

ANALYSIS OF PEMFC WITH 2-PASSES SERPENTINE FLOW CHANNELS CONFIGURATION USING COMPUTATIONAL FLUID DYNAMICS

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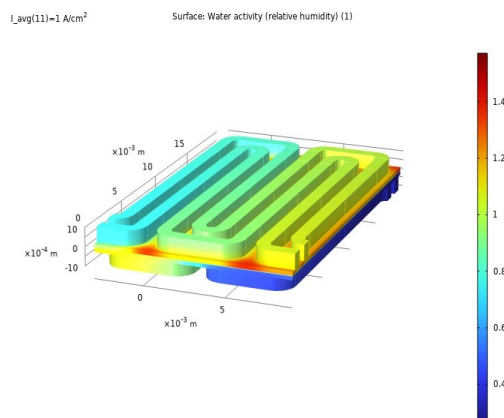
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Graphical abstract



Abstract

Proton exchange membrane fuel cells have attracted considerable attention for their potential as clean energy sources. The efficient operation of fuel cells depends greatly on proper water management, which directly influences performance by affecting mass transport and conductivity. This study aimed to simulate and analyze the evolution of parameters such as hydrogen and oxygen molar fractions, relative humidity in the channels, water activity, and electrolyte conductivity in the membrane on fuel cell performance. A three-dimensional proton exchange membrane model with 2-pass serpentine flow channels was developed using COMSOL Multiphysics software. The software was employed to numerically solve the complete model with governing equations of continuity, momentum, energy, and mass transport. Simulation results showed a significantly larger depletion of oxygen compared to hydrogen. Additionally, higher water activity near the air inlet led to increased oxygen content and local current density due to oxygen transport limiting the reaction rate. Furthermore, the membrane conductivity was significant where water activity was high, increasing current density distribution until 1A/cm². The developed fuel cell model's performance was evaluated by comparing it with experimental data, demonstrating favorable agreement. This work contributes to understanding fuel cell operation for enhanced efficiency and reliability in practical applications.

Keywords: PEMFC, 2-passes serpentine flow channels, simulations, water activity, molar fraction

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1.0 INTRODUCTION

Proton exchange membrane fuel cells (PEMFCs) exhibit significant potential as energy conversion systems applicable across various domains. This is

ascribed to their exceptional properties, including high efficiency, minimal emissions, adaptability to different fuels, reliability, low operating temperatures, high power density, low noise levels, and the capability for cogeneration [1-8]. The assessment of fuel cell

performance commonly involves the use of polarization curves, depicting the relationship between current density and cell voltage [9-11]. It is widely acknowledged that this performance curve is influenced by factors such as reactant distribution, effective water and thermal management, and electrochemical kinetics. These factors are generally determined by the properties of the catalyst layer and the membrane [12-14]. In this context, the modeling of fuel cells plays a pivotal role in designing new materials, establishing optimal configurations for reactant transport, and identifying the most favorable operating conditions to achieve maximum fuel cell efficiency [15].

Flow field plates (FFPs) play a vital role in improving the efficiency of fuel cells and are considered one of the most important components [16, 17]. Their main functions are to ensure the appropriate distribution of reactants such as hydrogen (H_2) and oxygen (O_2), remove excess water efficiently, recover the generated electrical energy, and support the membrane electrode assembly (MEA). The performance of fuel cells is largely determined by the interplay between electrochemical reactions, channel patterns, and plate configurations, all of which have a significant impact on mass transfer characteristics [18]. Therefore, achieving an optimal shape, orientation, size, and channel pattern is crucial for maximizing the performance of bipolar plates in fuel cell systems.

The fuel cells performance is significantly impacted by both design and operational factors. The effective distribution of reactants within the flow fields is facilitated by the design of the flow channels. Therefore, the geometry of the flow channels and the overall design of the flow field play a crucial role in determining the fuel cells performance. Among various flow field designs, the serpentine flow field demonstrates superior performance compared to others [19]. The serpentine flow field design has garnered considerable interest because of its ability to enhance mass transport within the fuel cell and promote uniform reactant distribution uniformity [20, 21]. Oxygen and hydrogen are important to be used because they are the reactants in the electrochemical reactions that occur within the fuel cell. They undergo oxidation and reduction reactions at the anode and cathode, respectively, generating electrical energy and water as byproducts [22, 23].

