



Research Article

Design and parametric evaluation of proton exchange membrane fuel cell for enhanced performance

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ABSTRACT

The objective of the study is to explore the influence of various operating conditions on the performance of the Proton exchange membrane fuel cell (PEMFC) using COMSOL software. The effects of gas diffusion layer porosity, membrane conductivity, electrolyte thickness and operating temperature are studied. A structured hexahedral mesh was employed for the simulations. Essential geometric and operational factors are calculated analytically. The computational analysis of the PEMFC is conducted using a coupled approach that integrates free and subsurface flow, species transport and current distribution modules. The governing equations used in the simulation included conservation of energy, momentum, mass and species. The Joule heating, Butler-Volmer and the Nernst equation were incorporated to enable the modeling of reaction kinetics and cell performance. The uniqueness of this study lies in its comprehensive examination of the interactions between gas diffusion layer, gas diffusion electrode and membranes under various conditions, an area that has been less thoroughly investigated in the existing literature. Results reveal that higher gas diffusion layer porosity, increased electrolyte conductivity and reduced membrane thickness enhance fuel cell performance. A 26.54% increase in power density is observed when electrolyte conductivity is raised from 5.05 to 10.6, and a 21.19% improvement is achieved by decreasing electrolyte thickness from 254 μm to 127 μm . This data is vital for applications requiring high power output, such as in transportation or portable devices. Higher conductivity permits for better ion transport within the electrolyte, which can lead to more efficient reactions at the electrodes. This characteristic makes such fuel cells suitable for applications that demand rapid response times and high energy outputs. This study presents a novel approach to optimizing the performance of PEMFCs by systematically investigating the effects of critical operating conditions.

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INTRODUCTION

Proton Exchange Membrane Fuel Cells (PEMFCs) have fascinated substantial interest as an innovative clean energy solution, compact structure, valued for their high efficiency and competence to reduce greenhouse gas emissions. The hydrogen and oxygen is supplied to PEMFCs and it produces electricity through electrochemical reactions along with water and heat as byproducts. These qualities make PEMFCs great options for use in transportation, portable power and energy systems that are spread out. They support the worldwide movement toward sustainable and renewable energy sources. To achieve the best performance and durability, careful design choices are important. It is also necessary to understand the complex interactions among the cell components. The performance of a PEMFC is affected by several important factors. These include the design and materials of the membrane, gas diffusion electrode (GDE) and gas diffusion layer (GDL) as well as operational factors like porosity, temperature and reactant flow rates. The catalyst layer is very important for PEMFC. It is made of platinum based materials and helps to speed up the reactions that involve hydrogen and oxygen which are essential for the fuel cell to work. Platinum is expensive. Improving how well the catalyst layer works is a big challenge in designing PEM fuel cells. Recent advancements in computational modeling have greatly enhanced the study of factors affecting fuel cells in controlled virtual environments. These improvements allow for detailed analysis of various parameters. COMSOL Multiphysics software enables simulations that can capture the intricacies of species transport, current distribution and the effect of various structural and operational conditions on fuel cell output. These models offer invaluable insights into optimizing PEMFC performance by evaluating factors like electrolyte conductivity, membrane thickness, and GDL porosity. PEMFCs have the potential to serve as an economical power source across various sectors, including stationary, mobile and automotive applications [1]. The materials used for the main components of PEMFC are discussed and highlighted that the low power density is one of the problem with the PEMFC [2]. A two dimensional analysis of PEMFC was carried out using FORTRAN and the effects of porosity and pressure on the electrolyte potential were studied. The performance of the fuel cell increased with porosity [3]. A two dimensional analytical model for high temperature PEMFC in the range of 160°C was developed and the results obtained from the model were validated [4]. The influence inlet gas flow rate of the cathode, humidification temperature at cathode inlet, cell temperature on the performance of PEM fuel cells with interdigitated flow field and conventional flow field were studied from the experiments. The results reveal that the performance of the fuel cell increased with the increase of these chosen parameters [5]. The effects of channel depths and anode flow rates on the performance of small three pass serpentine flow field PEMFC were studied

