W/cm^2 at 0.5V compared to the planar button cell (A_{B1} = 133mm^2) that achieve 0.52 W/cm^2 at 0.5V. Larger rectangular cells increase fuel utilisation efficiency, while smaller geometries promote higher peak power density, demonstrating a clear geometry-performance trade-off in planar PCFC design.

1. INTRODUCTION

A solid oxide fuel cell (SOFC) is a green technology that directly converts chemical energy into electrical power. Compared to traditional thermal power plant, this device has attracted a lot of interest due to its superior conversion efficiency and reduced carbon emissions [1]. However, due to its high operating temperature (800°C – 1000°C), it can cause many implications for the cell. To overcome the problem of conventional SOFC without affecting the efficiency of the cell, instead of using oxygen ions (O^{2-}), proton (H^+) is used as the charge carrier. Proton-conducting SOFC (H^+-SOFC), also known as proton ceramic fuel cell (PCFC), is more promising in terms of attaining good performance at moderate to low temperatures.

The study of the PCFCs performance mainly focuses on a few elements, such as current density, power density, conversion efficiency, and flow distribution of the fuel cell. Other than that, there are also studies on the model and the geometries of PCFCs, which can influence the performance of the fuel cell. These properties can be studied more effectively and affordably using Computational Fluid Dynamics (CFD) than through physical experimentation [2]. Several researchers

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have utilised CFD to study the performance of PCFC with various geometries, such as single-channel rectangular cell [3] and stack cell [4]. The study of CFD and the simulation of fluid dynamics can be done using software such as ANSYS.

This study investigates the effect of different shapes (button and single-channel rectangular) and sizes (135 mm^2 and 500 mm^2) of planar PCFCs on their performance, focusing on fuel utilisation efficiency and power density via computational fluid dynamics. A lot of experiments for BCZY-based PCFC in button cell shape were done by [5] and [6]. However, based on the available literature, the comparison for both button cell shape and single-channel rectangular shape PCFC using a CFD model has not been reported. Such comparison study is critical because engineering design is about optimisation and trade-offs. By understanding how geometry affecting the performance of PCFC will help engineers making decisions when designing scalable and reliable PCFC systems before physical fabrication.

In this study, the performance of PCFCs is simulated using CFD software, ANSYS R2, with two different shapes at different sizes while maintaining similar active areas. Through CFD approach, it allows the evaluation of electrochemical performance and fuel flow without the time constraints and complexity of physical experiments.

2. METHODOLOGY

The CFD software can be divided into three main processes, which are pre-processing, solver, and post-processing. The creation of the geometry for each PCFC model with different sizes was done in a pre-processing step using the Design Modeler. This includes the mesh generation, material selection, as well as the cell zones and boundary conditions. Using the Ansys FLUENT, the parameter input and solution were set up in the solver process based on past studies. The results of the simulation for all models are thus shown in the post-processing and then visualised.

2.1 Pre-processing

The first step of CFD is pre-processing, where the user is required to insert any important input parameters of the model used. The input parameters that are needed for the CFD modelling pre-processing step are the geometry of the model, the setup mesh or grid, the setup of the cell's boundary conditions, and the material selection. The geometry configuration that was chosen for this study are single-channel rectangular PCFC and planar button cell PCFC. The cell size for the PCFC geometry is changed throughout the experiment, while the parameters and the boundary conditions of the cells were kept constant.

The component layers of the planar PCFCs were still the same even though the shapes were differed. The current collector, flow channel, gas diffusion layer, and catalyst layer for both cathode and anode, and also the electrolyte membrane were the important components or regions that must be included for both models in the CFD modelling. The cell geometry parameters were inserted using the Design Modeler of Ansys, FLUENT, and were drawn. Planar Button PCFC with the geometry size of 13 mm (A_{B1} = 133 mm^2) and 25 mm (A_{B2} = 491 mm^2) in diameter were chosen for the input parameters while for the single-channel rectangular PCFC, geometry size of 27 mm (A_{R1} = 135mm^2) and 100 mm (A_{R2} = 500 mm^2) in length with the width of 5 mm were chosen for the cell length. Figures 1 and 2 show the button cell PCFC components and single-channel rectangular PCFC components, respectively.