Fuel cells have been studied both experimentally and theoretically. However, experimental studies on PEM fuel cells are often expensive and limited to laboratory settings, making these devices difficult to design and optimize for practical applications [24]. In contrast, the numerical simulation of fuel cells is complex, requiring sophisticated computational models and algorithms [25]. Theoretical studies have mainly focused on modeling fuel cells to improve their overall performance and understanding the transport phenomena and electrochemical kinetics that occur in fuel cells.

Many works have investigated the flow field design of PEMFCs for performance improvement through

experimental studies and numerical simulations. Jang *et al.* [26] created a three-dimensional numerical model for PEMFC with traditional flow field configurations to analyze fuel cell performance and transport phenomena. Their findings indicated that the serpentine flow field outperforms both Z-type and parallel flow fields. Guo *et al.* [27] developed a three-dimensional simulation model incorporating bio-inspired flow field designs to assess fuel cell performance through both numerical simulations and experimental testing. Their conclusion highlighted a substantial enhancement in cell performance, with bio-inspired designs yielding a 20-25% increase compared to conventional designs.

The main problem addressed throughout the entire study is the optimization of water management in PEMFCs. This encompasses ensuring a balance between avoiding excessive water accumulation, which can lead to flooding and mass transport limitations, and preventing the system from becoming too dry, which can result in poor performance due to low ionomer conductivity. More precisely, water is produced on the air (cathode) side in the oxygen reduction reaction, but may permeate through the membrane to the hydrogen (anode side). Running the cell under too wet conditions may result in mass transport limitations of gases due to flooding of liquid water in the pores, whereas running the cell under too dry conditions may result in poor performance due to a low ohmic conductivity in the ionomer (polymer electrolyte) used in the membrane and catalytic layers. The gap in the study lies in the need for a comprehensive analysis of the water management strategies within the PEMFC system utilizing 2-passes serpentine flow channels configuration.

In this study, a 3D mathematical model is developed to investigate the performance of the PEMFC with 2-passes serpentine flow fields using the Electrochemistry Module of COMSOL Multiphysics software. The aim of this research is to assess the impact of the 2-passes serpentine flow channels configuration on the performance of the PEMFC by analyzing several conditions such as hydrogen and oxygen molar fractions, relative humidity in the channels, water activity and electrolyte conductivity in the membrane and understanding major physicochemical processes within the fuel cell.

The paper is organized as follows: In Section 2, a comprehensive explanation of the model developed in this study is provided, including the governing equations and computational framework. Section 3 exhibits the implementation of our 3D PEMFC model with 2-passes serpentine flow channels using COMSOL Multiphysics. The obtained results of our investigation, along with a detailed analysis of the influence of various parameters on the performance of PEMFC with 2-passes serpentine flow fields are presented and discussed in Section 4. Finally, Section 5 concludes the study by summarizing the key findings.

2.0 METHODOLOGY

2.1 Geometric Model

The three-dimensional model with 2-passes serpentine gas flow channels is illustrated in Figure 1. The membrane electrode assembly (MEA) of the fuel cell is positioned between the anode and cathode gas diffusion layers (GDLs), along with serpentine channels for both hydrogen and oxygen. The oxygen side is situated above the MEA, whereas the hydrogen side is located below it. Indeed, oxygen and hydrogen have been used in this study rather than other fluids because they are the primary reactants in PEMFCs, which are commonly utilized in various applications due to their high energy efficiency, low emissions, and potential for clean energy generation. Figure 1 indicates the positions of the gas inlets. Table 1 reports the geometric parameters used in the developed model.