with 200, 400, 600µm channel depth and noticed that the cell with 400µm yielded better performance [6]. The effect of channel path length in flow fields on the performance of PEMFCs was studied experimentally [7]. Commercial flow solver STAR-CD 3.26 was employed and studied the influence of serpentine flow-fields with various rib/ channel's cross section areas on the effectiveness of PEMFC. The numerical analysis discovered that narrower channel with wider rib spacing gives higher performance for stationary condition and the trend is different for automotive condition [8]. The experimental study on PEMFC revealed that the performance of the fuel cell was improved with the decrease of the thickness of the GDL and PEM thickness [9]. The effect of working pressure and temperature on the effectiveness of a PEM fuel cell is investigated using a 3D computational model [10]. They noticed that the performance was improved with increased cell temperature and operating pressure. An experimental analysis was carried out to study the self-regulating capability of open-cathode PEM fuel cells at different fan operating conditions and noticed that the fan speed remarkably affects the thermal and water management of the PEMFC [11]. The PEM fuel cell system thermal stability of UAVs was analyzed using MATLAB/Simulink at different altitudes and noticed the variations of the cooling load with altitude [12]. The hydrogen chilling efficiency for aviation PEM fuel cells was studied with simulation and experimental approach. The results of this study revealed that that effective hydrogen cooling is critical for maintaining thermal stability in aviation applications [13]. A system-level dependability model of the hybrid marine power plant with four PEMFC systems and a battery has been developed for 500 kW capacities [14]. The techno-economic aspects of flow channel design were investigated using Nafion membranes [15]. Compared the S-shaped and two-stage micro channel designs with standard designs and optimum one is identified [16]. The study highlighted that, how ejector configurations can contribute to enhanced performance in large-scale applications [17]. A human memory optimizer algorithm was presented to improve the modeling and characterization of PEM fuel cells and sensitivity and uncertainty analysis also carried out [18]. The artificial rabbits optimization procedure was used for parameter extraction in PEM fuel cells and their study emphasized the substantial role of parameter optimization in improving fuel cell performance [19]. The significance of cathode design for PEM fuel cells in transport applications was deliberated and presented analysis of cathode material choice for maximizing power density [20]. Various applications and types of fuel cells, the importance of the PEM fuel cell and the current status and challenges of the fuel cells are discussed [21]. The authors opined that hydrogen fuel cells show great promise in transforming clean energy resolutions and justifying the injurious properties of outdated fossil fuel-based systems on the atmosphere. PEMFCs have a relatively high specific power above 1,000 W/kg and are used in transportation, Aerospace,

stationary power applications. PEM fuel cells play a vital role in Sustainable energy systems and ecofriendly sustainability. Current developments in mathematical modeling of Proton Exchange Membrane (PEM) fuel cells have presented inventive iterative methods for parameter estimation, improving the correctness of voltage-current characteristic estimates [22, 23]. The previous investigators focused their studies on the materials and designs of components such as the gas diffusion layer (GDL), gas diffusion electrode (GDE) and membrane and channel designs. The effect of porosity, temperature and reactant flow rates, humidification levels on performance of fuel cell are studied experimentally. The interactions between GDL, GDE and membrane under varying conditions remain underexplored. There are gaps in realizing the interactions under varying operational conditions. The integration of advanced computational models for multi-scale phenomena is still emerging with limited studies focusing on parametric analysis using COMSOL Multiphysics software. Therefore, comprehensive studies are required to understand the interactions among PEMFC components. The aim of the current study is to evaluation of the influence of the operating conditions on the performance of the PEM fuel cell using COMSOL software with the intension of recognizing optimal operating conditions which enhances the performance of fuel cell.

MATERIALS AND METHODS

The platinum is chosen as the catalyst for the electrode surface. The design parameters for the PEMFC gas diffusion layer and catalyst layer were chosen based on established thumb rules, ensuring a balance between performance and durability. The PEMFC is designed based on the empirical relations available in the literature [24]. Three equations are used to calculate the catalyst layer. Equation (1) defines the catalyst loading, Equation (2) relates the geometric area to the platinum-to-carbon ratio and Equation (3) calculates the active surface area based on particle size and density.

$$L_a = \frac{m_{Pt}A_o}{A_c} \quad (1)$$

$$A_o = 2.2779 * 10^6 \left(\frac{P_t}{C}\right)^3 - 1.5857 * 10^6 \left(\frac{P_t}{C}\right)^2 - 2.01538 * \left(\frac{P_t}{C}\right) - 1.595 * 10^6 \quad (2)$$

$$A_c = \frac{6}{d_{Pt} \times \rho_{Pt}} \quad (3)$$

The thumb rules were applied to select the design parameters based on existing literature [13, 14]. Diameter of platinum particles ranges from 2 nm to 7 nm for pure platinum and 3.5 nm to 15 nm for platinum alloy. Platinum Carbon ratio ranges from 0.1 to 0.6. The mass loading of platinum is between 0.033 mg/cm² to 0.15 mg/cm². The porosity of the catalyst layer varies from 0.1 to 0.5. The thickness of the

gas diffusion layer is in the range of 0.11mm to 0.37mm. The porosity of the gas diffusion layer ranges from 0.78 to 0.8. The anode side of the fuel cell is designed with a linear gas channel, the dimensions of which are determined analytically based on the catalyst layer's characteristics. The specific dimensions used for creating the fuel cell geometry including the GDL, GDE and electrolyte are outlined in Table 1. Figure 1 illustrates the three-dimensional model of the designed fuel cell, which integrates these components to simulate the fuel cell's operational environment.

