

## ORIGINAL RESEARCH ARTICLE

# Enhancing performance of planar structure single unit 800 °C O<sup>2</sup>-SOFC at atmospheric pressure: A numerical modeling approach for electric power production

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## ABSTRACT

Solid oxide fuel cells generate electricity with high electrical efficiency and flexibility in fuel use without emitting pollutants, such as carbon dioxide, nitrogen oxides, sulfur oxides and particulates. Nevertheless, they still face several obstacles and challenges that pose problems and questions driving researchers to find solutions. Numerical simulation is a key tool for integrating various physical fields, including charge dynamics, electrochemical pathways, chemical species kinetics, fluid flow, and energy transformations. The Butler-Volmer equation, in its various forms and approximations, is the most widely used equation for relating electrochemical pathways to current density in solid oxide fuel cell modeling. The main objective of this research is to model and simulate a high-temperature solid oxide fuel cell at atmospheric pressure, in order to test the effect of changing some properties values on the electrical power density produced. The results obtained revealed several techniques for enhancing the fuel cell performance, by improving the physical behaviors appropriate to each property on the corresponding side. It was found that fuel cell performance improves with increasing values of porosity rate, exchange current density, and pressure drop, and with decreasing both cell length and electrolyte thickness. Furthermore, since the electrolyte's conductivity class is oxygen ion carrier, the effect of parameters at the cathode side was more significant compared to the anode side. The results of this research are consistent with well-documented theories, and it is usable for developing other numerical models.

**Keywords:** solid oxide fuel cell; electrochemical; cathode; anode; electrical power

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## 1. Introduction

Increasing electricity production with reducing polluting emissions is a pressing global necessity. Throughout history, diverse energy sources have been discovered, studied, and exploited, all contributing to meeting human needs. Suitable sources for producing electrical energy, such as the sun, wind, tides, and biomass, have proven their effectiveness<sup>[1]</sup>. Fuel cells have recently become a major focus of research; they are electrochemical technologies that can be classified according to operating temperature, fuel type, electrolyte material, and construction engineering<sup>[2,3]</sup>. The most commonly used fuel cell types are: Solid Oxide Fuel Cells (SOFCs), Polymer Electrolyte Fuel Cell or Proton Exchange Membrane Fuel Cells (PEMFCs), Phosphoric Acid Fuel Cells (PAFCs), Molten Carbonate Fuel Cells (MCFCs), Alkaline Fuel Cells (AFCs), and Direct Methanol Fuel Cells (DMFCs)<sup>[4]</sup>. Fuel cells are divided into two main categories

based on their operating temperature: low-temperature fuel cells and high-temperature fuel cells. Low-temperature fuel cells are suitable for transportation applications such as electric vehicles and include PEMFCs, PAFCs, DMFCs, and AFCs. High-temperature fuel cells are suitable for stationary power applications and include SOFCs and MCFCs<sup>[5,6]</sup>. SOFCs have high electrical efficiency up to 70%, high combined heat yield, long-term stability, fuel flexibility, low emissions, low maintenance costs, and a long theoretical life<sup>[7]</sup>. The solid electrolyte allows the cell to be manufactured in various self-supporting configurations, such as planar, monolithic, roll, and tubular<sup>[8-10]</sup>. However, the high operating temperature leads to long start-up times and mechanical and chemical compatibility problems<sup>[11]</sup>. The materials must possess unique and stringent properties due to the constraints and requirements imposed by the engineering of SOFCs, such as durability to prevent unwanted reactions and reliable thermal expansion<sup>[12]</sup>. The creation of SOFCs requires the development of chemically compatible materials with suitable conductivity, dimensional stability, strength, and high density<sup>[13]</sup>. Depending on the types of charge carriers in the electrolyte, two types are distinguished: oxygen-ion conducting ( $O^{2-}$ SOFC) and hydrogen-ion conducting ( $H^+$ SOFC)<sup>[14]</sup>.

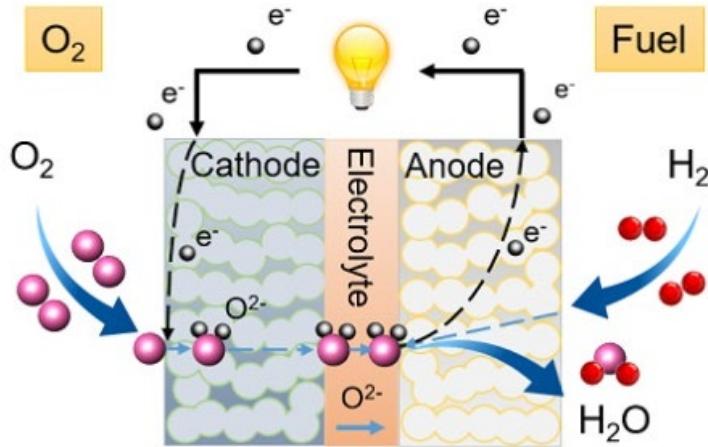
Numerical simulation is a very useful tool for understanding the various mechanisms and phenomena related to the behavior of fuel cells from several aspects. For example, Wei Kong et al. studied the effect of anode and cathode rib widths on gas diffusion and cathode-supported SOFC performance. They found that SOFC performance is strongly affected by rib width and that the optimal anode rib width is smaller than the optimal cathode rib width<sup>[15]</sup>. Jee Min Park et al. investigated how electrolyte thicknesses ranging from 80 to 100  $\mu$ m and operating temperatures ranging from 700 to 800 °C affect electrochemical reactions and thermo-fluidic characteristics within a planar SOFC unit. They found that the maximum electrical power density increases with decreasing electrolyte thickness and that cell performance improves with increasing operating temperature<sup>[16]</sup>. Xuan-Vien Nguyen investigated how operating conditions, fuel concentration, and electrode porosity affect the electrochemical performance of electrodes. The results showed that improving fuel mass transfer requires higher electrode porosity and that increasing the operating temperature improves electrical potential distribution across electrode surfaces<sup>[17]</sup>.