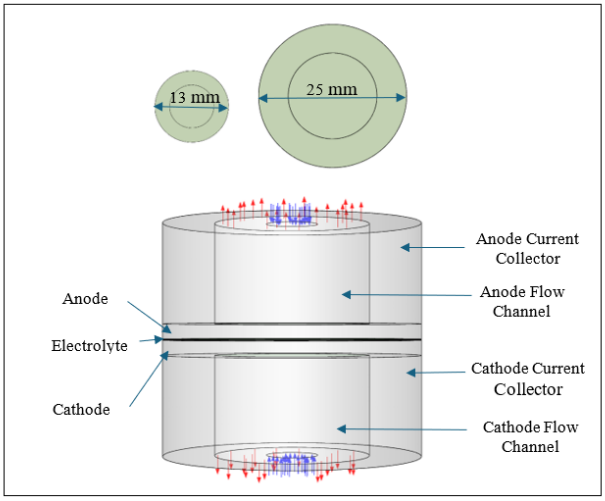

Fig. 1. Button Cell PCFC Components

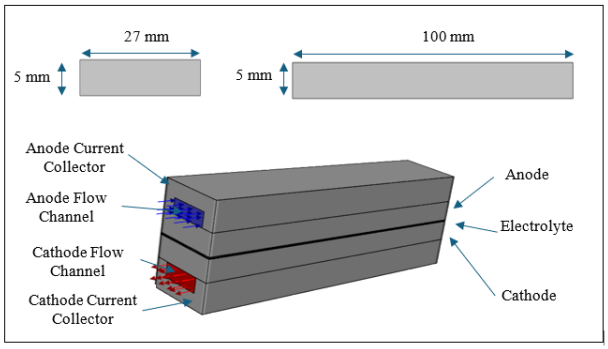

Fig. 2. Single Channel Rectangular PCFC Components

After the 3D geometry for both models with different sizes was drawn, meshing was then generated for all models. Meshing is an important part of CFD pre-processing, which involves breaking up complex geometrical components that can be used to discretise a domain [7]. This will form the foundation of the governing equations of the simulation. The accuracy of the calculations is impacted by the mesh density. More accurate results are obtained as the mesh density increases. Table 1 shows the mesh size for all PCFC models.

Table 1. PCFCs Mesh Size

PCFC Model	Size (mm)	Active Bodies	Elements	Element Size (mm)
Button Cell	13	9	52582	0.4
	25	9	92953	0.5
Single Channel Rectangular	5 x 27	11	46980	0.3
	5 x 100	11	174348	0.3

2.2 Solver

Solver is the fundamental process in CFD simulation, where it involves numerically solving the governing equations of fluid flow to determine the flow behaviour, temperature,

pressure, and other variables [8]. The species mass fraction and power density of the button cell and single-channel rectangular PCFCs with various sizes were modelled and simulated by using hydrogen with a concentration of 60%. The species that were selected for this simulation are hydrogen, oxygen, and water. The hydrogen mass fraction at the anode side is 0.6 (60%) while the oxygen mass fraction is zero with the water percentage held constant at 0.03. On the cathode side, the hydrogen and water mass fraction is zero, while oxygen is 1.0 as presented in Table 2. The simulation is in steady state with laminar flow regime. The porous electrodes are assumed to be isotropic. Parameters of the models for the simulation are taken from [9] and are tabulated in Table 3. All models were simulated using 60% hydrogen each with ten different voltages (0.1V to 1.0V) for 200 iterations.