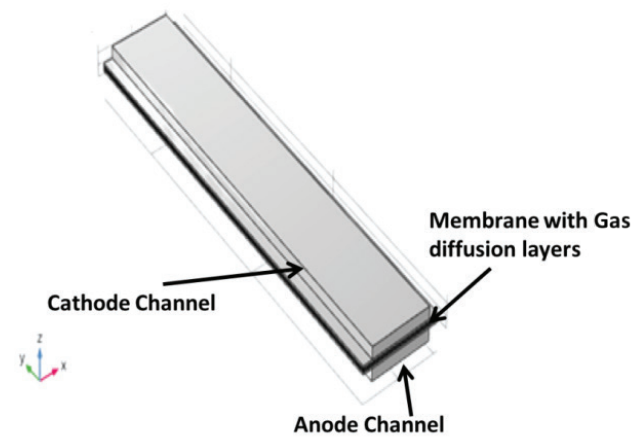


Figure 1. Model of the designed fuel cell for parametric study.

Table 1. Geometry and Operating parameters

S No.	Parameter	Value
1	Length of the channel (mm)	50
2	Channel height (mm)	1
3	Channel width (mm)	8
4	Rib Width (mm)	2.5
5	Thickness of GDL(μm)	190
6	Thickness of Membrane (μm)	127
7	Thickness of GDE (μm)	100
8	GDL Porosity	0.8
9	Conductivity of GDE (S/m)	222
10	Conductivity of Membrane (S/m)	9.825
11	Operating Temperature	800C
12	Inlet mass flow rate of H ₂ (kg/s)	0.1576
13	Inlet mass flow rate of O ₂ (kg/s)	0.6255
14	Mole fraction of H ₂ at inlet	0.96
15	Mole fraction of O ₂ at inlet	0.20
16	Mole fraction of H ₂ O at inlet	0.034
17	Mole fraction of N ₂ at inlet	0.76
18	Anode stoichiometry	2
19	Cathode stoichiometry	4

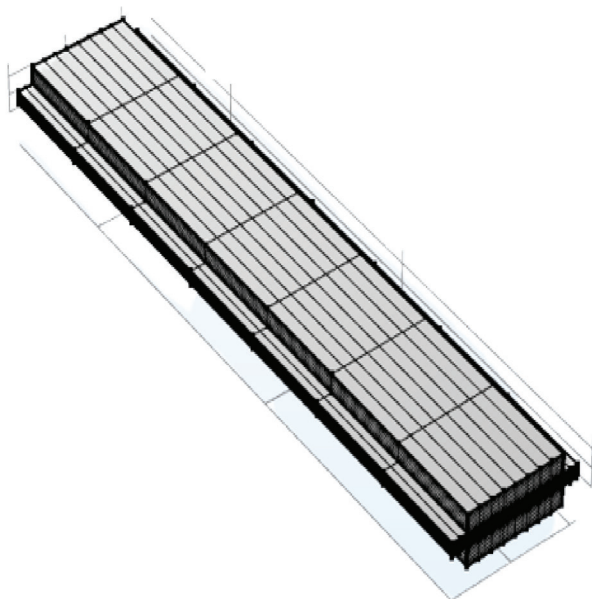


Figure 2. Meshed image of the modeled fuel cell.

In COMSOL multi-physics software, the computational domain of PEMFC is discretized using hexahedral elements and the mesh generated is depicted in Figure 2. The use of hexahedral mesh for the simulation provides good convergence and good results to capture the flow, heat and mass transfer physics. The computational domains include the air and fuel flow channels, as well as the GDL, GDE, and membrane. The geometry of fuel cell is a rectangular geometry and it is convenient to employ the structured mesh in computational domain. The number of elements used for fuel cell in computational domain is 1876.