This article focuses on testing the effect of certain structural and electrochemical properties on the change in electrical power produced by a single-unit fuel cell. In section 2, the computational model of  $O^{2-}$ SOFC is described, including the operating process of  $O^{2-}$ SOFC, computational settings, and governing equations. In section 3, the simulation results are presented. In section 4, a conclusion highlighting the findings of this work is available.

## 2. Computational Model of $O^{2-}$ SOFC

### 2.1. Operating mechanism of $O^{2-}$ SOFC

In  $O^{2-}$ SOFCs, humidified air flows through the cathode channel while humidified hydrogen flows through the anode channel. The movement of electrons from the anode to the cathode generates electrical energy via an external circuit, as illustrated in **Figure 1**.



**Figure 1.** Operating principle of O<sup>2</sup>-SOFC<sup>[18]</sup>.

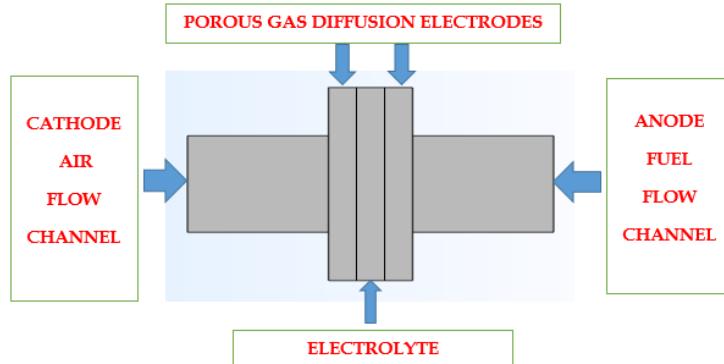
The two half reactions at both electrodes, and the full reaction are listed in **Table 1**.

**Table 1.** Electrochemical reactions in O<sup>2</sup>-SOFC.

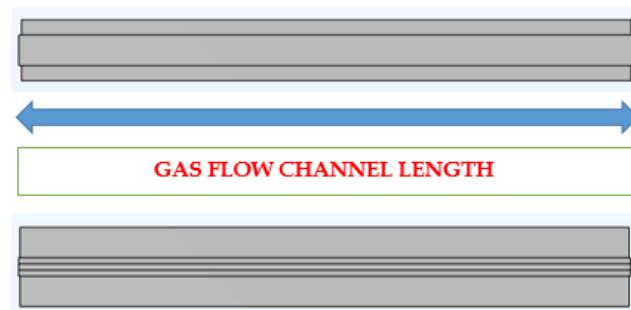
Side	Chemical/Electrochemical Reactions
Cathode	$1/2O_2 + 2e^- \rightarrow O^{2-}$
Anode	$H_2 + O^{2-} \rightarrow H_2O + 2e^-$
Overall	$1/2O_2 + H_2 \rightarrow \text{Electric Power} + \text{Heat} + H_2O$

## 2.2. Planar-structure single-unit of O<sup>2</sup>-SOFC

The planar-structure single-unit of O<sup>2</sup>-SOFC model comprises two gas flow channels, two porous gas diffusion electrodes, and a single electrolyte. **Figure 2** shows the YZ plan, and **Figures 3** shows the XY and XZ plans.



**Figure 2.** YZ-Plan Design for Planar-Structure Single-Unit O<sup>2</sup>-SOFC Model.



**Figure 3.** XY and XZ Plans Design for Planar-Structure Single-Unit O<sup>2-</sup>-SOFC Model.

**Table 2** lists the initial structural properties of the O<sup>2-</sup>-SOFC model.

**Table 2.** Initial Structural Settings of O<sup>2-</sup>-SOFC Computational Model<sup>[19]</sup>.

Structural Settings	Value and Unit
Gas Flow Channel Width	0.5 mm
Rib Width	0.5 mm
Porous Gas Diffusion Electrode Thickness	0.1 mm
Electrolyte Thickness	0.1 mm
Gas Flow Channel Height	0.5 mm
Cell Length	10 mm

### 2.3. Boundary conditions

The boundary conditions at the cathode and anode inflow are listed in **Table 3**.

**Table 3.** Boundary Conditions of O<sup>2-</sup>-SOFC Computational Model.

Boundary Conditions	Cathode-Side Inflow	Anode-Side Inflow
Electric Potential	1 V	0 V
Species Mass Fraction	O <sub>2</sub> : N <sub>2</sub> : H <sub>2</sub> O = 0.15 : 0.48 : 0.37	H <sub>2</sub> : H <sub>2</sub> O = 0.4 : 0.6
Pressure Drop	6 Pa	2 Pa

### 2.4. Kinetic species settings

**Table 4** and **Table 5** list the properties relating to the diffusivity of the fuel and air species, including effective diffusivity, kinetic volume, molar mass, reference diffusivity, and binary diffusivity.