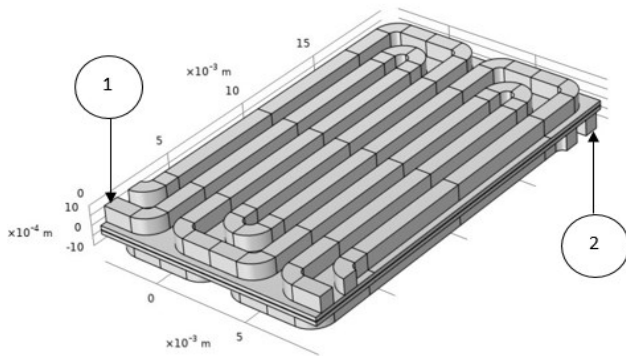


Figure 1 Geometry of 2-passes serpentine flow channels fuel cell (1: Oxygen inlet; 2: Hydrogen inlet)

Table 1 Design parameters

Description	Value
Minimum plate width (m)	0.02
Number of channels	2
Number of repeating units	2
Rib width (m)	7e-4
Channel width (m)	8e-4
Channel height (m)	8e-4
Gdl height (m)	2e-4
Membrane thickness (m)	3e-5
Use 1 for counter flow, 0 for coflow	1
Plate width (m)	0.01
Channel-to-channel distance (m)	0.0015
Length of repeating unit (m)	0.006
Plate length (m)	0.012

2.2 Basic Assumptions

Our model operates under the following assumptions:

- 3D domain
- Cell temperature is held constant
- Stationary model
- Membrane is impermeable to reactant species
- All gases are treated as ideal gas
- Gas diffusion layer is isotropic and homogeneous

2.3 Governing Equations

The following expressions encapsulate the mathematical equations that govern continuity, momentum, energy, species, and charge:

Continuity equation

$$\nabla \cdot (\rho \vec{V}) = 0 \quad (1)$$

Momentum conservation

$$\rho (\vec{V} \cdot \nabla) \vec{V} = -\nabla p + \mu \Delta \vec{V} \quad (2)$$

Conservation of energy equation

$$\nabla \cdot (\rho u H) - \nabla \cdot (k \nabla T) = 0 \quad (3)$$

Mass transport

$$\nabla \cdot (\rho u Y_i) - \nabla \cdot (\rho D_{ii} \nabla Y_i) = \nabla \cdot (\rho D_{ij} \nabla Y_j) \quad (4)$$

where \vec{V} is the velocity vector (u , v , and w) in the (x , y , and z) directions, respectively (SI unit: m/s), ρ is the density of reactant gases (SI unit: kg/m³); p is the pressure (SI unit: Pa), μ is the viscosity (SI unit: kg/m.s), T is the temperature (SI unit: K), H is the total specific enthalpy (SI unit: J/kg), k is the conductivity (SI unit: S/m), Y_i is the mass fraction, u is the reference velocity and the index i represents O₂ on the cathode side and H₂ on the anode side, while j signifies H₂O vapor in both sides. The Stefan-Maxwell ternary diffusion coefficients, denoted as D_{ii} and D_{ij} , are derived in accordance with the methodology outlined by [28].

2.4 Boundary Conditions

In order to model the operational conditions of the PEMFC with 2-passes serpentine flow channels, we set up boundary conditions. Table 2 furnishes boundary conditions of the simulation model. This simulation requires defining operational parameters such as temperature, stoichiometry levels at the anode and cathode, as well as relative humidity at both sides.

Table 2 Boundary conditions

Specifications	Value
H ₂ flow stoichiometry	1.2
O ₂ flow stoichiometry	2.5
Inlet relative humidity, anode side	0.25
Inlet relative humidity, cathode side	0.75
Cell temperature (K)	343.15
H ₂ mass flow rate, anode side (kg/s)	9.3278e-10
O ₂ mass flow rate, cathode side (kg/s)	6.2186e-9
Humidification temperature (K)	343.15

2.5 Numerical Procedure

A structured computational model of the PEMFC with 2-passes serpentine flow fields was created using the COMSOL Multiphysics software (Figure 2). The developed model is assumed as 3-D, steady, isothermal and the gases at the inlet as ideal, the flow as laminar, the fluid as incompressible, the porous layers such as Gas Diffusion Layers (GDLs), Catalyst Layers (CLs) and the membrane (PEM) as isotropic and the thermo-physical properties as constant. Meshing is done by using triangular and tetrahedral methods. This model requires a costume mesh for accurate calculations. Mapped and swept meshing are used in this model. Using COMSOL boundary conditions and a simple algorithm based on the finite element technique, the governing equations were solved [29]. This study investigates the influence of the number of meshes on the simulation results to ensure independence. The model geometry in Figure 1 is used to test mesh independence. As shown in Figure 3, it can be obviously seen that the polarization curves are consistent when the mesh numbers are 107763, 339410, and 561874, respectively. Results show that the calculation error is within 1% when the number of meshes exceeds 339410. In the analysis of PEMFC with 2-passes serpentine flow channels configuration using COMSOL Multiphysics, various numerical methods were employed to simulate the complex multiphysics phenomena involved. Finite element method (FEM) was utilized for solving the governing equations, including the Navier-Stokes equations for fluid flow, species transport equations for mass transport, and the electrochemical reactions at the electrode-electrolyte interface and to capture fluid flow behavior, accounting for the serpentine flow channels. Additionally, the numerical methods was utilized the Butler-Volmer equation to model the kinetics of the electrochemical reactions.