Table 2. Species Mass Fractions

Inlet	Species mass fraction		
	Hydrogen	Oxygen	Water
Anode	0.6	0	0.03
Cathode	0	1.0	0

Table 3. Parameters of the Models Using Experimental Data

Parameter	Value
Operating temperature	700°C
Operating pressure	101235 Pa
Anode fuel	H_2, H_2O
Cathode fuel	O_2
Porous electrode porosity	
Anode	0.26
Cathode	0.3
TPB layer catalyst porosity	
Anode	0.26
Cathode	0.26
Reference current density	
Anode	4000 A/m^2
Cathode	1300 A/m^2

2.3 Post-processing

Post-processing is the final step of CFD simulation, where the solver's numerical data is converted into useful analysis, visualisation, and outcomes. This allows the user to analyse and interpret the results of the simulation. Several visualization tools were used in Ansys FLUENT, such as surface and contour plots in either 2D or 3D. The distribution of the mass species across each of the PCFC models were analysed by using this plot. The current density's results obtained from the simulations was shown on the console tab. The power density of the cell can be determined by the results of the current density after the simulations of each cell. The value of the mass flow rate of hydrogen was shown from the surface integrals section and is used to calculate the fuel utilisation efficiency using Equation [1].

$$\mu = \frac{\dot{m}_{H_2,in} - \dot{m}_{H_2,out}}{\dot{m}_{H_2,in}} \times 100\% \quad (1)$$

where,
μ = Fuel utilization efficiency
$\dot{m}_{H_2,in}$ = Hydrogen inlet flow rate
$\dot{m}_{H_2,out}$ = Hydrogen outlet flow rate

3. RESULTS AND DISCUSSION

3.1 Fuel Utilisation Efficiency

Fuel utilization or fuel efficiency describe how effectively a fuel cell converts its fuel into electrical energy rather than becoming waste. This parameter is important for determining the fuel cell performance and economic viability. In practice, not all hydrogen fuel is consumed, and some of it flows through without reacting [10]. The hydrogen flow rate values for each PCFC model simulated at 0.8V are presented in Table 4, along with the fuel utilization efficiency calculated using Equation [1].

Table 4. Hydrogen Mass Flow Rate and Fuel Utilisation Efficiency

PCFC Model	Size, (mm)	Area. (mm^2)	Hydrogen Inlet Flow Rate, $\dot{m}_{H_2,in}$, (kg/s)	Hydrogen Outlet Flow Rate, $\dot{m}_{H_2,out}$, (kg/s)	Fuel Utilization Efficiency, μ, (%)
Button Cell	13	133	6×10^{-8}	4.639×10^{-8}	22.7
	25	491	6×10^{-8}	3.528×10^{-8}	41.2
Single Channel Rectangular	5 x 27	135	6×10^{-8}	4.401×10^{-8}	26.7
	5 x 100	500	6×10^{-8}	1.729×10^{-8}	71.2

The simulation results show that a single-channel rectangular PCFC with 100 mm of length (AR2 = 500 mm2) has the highest fuel utilisation efficiency, at 71.2%. When the identical model of PCFC is compared with different sizes, those with a larger surface area demonstrate better fuel efficiency than their smaller counterparts. Additionally, single-channel rectangular PCFC models exhibit higher fuel utilization efficiency compared to planar button cell PCFC models, provided their sizes are almost similar. For better visualisation of the hydrogen consumption, the contour of the hydrogen mass fraction for each PCFC model is shown in Figures 3 and 4. The fuel utilisation efficiency of PCFC is highly dependent on hydrogen flows and consumption, as seen in the contour of both button cells and single-channel rectangular cells.

The larger size of the single-channel rectangular cell (A_{R2} = 500 mm^2) and button cell (A_{B2} = 491 mm^2) exhibits the highest value of fuel utilisation efficiency of 71.2% and 41.2% respectively. This may be due to the uniform hydrogen distribution showed by the larger size which can optimize electrochemical reactions across the cell active region, thus potentially improving total efficiency. Fuel utilisation increased due to the higher electrochemical conversion of the supplied fuel [11]. Higher fuel utilisation means that more fuel is fully oxidised, which can generate more electrons and current, thus improving system efficiency [12]. While both models have their advantages, the single-channel rectangular cell model is more efficient in fuel utilization due to its directed flow distribution, resulting in minimal fuel wastage. This behaviour may be due to the unidirectional flow arrangement, which increases reactant residence time and promotes more effective

electrochemical conversion than radial diffusion in button type cell.