**Table 4.** Kinetic Species Characteristics<sup>[20,21]</sup>.

Species	Effective Diffusivity	Kinetic Volume	Molar Mass
O <sub>2</sub>	1.2018 × 10 <sup>-5</sup> m <sup>2</sup> /s	16.3 × 10 <sup>-6</sup> m <sup>3</sup> /mol	0.032 kg/mol
N <sub>2</sub>	1.2342 × 10 <sup>-5</sup> m <sup>2</sup> /s	18.5 × 10 <sup>-6</sup> m <sup>3</sup> /mol	0.028 kg/mol
H <sub>2</sub>	4.9825 × 10 <sup>-5</sup> m <sup>2</sup> /s	6.12 × 10 <sup>-6</sup> m <sup>3</sup> /mol	0.002 kg/mol
H <sub>2</sub> O	2.7041 × 10 <sup>-5</sup> m <sup>2</sup> /s	13.1 × 10 <sup>-6</sup> m <sup>3</sup> /mol	0.018 kg/mol

**Table 5.** Binary Diffusivity Data of O<sup>2-</sup>-SOFC Computational Model<sup>[20,21]</sup>.

Diffusion Parameters	Value and Unit
Reference diffusivity	3.16 × 10 <sup>-8</sup> m <sup>2</sup> /s
Binary diffusivity of O <sub>2</sub> and N <sub>2</sub>	1.9235 × 10 <sup>-4</sup> m <sup>2</sup> /s
Binary diffusivity of H <sub>2</sub> and H <sub>2</sub> O	8.1794 × 10 <sup>-4</sup> m <sup>2</sup> /s
Binary diffusivity of O <sub>2</sub> and H <sub>2</sub> O	3.2674 × 10 <sup>-5</sup> m <sup>2</sup> /s
Binary diffusivity of N <sub>2</sub> and H <sub>2</sub> O	2.4477 × 10 <sup>-4</sup> m <sup>2</sup> /s

### 2.5. Electrochemical properties of SOFC model

The electrochemical settings are listed in **Table 6**.

**Table 6.** Electrochemical Settings of O<sup>2-</sup>-SOFC Computational Model<sup>[22-26]</sup>.

Electrochemical properties	Cathode-Side	Anode-Side	Electrolyte-Side
Exchange Current Density	0.01 A/m <sup>2</sup>	0.1 A/m <sup>2</sup>	-

Electrochemical properties	Cathode-Side	Anode-Side	Electrolyte-Side
Equilibrium Voltage	1 V	0 V	-
Permeability	$10^{-10} \text{ m}^2$	$10^{-10} \text{ m}^2$	-
Porosity Rate	40%	40%	-
Viscosity	Air : $4.4574 \times 10^{-5} \text{ Pa.s}$	$\text{H}_2 : 2.4320 \times 10^{-5} \text{ Pa.s}$	-
Specific Surface Area	$10^9 \text{ m}^{-1}$	$10^9 \text{ m}^{-1}$	-
Electrolyte Effective Conductivity	$1 \text{ S.m}^{-1}$	$1 \text{ S.m}^{-1}$	-
Solid Effective Conductivity	$1000 \text{ S.m}^{-1}$	$1000 \text{ S.m}^{-1}$	-
Electrolyte Conductivity	-	-	$5 \text{ S.m}^{-1}$

Table 6. (Continued)

## 2.6. Related equations

To activate various mechanisms and balance the behavior of phenomena, certain processes must be included in fuel cell modeling. Solid oxide fuel cell modeling is primarily based on electronic and ionic charge balances, charge transfer kinetics, mass balances, and flow distribution.

The current densities in the electrolyte  $i_l$  and solid electrode  $i_s$ , as well as the electron  $Q_s$  and ion  $Q_l$  current densities, are given by OHM's law with charge balance<sup>[27]</sup>:

$$i_l = -\sigma_l \nabla \phi_l \quad (1)$$

$$i_s = -\sigma_s \nabla \phi_s \quad (2)$$

$$Q_s = \nabla \cdot i_s \quad (3)$$

$$Q_l = \nabla \cdot i_l \quad (4)$$

Here  $\sigma_l$  and  $\sigma_s$  are the ionic and solid electrode conductivities, respectively, and  $\phi_l$  and  $\phi_s$  are the electrolyte ionic and solid electrode potentials, respectively.

Several expressions of the BUTLER-VOLMER equation are considered depending on the cases of electrochemical electrode kinetics cases<sup>[28]</sup>. The concentration-controlled BUTLER-VOLMER equation governs the charge transfer current density at the anode  $i_{act}$  and the cathode  $i_{cct}$ :

$$i_{act} = i_{0a} \left[ \frac{c_{H_2}}{c_{H_2}^{ref}} \exp\left(\frac{0.5F}{RT}\eta\right) - \frac{c_{H_2O}}{c_{H_2O}^{ref}} \exp\left(\frac{-1.5F}{RT}\eta\right) \right] \quad (5)$$

$$i_{cct} = i_{0c} \left[ \exp\left(\frac{3.5F}{RT}\eta\right) - x_{O_2} \frac{c_t}{c_{O_2}^{ref}} \exp\left(\frac{-0.5F}{RT}\eta\right) \right] \quad (6)$$

Where  $i_{0a}$  : Initial anode-side exchange current density,  $c_{H_2}$  : Hydrogen concentration,  $c_{H_2O}$  : Water concentration,  $c_{H_2}^{ref}$  : Hydrogen reference concentration,  $c_{H_2O}^{ref}$  : Water reference concentration,  $R$ : Gas constant,  $F$ : Faraday's constant,  $T$ : Operating temperature,  $\eta$  : Activation over-potential,  $i_{0c}$  : Initial cathode-side exchange current density,  $c_{O_2}^{ref}$  : Oxygen reference concentration,  $x_{O_2}$  : Oxygen fraction,  $c_t$  : Total concentration.