Three-dimensional computational analysis is carried out by assuming steady flow conditions and the inlet gases are considered as ideal gases. The flow is presumed to be smooth and the fluid is immiscible. In the analysis of the PEM fuel cell, the flow is assumed to be laminar, considering the operating conditions and the dimensions of the flow channels. The working fluid is modeled as incompressible, as density variations due to pressure changes are negligible. The porous GDL, catalyst layers, and membrane are

treated as isotropic, implying uniform material properties in all directions. Additionally, the thermal properties of the materials are considered constant throughout the analysis and the membrane, catalyst layers, GDL are assumed to be homogeneous, ensuring uniform structural characteristics for simplification and consistency in the numerical model. The computational analysis of the PEMFC was conducted using a coupled approach integrating the free and subsurface flow, species transport, and current distribution modules. The free and subsurface flow module simulated the flow dynamics of the species under specified boundary conditions such as pressure and velocity, while the species transport module accounted for chemical reactions based on a defined diffusivity matrix. The current distribution module calculated the current density generated from the electrochemical reactions. A coupled analysis of these modules was performed to deduce the power density from the polarization curve. The numerical solution employed governing equations that encompassed the conservation of mass, momentum, energy and species. The solver also utilized the Butler-Volmer equation, Joule heating equation, and Nernst equation. This framework helped the modeling of reaction kinetics and cell performance [25-31]. The study takes into account the species transfer tool, current distribution node, open and permeable medium flow plugin, and fuel- cell component. The flow component is focused on the movement of substances in accordance to specific model parameters like pressure, velocity. The fuel-cell engine is in responsibility of connecting the electrochemical interactions with the other programs boundary conditions. The chemical reactions that take place for the selected diffusion matrix are under the control of the species transport module. The energy distribution element determines how much current density is produced by the process. As a consequence, a connected analysis of every module in the application was performed and the characteristic plot is used to evaluate the overall output of fuel cell. The materials selected for the Proton Exchange Membrane Fuel Cell (PEMFC) include copper for the current collectors due to its excellent electrical conductivity, which ensures efficient current collection and transport. For GDLs and GDEs, porous graphite is chosen for its high porosity, enabling efficient gas distribution and water removal. Additionally, platinum is coated on the GDE to

Table 2. Parameters varied for analysis

S No.	Parameter	Value
1	GDL Porosity	0.6 to 0.8 in the steps of 0.1
2	Operating Temperature	60 °C to 80 °C in the steps of 10 °C
3	Membrane Conductivity	5 S/m to 11 S/m
4	Membrane Thickness	Nafion 115,117 and 1110 membranes
5	Catalyst layer thickness	100µm to 60µm in the steps of 20µm

enhance catalytic activity for both the hydrogen oxidation reaction and oxygen reduction reaction. The membrane material selected is Nafion 117, a sulfonated tetrafluoroethylene-based copolymer, which offers superior proton conductivity, chemical stability, and mechanical strength, making it ideal for PEMFC applications. A set of parameters, as outlined in **Table 2**, has been chosen for a systematic study of the fuel cell's performance under various operating conditions, enabling an in-depth analysis of its efficiency and overall effectiveness.

RESULTS AND DISCUSSION

Validation

The following are the geometrical parameters used for the geometric model of the PEMFC. The width and depth of the anode and cathode flow channels are 50mm and height is 10mm. The thickness of gas diffusion layer and gas diffusion electrode is 190 μm and 10 μm respectively. Thickness of the membrane is 127 μm . Thickness of the current collectors is 2 mm. The PEMFC model was created in COMSOL software for validation is depicted in Figure 3.

The computed V-I characteristics of the PEMFC were compared with the experimental data [9] at 80°C and RH 80% as shown in Figure 4. The characteristic curve demonstrates the current density variation with the voltage for both the experimental and computational results. The results establish a strong agreement with the experimental findings. However, the minor deviations are noticed due to the stimulation over potentials govern at low current densities because of slow electrochemical reaction rates. This validated computational approach was used for the subsequent parametric analysis.

Polarization curve

The plot depicted in Figure 5 is a polarization curve of a fuel cell, shows the dependency between the current

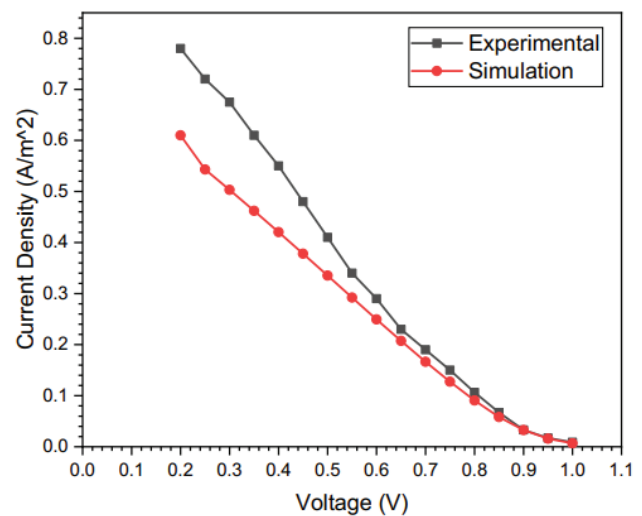


Figure 4. Validated V-I Characteristics.

density and voltage within the operational voltage range of a fuel cell. The data indicates that the proposed fuel cell generates higher power outputs specifically within the voltage range of 0.3 to 0.5 V. The slope of the curve is more at low current densities due to activation losses caused by sluggish reaction rates. The voltage decreases slowly with the increase in current densities and this trend indicates that the prevalence of ohmic losses arising from resistance to ion transport in the electrolyte and electron flow in the cell [3].