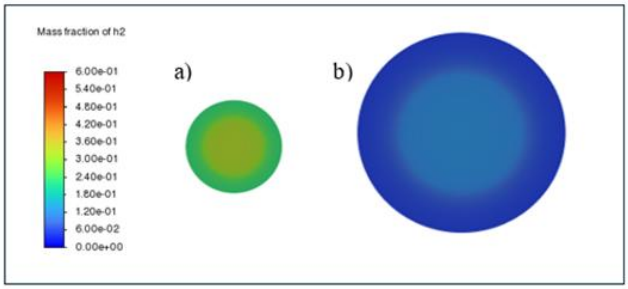

Fig. 3. Contour of Hydrogen Mass Fraction of a) 13 mm Diameter and b) 25 mm Diameter Button Cell at 0.8V

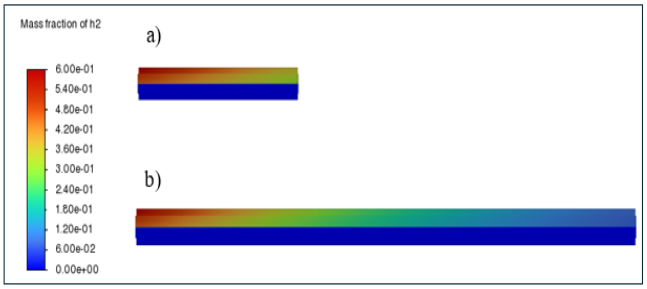

Fig. 4. Contour of Hydrogen Mass Fraction of a) 27 mm Length and b) 100 mm Length Single Channel Rectangular Cell at 0.8V

3.2 Power Density and Polarisation Curve

Power density in fuel cells refers to the amount of electrical power generated per unit area of the electrode, and it is usually expressed in watts per square centimetre, W/cm^2 [13]. It is an important parameter that indicates how efficiently a cell generates electrical energy from a chemical reaction. In this simulation, the power density, P, of the PCFC models is determined from the product of voltage, V (V), and the average current density, I-average (A/cm^2).

The polarisation curve of a fuel cell is a graphical representation of the relationship between cell voltage used and the current density produced as a tool to evaluate the performance of the fuel cell. The polarisation curve is also referred to as the electrochemical characterisation of a fuel cell (V-I and P-I curve) [14]. For PCFCs that operate at intermediate temperature, the polarisation curve indicates the efficiency of proton conduction through the ceramic electrolyte and electrode reactions. By analysing the polarisation curve, researchers can identify the performance bottlenecks and optimize materials and operating conditions to improve the efficiency of the fuel cell. The result of the power density of button cells is shown in Figures 5 and 6, while single-channel rectangular cells are in Figures 7 and 8.

The power density of PCFCs is controlled by both structural design and operating voltage. The smaller size of both models exhibits higher peak power density than their respective larger sizes. [11] mentioned that power density is reduced as the electroactive area of the cell is increased.