The activation over-potential is related to the equilibrium electrode potential  $E_{eq}$ , as follows:

$$\eta = \phi_s - \phi_l - E_{eq} \quad (7)$$

The expression of cell voltage  $V_{cell}$  depends on the cell polarization  $V_{pol}$ , as shown below:

$$V_{cell} = \phi_c - \phi_a - V_{pol} \quad (8)$$

Where  $\phi_c$  and  $\phi_a$  are the electric potential at the cathode-side inlet and anode-side inlet, respectively.

### 3. Results and discussion

#### 3.1. Voltage-current-power curves

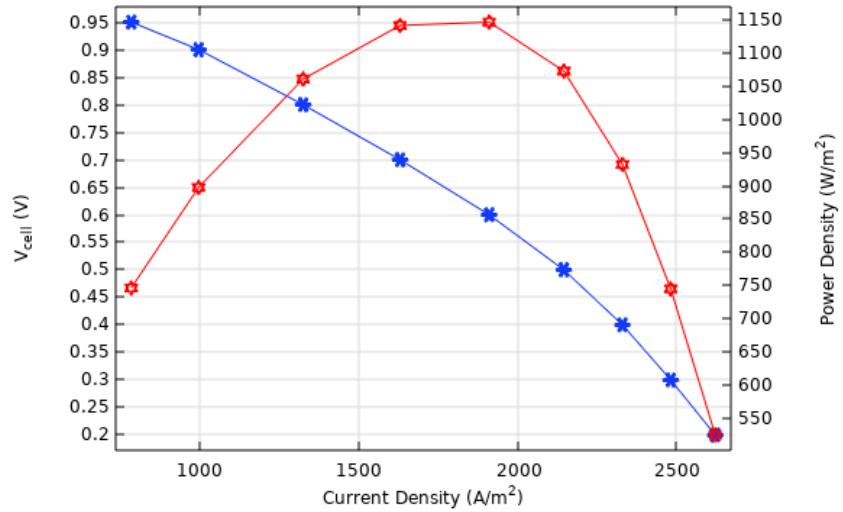
The cell current density is low when the cell voltage is high and high when the cell voltage is low<sup>[29]</sup>. The change in cell current density  $I_{cell}$  as a function of the input cell voltage range can be expressed as follows:

$$I_{cell} = f(V_{cell}) \quad (9)$$

The produced cell power density  $P_{cell}$  is calculated, as follows:

$$P_{cell} = V_{cell} \times I_{cell} \quad (10)$$

Under the same operating conditions, the cell voltage is inversely proportional to the cell current density. On the other hand, the cell power density initially increases to reach a peak value of 1132 W/m<sup>2</sup>, and then decreases as the cell current density increases, as illustrated in **Figure 4**. These results are consistent with the available literature<sup>[30]</sup>.



**Figure 4.** V-I-P Curves for Initial Operating Conditions.

#### 3.2. Effect of porous gas diffusion electrodes porosity

The porosity is defined as the percentage of a material's volume occupied by pores or voids<sup>[31]</sup>. It is expressed as a fraction or percentage, given by the following formula:

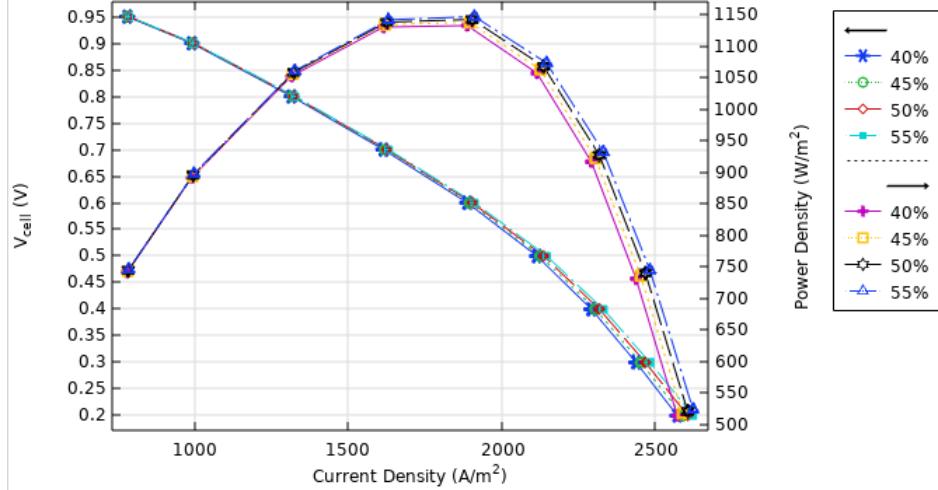
$$P(\%) = \frac{V_p}{V_b} \times 100 \quad (11)$$

Here  $P$  is the porosity rate,  $V_p$  is the total pores volume per unit volume,  $V_b$  is the bulk volume of the porous materials per unit volume.