Electrode potential

The contours of electrode potential are depicted in Figure 6. The cell voltage differential is greater at the middle of the cell than the ribs. This is because the interaction of the reagents occurs at the center of the cell, whilst the reaction at the ribs is gradual.

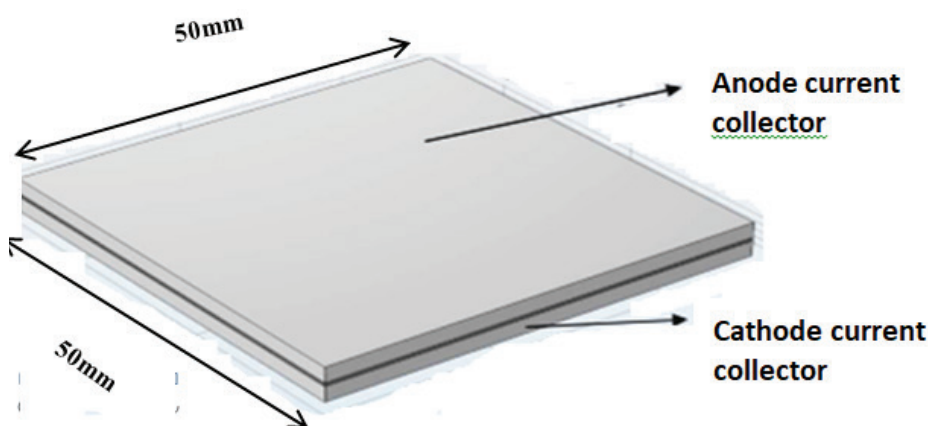


Figure 3. Fuel cell model employed for validation.

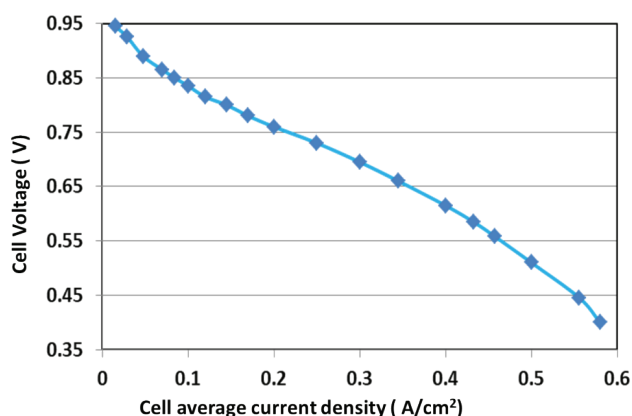


Figure 5. V-I Characteristics of the designed fuel cell.

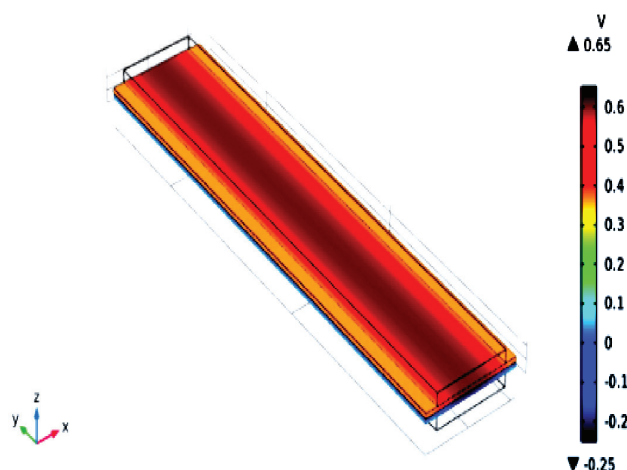


Figure 6. Contours of electrode potential of the fuel cell.

Mole fraction of hydrogen and oxygen

The hydrogen mole fraction decreases progressively from inlet to outlet of the fuel cell. This reduction is attributed to the consumption of hydrogen in electro-chemical reactions on the anode side, where it contributes to generating electricity. As hydrogen molecules react, protons move across the electrolyte membrane and the electrons are directed along the external circuit an electric current is produced. Figures 7 and 8 illustrate the hydrogen and oxygen mole fractions through the cell. The drop in hydrogen mole fraction in Figure 7 confirms its utilization during the reaction process. Figure 8 shows the oxygen mole fraction trends, which mirror those of hydrogen on the cathode side. Oxygen consumption increases towards the output as it reacts with protons and electrons to form

water, completing the electrochemical process and confirming effective reaction kinetics within the cell.