The model was run at a constant temperature of 343.15 K. Table 3 reports the physicochemical parameters used in this model.

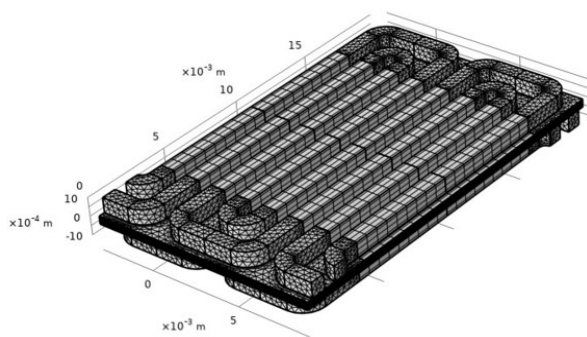


Figure 2 Structure after meshing

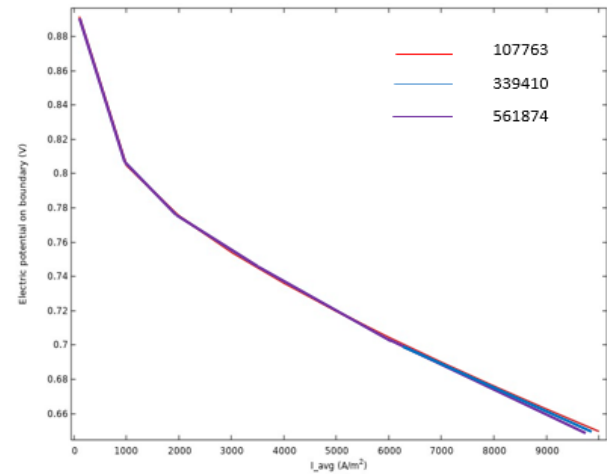


Figure 3 Results of the mesh independent test

Table 3 Physicochemical parameters

Parameter	Value
H ₂ flow stoichiometry	1.2
O ₂ flow stoichiometry	2.5
Inlet relative humidity, anode side	0.25
Inlet relative humidity, cathode side	0.75
Cell temperature (K)	343.15
Initial average current density in sweep (A/m ²)	100
Final average current density in sweep (A/m ²)	10000
Catalytic layer thickness (m)	1e-5
Exchange current density, H ₂ oxidation (A/m ²)	100
Exchange current density, O ₂ reduction (A/m ²)	1e-4
Specific area, catalytic layers (1/m)	5e7
Electric in-plane conductivity, GDL (S/m)	5000
Electric thru-plane conductivity, GDL (S/m)	200
Gas permeability, GDL (m ²)	5e-12
Anodic transfer coefficient, O ₂ reduction	3
Gas phase volume fraction, GDLs	0.6
Solid phase volume fraction, GDL	0.4
Average cell current density (A/m ²)	100
Cell area (m ²)	3e-5
Total current for stoichiometric flow calculations (A)	0.03
Total cell current (A)	0.003
H ₂ molar flow rate (mol/s)	4.6639e-7
Vapor molar flow rate, anode side (mol/s)	8.4876e-8
Vapor molar flow rate, cathode side (mol/s)	2.7789e-7
N ₂ molar flow rate (mol/s)	7.3105e-7
O ₂ molar flow rate (mol/s)	1.9433e-7
Anode total mass flow rate (kg/s)	2.4606e-9
Cathode total mass flow rate (kg/s)	3.169e-8
H ₂ mass flow rate (kg/s)	9.3278e-10
Vapor mass flow rate, anode side (kg/s)	1.5278e-9
Vapor mass flow rate, cathode side (kg/s)	5.0021e-9
N ₂ mass flow rate (kg/s)	2.0469e-8
O ₂ mass flow rate (kg/s)	6.2186e-9
Water mass fraction in anode flow stream	0.6209
Water mass fraction in cathode flow stream	0.15784
N ₂ mass fraction in cathode flow stream	0.64593
H ₂ molar fraction in anode flow stream	0.84604
Humidification temperature (K)	343.15
Vapor pressure (Pa)	31201
Vapor molar fraction in anode flow stream	0.15396
Vapor molar fraction in cathode flow stream	0.23095
N ₂ molar fraction in cathode flow stream	0.60755
O ₂ molar fraction in cathode flow stream	0.1615