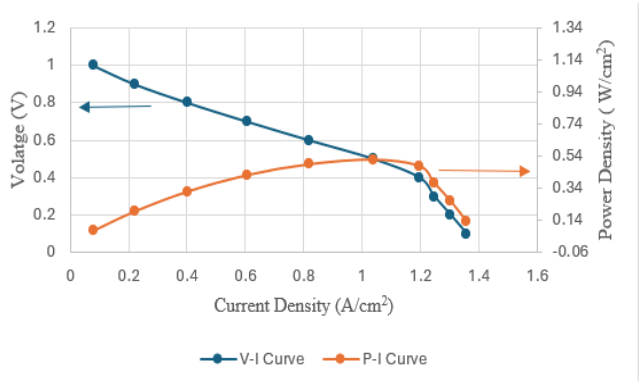

Fig. 5. Polarisation Curve of 13 mm Button Cell PCFC at T=700°C

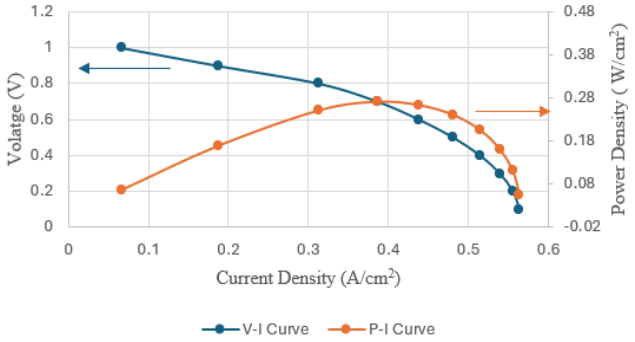

Fig. 6. Polarisation Curve of 25 mm Button Cell PCFC at T=700°C

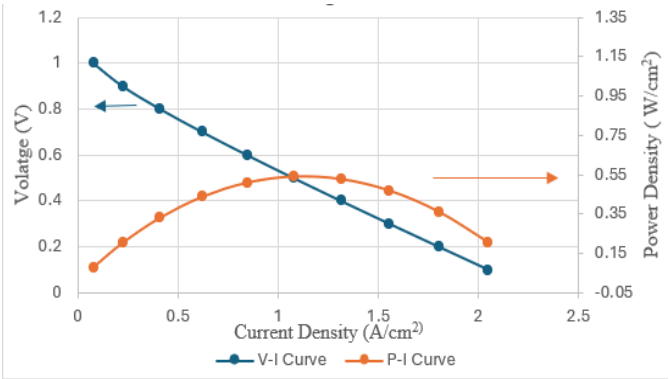

Fig. 7. Polarisation Curve of 27 mm Single Channel Rectangular PCFC at T=700°C

The A_{R1} =135 mm^2 single channel rectangular cell exhibits the highest power density, reaching 0.54 W/cm^2 at 0.5V, while A_{B1} = 133 mm^2 button cell shows slightly lower peak power density of 0.52 W/cm^2 at 0.5V. These results are comparable with the experimental values done [15] and [16] that achieve peak power density of 0.56 W/cm^2 at 600°C for a single-channel rectangular cell and 0.53 W/cm^2 at 650°C for a button cell, respectively.

The larger size for both models shows significantly lower peak power density of 0.44 W/cm^2 (A_{R2} = 500 mm^2 single channel rectangular cell) and 0.27 W/cm^2 (A_{B2} = 491 mm^2 button cell). This suggests that larger area cells may maintain high output but could experience slight performance loss due to resistance increasing or gas transport constraints. Parasitic

electron current in an electrolyte can lower the power density due to nonelectrochemical fuel oxidation [17]. Overall, a single-channel rectangular models produce higher peak power compared to a button cell; meanwhile, the smaller size of both PCFC geometries produces higher peak power density than the larger size cell.

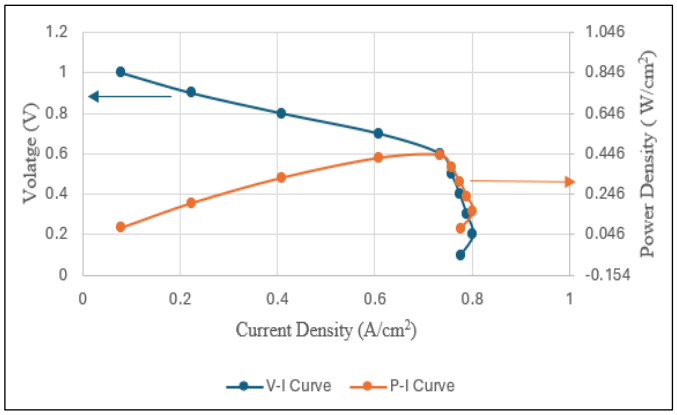

Fig. 8. Polarisation Curve of 100 mm Single Channel Rectangular PCFC at T=700°C

4. CONCLUSION

This study aimed to identify the impact of PCFC geometries on power density and evaluate fuel utilization efficiency. With the help of Ansys FLUENT, single-channel rectangular cells have been found to have better efficiency in terms of fuel utilisation. This is due to their directed hydrogen flow, which encourages controlled consumption and minimises fuel waste; meanwhile, planar button cells demonstrate uniform distribution but less precise flow control. The smaller size of geometries shows the highest peak power density compared to the larger size cells. The single-channel rectangular cell has been found to exhibit higher peak power density than the button cell. The study also found that higher fuel utilisation efficiency leads to lower peak power density. Future study will continue this CFD framework to multi-channel or stack configurations with experimental validation to confirm the observed geometry-performance relationships.

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