Velocity profiles

The simulated flow within the fuel cell operates under laminar conditions, as evidenced by the velocity contours shown in Figure 9 and Figure 10 at cell voltage is 0.5 V.

These contours illustrate that velocity reaches its peak at the center of the flow channel, where the reactant gases have unobstructed movement. This high central velocity facilitates effective passage of reactants to the reaction sites, crucial for sustaining the electrochemical reactions. At the channel edges, however, the velocity of the reactant gases drops to zero, adhering to the no-slip condition imposed by the channel

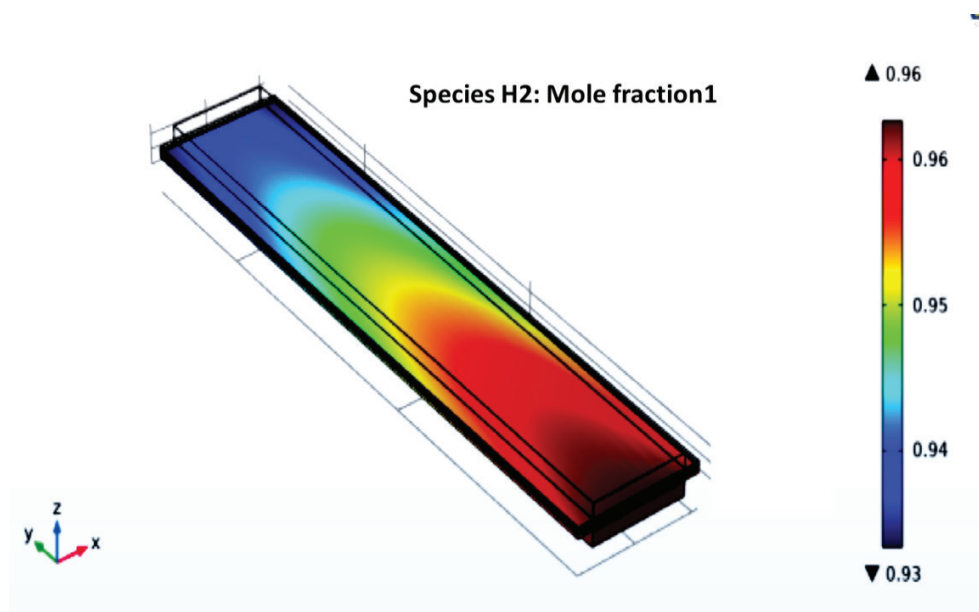


Figure 7. Hydrogen mole fraction contour of designed fuel cell.

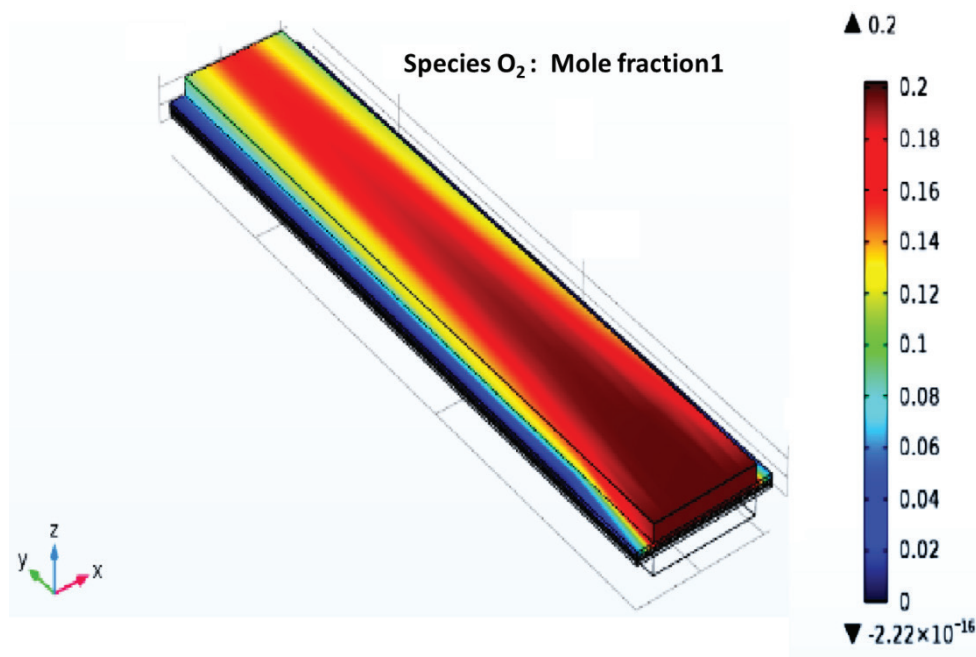


Figure 8. Oxygen mole fraction contour of designed fuel cell.