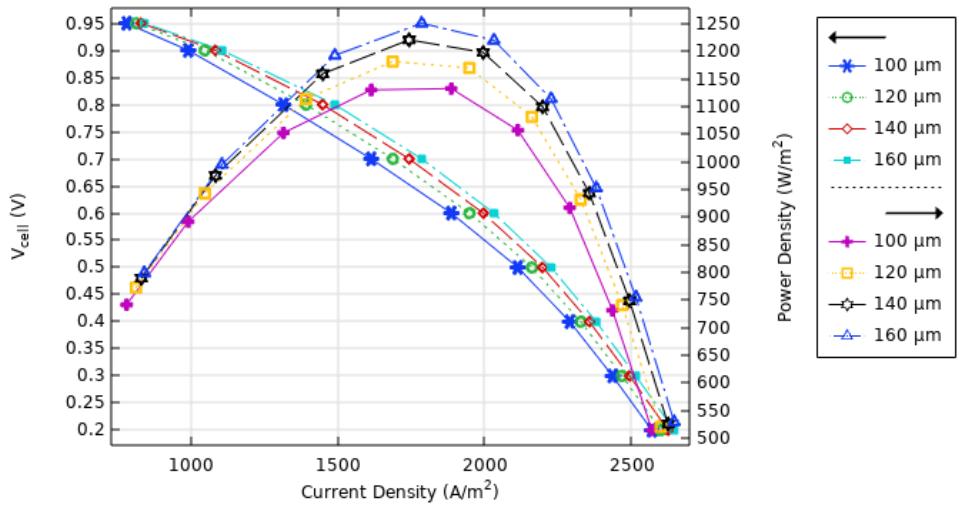
In materials physics, an increase in porosity rate refers to an increase in the size or number of pores embedded in the porous material. This improves the diffusion rate of chemical species through porous gas diffusion electrodes (PGDEs) in solid oxide fuel cells. Taking into account the independence of the porosity rate from any other physical or fluid property and maintaining the same initial operating conditions. This approach opens the possibility of increasing the porosity rate directly as a percentage as illustrated in **Figure 5** where the peak power density reaches 1146 W/m<sup>2</sup> at 55% or by increasing the thickness of PGDEs as illustrated in **Figure 6** where the peak power density reaches 1250.8 W/m<sup>2</sup> for 160 µm PGDEs thickness. This defines a direct proportionality that can be expressed as follows:

$$P^{\text{new}}(\%) = \frac{P^{\text{old}}(\%) \times V_b^{\text{new}}}{V_b^{\text{old}}} \quad (12)$$

Here  $P^{\text{new}}$  is the new porosity rate after changing (increasing or decreasing) the bulk volume of the porous material,  $P^{\text{old}}$  is the initial porosity rate before changing the bulk volume of the porous material.  $V_b^{\text{new}}$  and  $V_b^{\text{old}}$  are the new bulk volume and the initial bulk volume of the porous material, respectively.



**Figure 5.** Effect of PGDEs Porosity Percentage on V-I-P Curves.

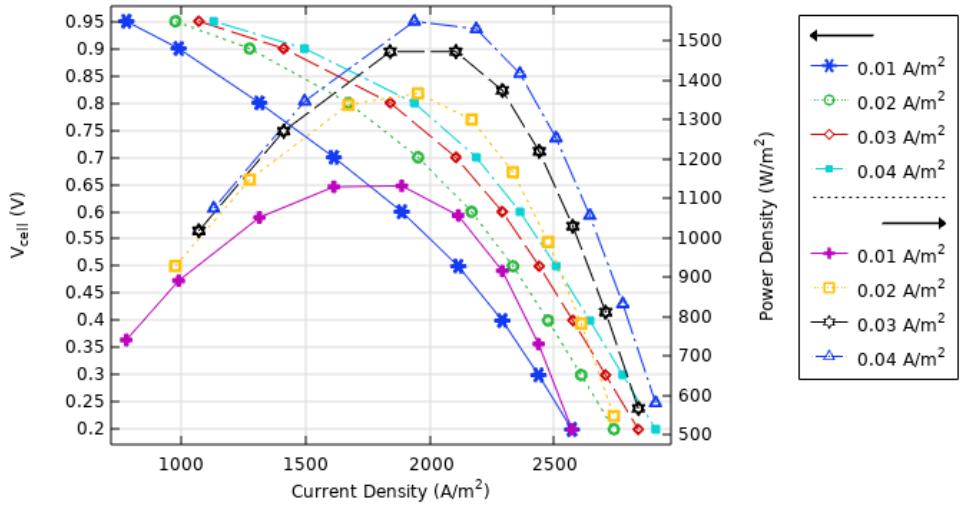


**Figure 6.** Effect of PGDEs Thickness on V-I-P Curves.

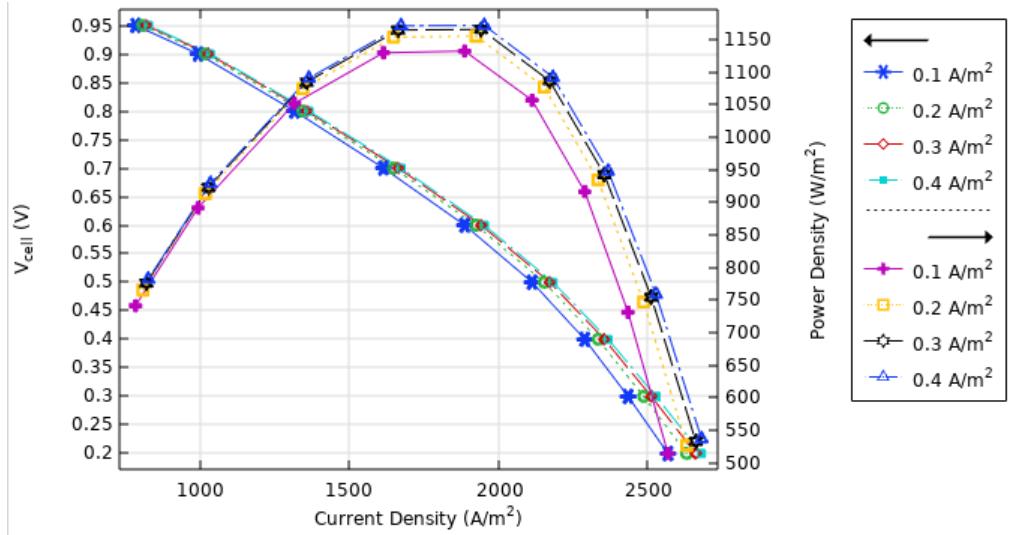
### 3.3. Effect of exchange current density