3.0 RESULTS AND DISCUSSION

An examination of the performance of the PEMFC with 2-passes serpentine flow field was conducted using computational fluid dynamics. Key parameters, including hydrogen and oxygen molar fractions, relative humidity within the channels, water activity, and electrolyte conductivity in the membrane of the 2-passes serpentine flow fields PEMFC, are illustrated in Figures 4-9. The polarization curve in Figure 10 depicts the performance voltage versus current density of the PEMFC.

Figure 4 and Figure 5 show the streamlines of hydrogen and oxygen within the 2-passes serpentine flow channel, and the corresponding molar fractions for a current density of 1 A/cm^2 . At the channel inlet, the molar fractions of both H_2 and O_2 are higher, gradually diminishing towards the outlet. This reduction in species molar fraction within the fields is because of the consumption of reactants during the reaction. The molar fractions of O_2 and H_2 are high until the final turn of the serpentine fields with the exception of the outlet side of the field. This can be enhanced by increasing the flow of reactants, allowing for a more even distribution across the entire active area of the cell.

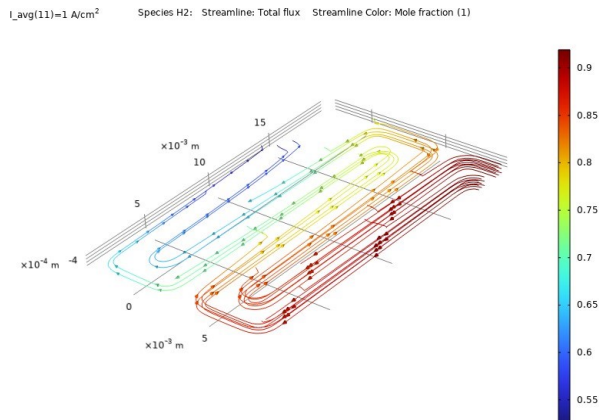


Figure 4 Plot of the hydrogen molar fraction at the current density of 1 A/cm^2

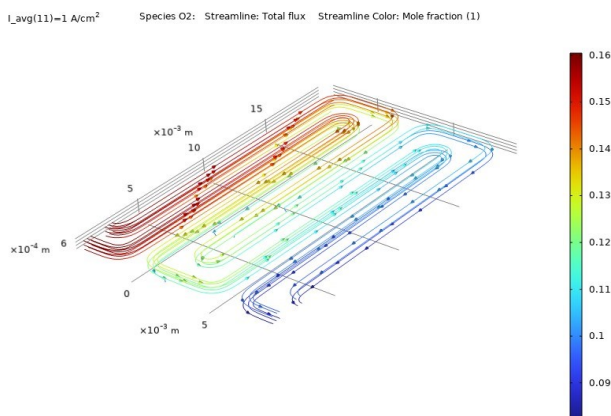


Figure 5 Plot of the oxygen molar fraction at the current density of 1 A/cm^2

Figures 6 and 7 show the water activity, which corresponds to the relative humidity in the gas phase, within both the channels and the membrane at the applied current density of 1 A/cm^2 . It is shown that the relative humidity increases toward the outlet for both gas streams. On the oxygen side (above the MEA), the increased water activity is a direct effect of the water being produced in the cell. On the hydrogen side (below the MEA), the increase in its water activity is due to the depletion of hydrogen. This implies that the water fraction (at 25% relative humidity at the inlet) of the gas stream increases as hydrogen is consumed. Additionally, this increase in water activity is because of the transport of water across the membrane between the two gas compartments, as depicted in Figure 6.