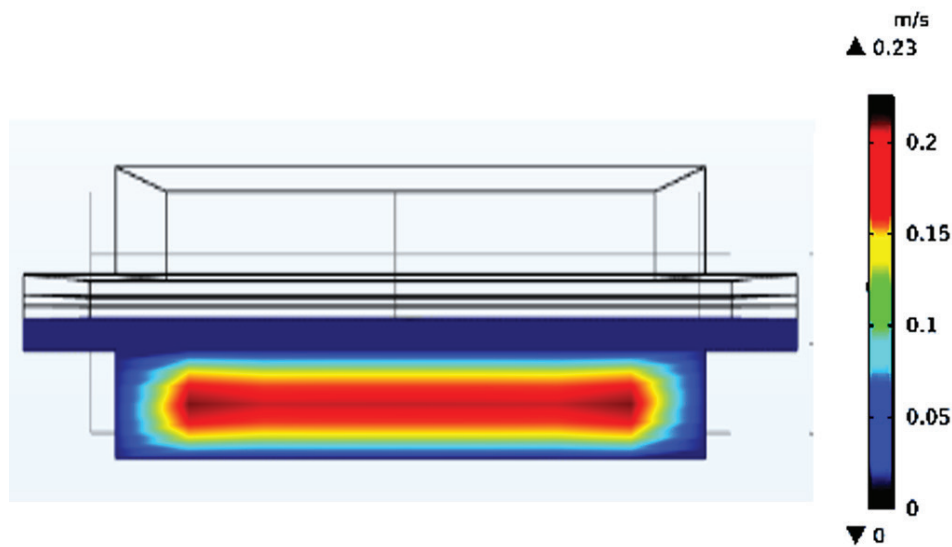


Figure 9. Velocity contours of fuel cell on anode side.

walls. This boundary condition leads to a steady reduction in velocity from the channel center to the walls, characteristic of laminar flow profiles. The resulting velocity gradient not only impacts reactant distribution but also influences mass transfer rates, highlighting the role of channel geometry and flow conditions in optimizing fuel cell performance.

Effect of GDL porosity

Figure 11 presents the fluctuation of current density with voltage, demonstrating that fuel cell effectiveness is

positively influenced by higher porosity values of the GDL, particularly at lower operating voltages. At these voltages, the effect of GDL porosity is more pronounced, as greater porosity facilitates enhanced gas diffusion. However, it leads to uneven distributions temperature inside the cell. These changes influence the local kinetics of reaction, as higher temperatures enhance electrochemical reactions rate, while lower temperatures can decrease reactant consumption and the performance decreases. Thus, the interaction between GDL porosity and temperature changes is important for

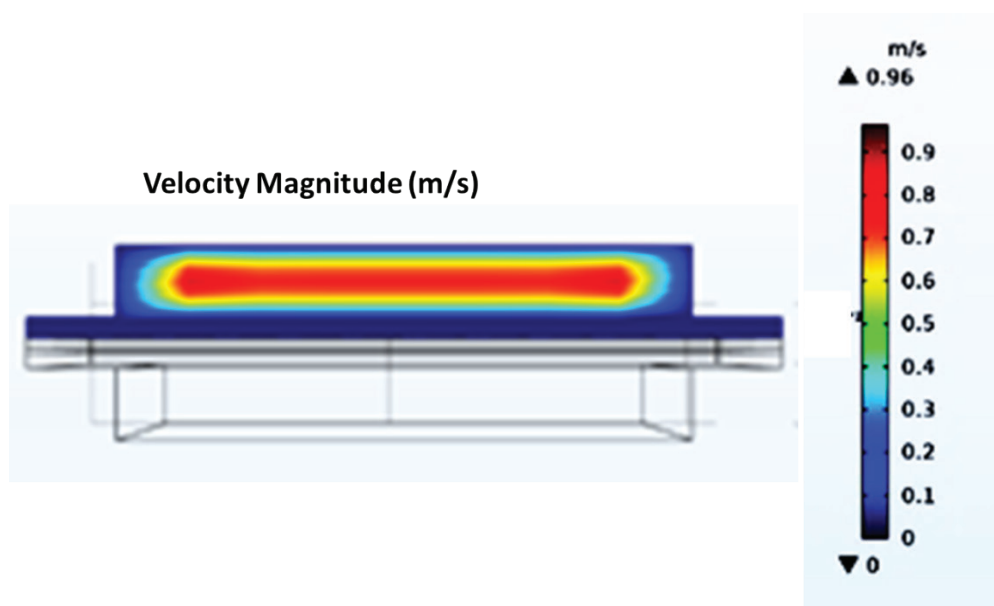


Figure 10. Velocity profile of fuel cell cathode side.

optimizing cell performance This improved diffusion allows for a more consistent and ample supply of reactant gases, such as hydrogen and oxygen, at the reaction zones, thus increasing the generation of electrons and improving overall cell efficiency. This phenomena also noticed by Larbi et al [3]. This is likely due to the reduced role of diffusion limitations at higher voltages, where other factors such as ohmic resistance and reaction kinetics become more dominant. Consequently, optimizing GDL porosity is especially beneficial at lower voltages, where it plays a crucial role in maintaining efficient fuel cell operation by ensuring a steady supply of reactants to the electrodes.