The reaction rate coefficient in chemistry is analogous to the exchange current density in electrochemistry<sup>[32]</sup>, meaning that chemical reactions with a high reaction rate coefficient are more significant than those with a lower reaction rate coefficient, some of which are neglected in certain studies. Similarly, the higher the exchange current density, the better the performance of the electrochemical fuel cell, and vice versa. Numerous examples in the literature demonstrate the direct relationship between increasing exchange current density and the efficiency of electrochemical systems. For example, Raj Kamal Abdul Rashid et al. reported that exchange current density is a good measure of catalyst reaction rate, and that a higher value indicates better electrochemical performance of a pulsed electrochemical fuel cell<sup>[33]</sup>. Harshad Bandal et al. suggest that exchange current density reflects the intrinsic interconnection and charge-transfer interactions of electrocatalysts. In other words, high exchange current densities generally indicate excellent catalytic activity<sup>[34]</sup>. The

results obtained are in satisfactory agreement with the outcomes of the aforementioned examples, where the peak power density reaches  $1550 \text{ W/m}^2$  for  $0.04 \text{ A/m}^2$  cathode-side exchange current density as shown in **Figure 7** and  $1172 \text{ W/m}^2$  for  $0.4 \text{ A/m}^2$  anode-side exchange current density as shown in **Figure 8**.



**Figure 7.** Effect of Cathode-Side Exchange Current Density on V-I-P Curves.



**Figure 8.** Effect of Anode-Side Exchange Current Density on VI-P Curves.

### 3.4. Effect of pressure drops

A pressure drop occurs when a gas experiences a decrease in pressure as it flows through a channel. This results in a pressure difference between the gas inflow and gas outflow<sup>[35]</sup>. When gas (such as air or fuel) flows, a frictional forces are created due to the channel's resistance, which drops the gas pressure. The resistance to gas flow through channels depends on the dynamic and fluid properties of the gases, such as viscosity and velocity. The greater the gas flow rate, the greater the pressure drop at the related electrode (anode for fuel and cathode for air). Therefore, if the gas is highly flowing, the pressure drop will also be higher, and vice versa. The peak power density reaches the values of  $1316 \text{ W/m}^2$  for 9 Pa at the cathode-side and  $1142 \text{ W/m}^2$  for 5 Pa at the anode-side, as illustrated in **Figure 9** and **Figure 10** respectively. Another solution to make the pressure drop effect more pronounced is to increase the resistance of the gas flow channels by decreasing the cell length. **Figure 11** shows that as the cell length decreases, the peak power density increases, reaching  $1515 \text{ W/m}^2$  at a cell length of 7 mm.

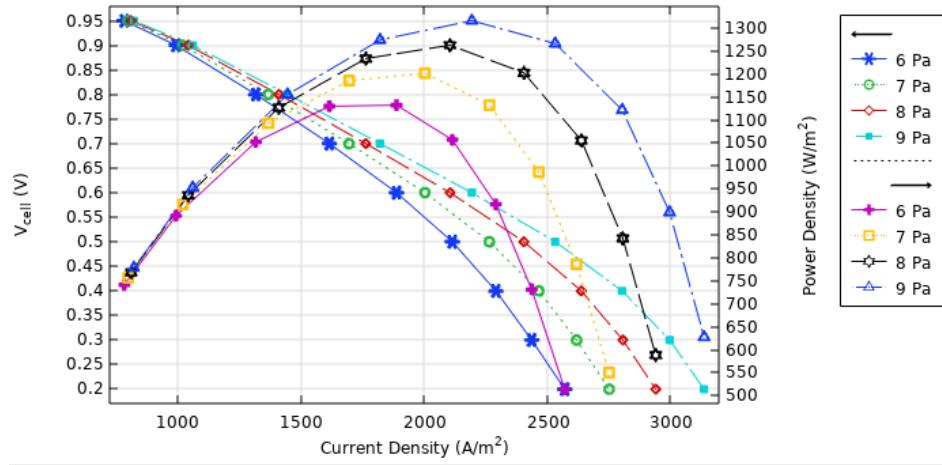


Figure 9. Effect of Cathode-Side Pressure Drop on V-I-P Curves.