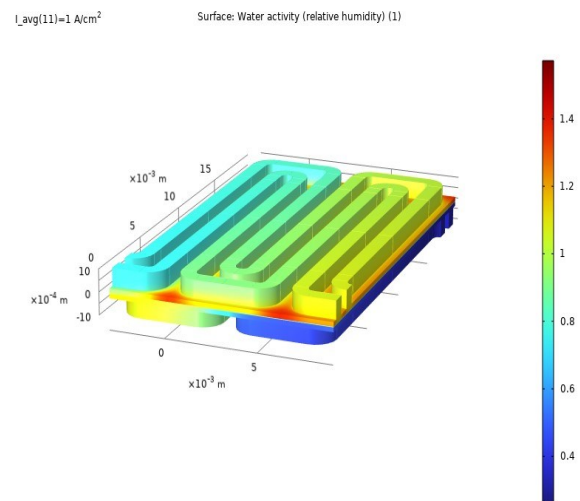


Figure 6 Distribution of the water activity in the channels at the current density of 1 A/cm^2

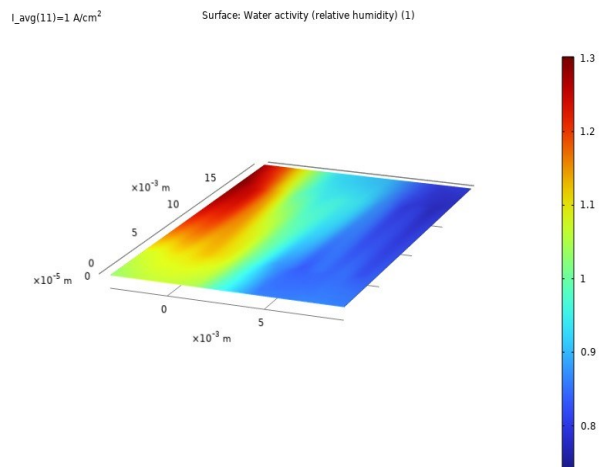


Figure 7 Distribution of the water activity in the membrane at 1 A/cm^2

The electrolyte conductivity of the membrane is shown in Figure 8. This property is related to the water activity within the system, which has an important

effect on the distribution of the current density across the cell. In this figure, regions characterized by lower conductivity (blue color) tend to exhibit reduced current densities.

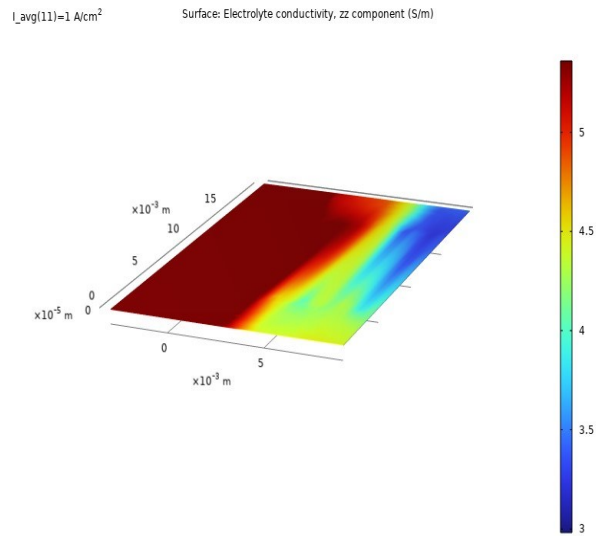


Figure 8 Distribution of the electrolyte conductivity in the membrane at 1 A/cm²

Figure 9 illustrates the electrolyte current density along the z-direction within the membrane. This current density distribution is related to varying levels of oxygen molar fraction. It is evident that regions less accessible to oxygen (blue color) exhibit lower current densities, highlighting the vital role of oxygen availability in influencing electrochemical activity within the PEM fuel cell.