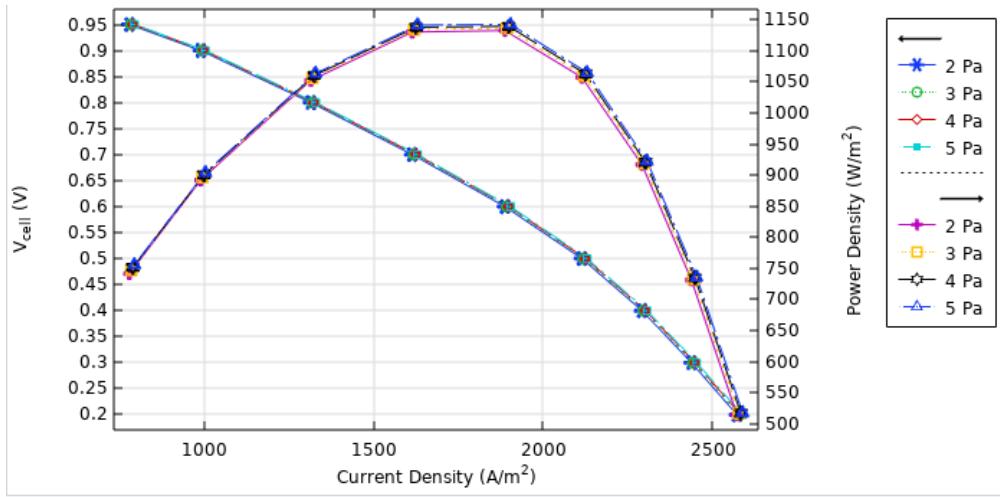


Figure 10. Effect of Anode-Side Pressure Drop on V-I-P Curves.

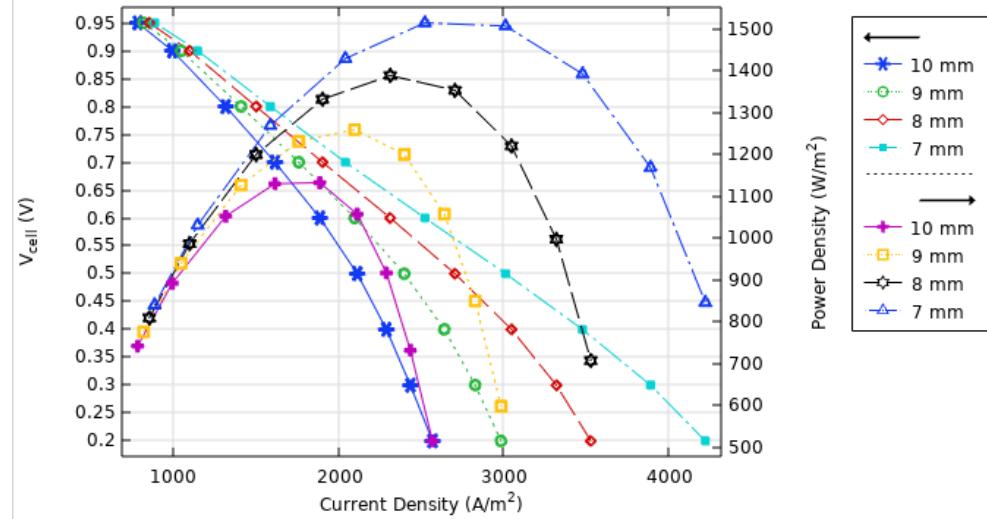
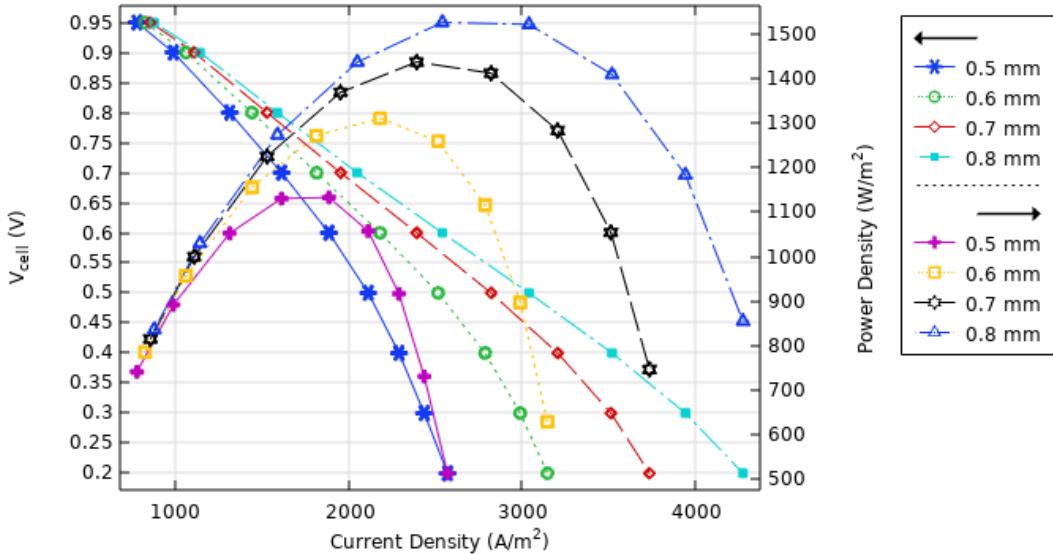


Figure 11. Effect of Single-Unit Cell Length on V-I-P Curves.

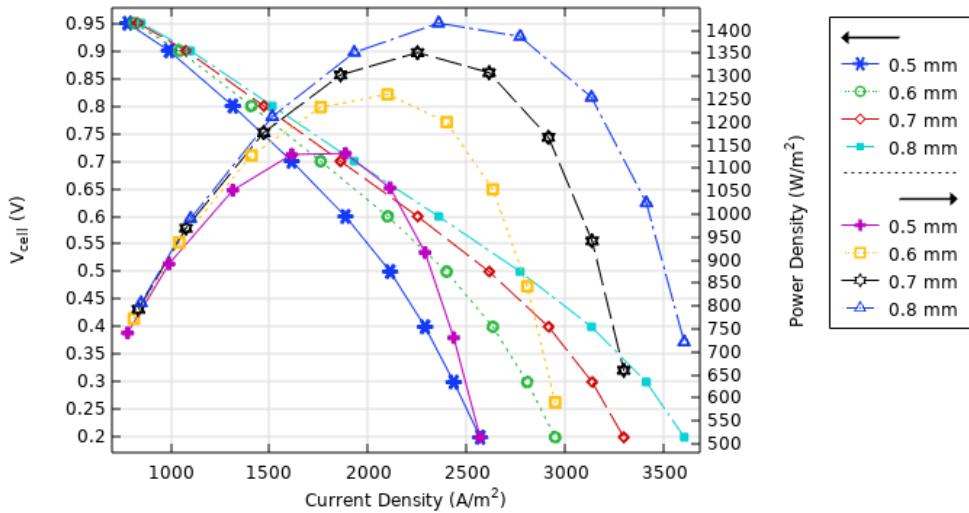
### 3.5. Effect of gas flow channel dimensions

Increasing the height or width of the gas flow channels increases their gas capacity, which improves the amount of gas flowing through them in terms of mass transfer, distribution, diffusion, and flow. Consequently,

the fuel cell performs more efficiently. As the height of the gas channels increases, the fluid and physical properties of the gases inside the channels improve vertically. And as the width of gas channels increases, the fluid and physical properties of the gases across the channels improve horizontally. The peak power density reached a values of  $1525 \text{ W/m}^2$  and  $1416 \text{ W/m}^2$  for 0.8 mm height and 0.8 mm width , as illustrated in **Figure 12** and **Figure 13**, respectively.



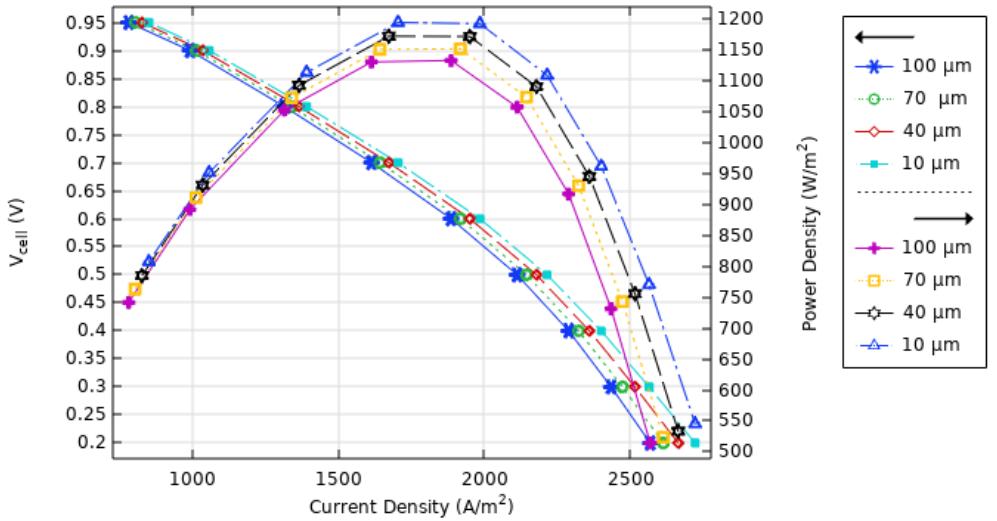
**Figure 12.** Effect of Gas Flow Channel Height on V-I-P Curves.



**Figure 13.** Effect of Gas Flow Channel Width on V-I-P Curves.

### 3.6. Effect of electrolyte thickness

The electrolyte is the core of a fuel cell, acting as an ionic conductor between the electrodes. The thickness of the electrolyte plays a key role in the overall performance of the cell. Reducing the electrolyte thickness results in better ionic conductivity and less heat loss. As reported by Jee Min Park et al<sup>[16]</sup>, the thinner the electrolyte, the better the solid oxide fuel cell performs. The peak power density reaches  $1190 \text{ W/m}^2$  for electrolyte thicknesses of  $10 \mu\text{m}$  as shown in **Figure 14**.



**Figure 14.** Effect of Electrolyte Thickness on V-I-P Curves.

**Table 7** summarizes the key elements related to improving cell performance and linking them to the corresponding component.

**Table 7.** Summary linking appropriate physical switches to the fuel cell component.

O <sup>2</sup> -SOFC Component	Physical properties	Related physical behaviors
Electrodes	Porosity rate	Species diffusion rate
Electrodes	Exchange current density	Charge transfer
Gas flow channels	Pressure drops	Frictional forces Channel's resistance Gas flow rate Gas viscosity and/or velocity
Gas flow channels	Dimensions (Height and Width)	Species mass transfer, propagation, distribution, and flow rates
Electrolyte	Thickness	Ionic conductivity

## 4. Conclusion

In conclusion, fuel cells are a leading technology in the field of renewable energy, and aim to produce electrical power to operate external circuits. This paper has presented a numerical simulation of a high-temperature solid oxide fuel cell for finding the best ways to improve fuel cell performance. The theoretical model was based on Ohm's law with charge balance, the Butler-Volmer equation, and activation over-potential. The findings revealed several methods to improve oxygen mass transport, ultimately optimizing the output electric power density. Overall, to improve the yield of a O<sup>2</sup>-SOFC, strategies can be summarized through:

- Bettering the ionic conductivity through reducing the electrolyte thickness.
- Enhancing the physics behaviors of the chemical species.
- Optimizing the structure dimensions.

## Conflict of interest

The authors declare no conflict of interest.

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