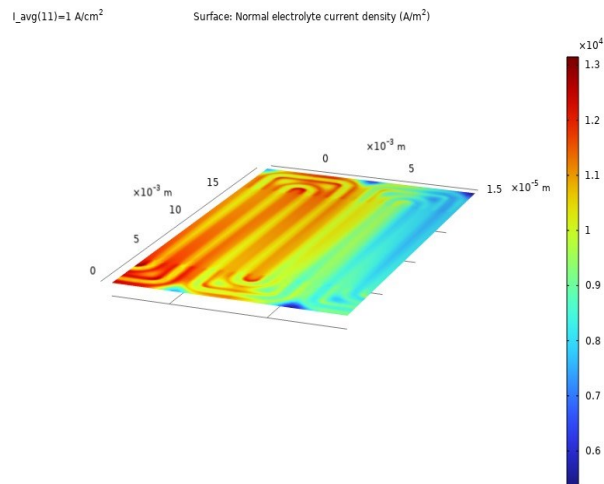


Figure 9 Distribution of the electrolyte current density in the z-direction in the membrane at 1 A/cm²

The performance of the 2-passes serpentine flow channels configuration in the PEMFC were evaluated by comparing the obtained polarization curve with

experimental data, as depicted in Figure 10. Experimental polarization data of Wang et al. [30] were employed to validate the developed model. A good agreement is found between the numerical simulations and the experimental results above almost 0.71 V. This alignment suggests that the simulation model effectively captures the system's behavior under operating conditions. However, below this value, the numerical predictions tend to slightly overestimate. The observed phenomenon can be explained by the flow channel's improved ability to expel water, resulting in a reduction in concentration losses. Also, the discrepancy could be attributed to the model's simplified representation of certain phenomena, electrode degradation or inaccuracies in parameter estimation. Nonetheless, the consistent correlation between the simulation and experimental data underscores the model's validity in predicting PEMFC performance, albeit with some limitations at lower voltages.

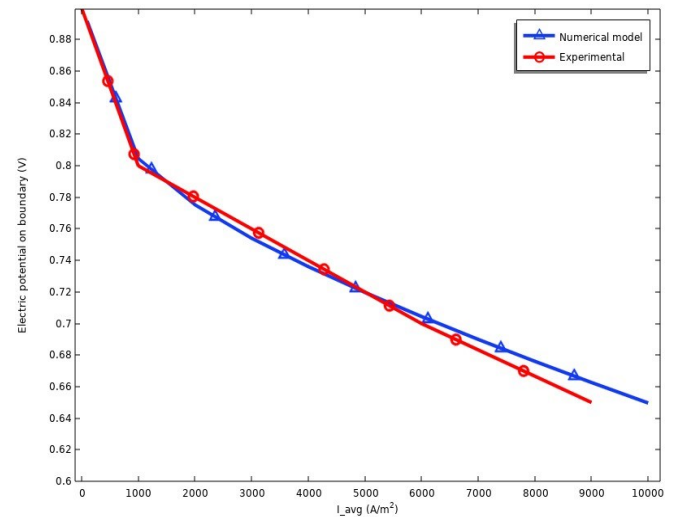


Figure 10 Comparison of current modeling results with experimental data

4.0 CONCLUSION

This study on the analysis of proton exchange membrane fuel cells (PEMFC) with 2-pass serpentine flow channels configuration using COMSOL Multiphysics software was conducted to address the crucial aspect of water management for optimizing fuel cell performance. By simulating parameters such as hydrogen and oxygen molar fractions, relative humidity, water activity, and electrolyte conductivity, the research aimed to deepen the understanding of how these parameters influence PEMFC operation. The findings underscored the significant impact of water activity on oxygen depletion and local current density distribution, highlighting the importance of effective water management strategies. The result simulation showed a substantially larger depletion of oxygen than hydrogen. Besides, the water activity is

higher near the air inlet, leading to increased oxygen content and local current density due to oxygen transport limiting the reaction rate. Also, the membrane conductivity is significant where water activity is high, impacting current density distribution, with oxygen and water content increasing current density until liquid water impedes gas transport in the cathode gas diffusion electrode at 1 A/cm². Furthermore, the outcomes obtained from the constructed model align well with the existing experimental data. This research contributes to advancing our understanding of the PEMFC with 2-passes serpentine flow channels configuration, emphasizing its practical applicability and reliability in real-world scenarios.

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Conflicts of interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper.

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