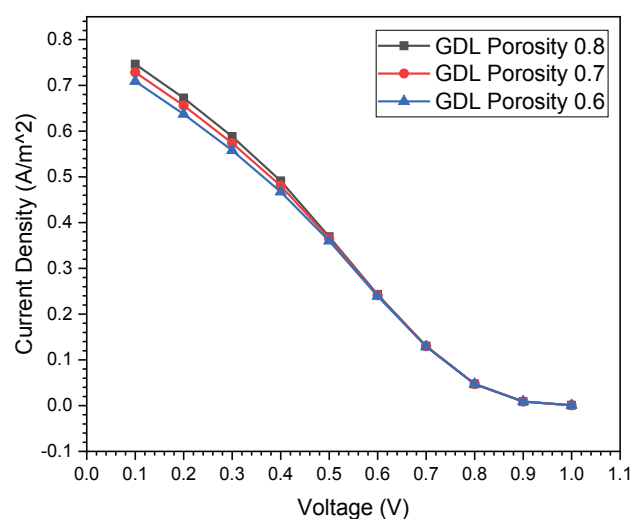


Figure 11. Polarization graph at different GDL porosity.

Effect of Operating Temperature

Figures 12 and 13 illustrate the voltage-current (V-I) characteristics and power density variation with voltage across a temperature range of 60 to 80°C. The V-I curves and power density profiles display only slight changes over this temperature range, indicating that the PEM fuel cell (PEMFC) maintains stable performance within these operational temperatures. This consistency suggests that moderate temperature variations between 60 and 80°C do not substantially affect the electrochemical reaction rates or the overall efficiency of the PEMFC. As a result, the fuel cell can function effectively within this temperature range

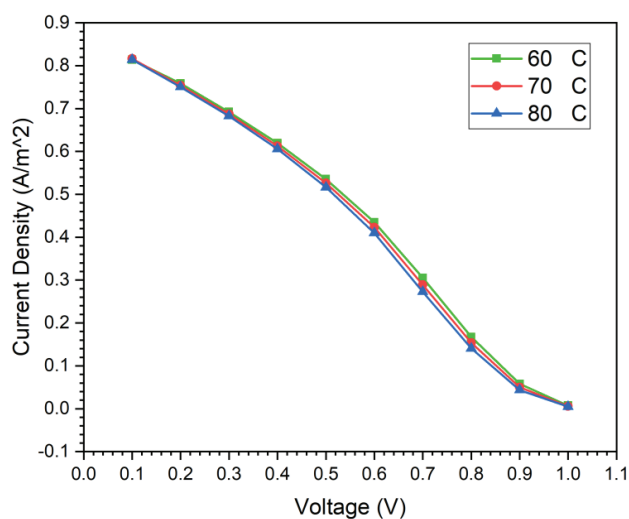


Figure 12. Polarization graph for the effect of operating temperature.

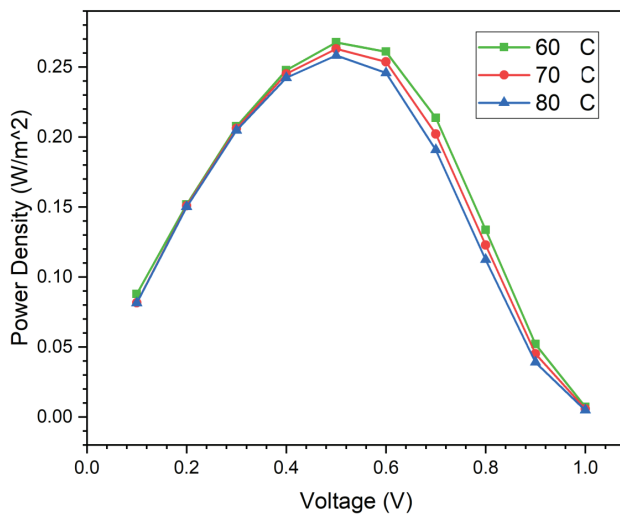


Figure 13. Power density curve for the effect of operating temperature.

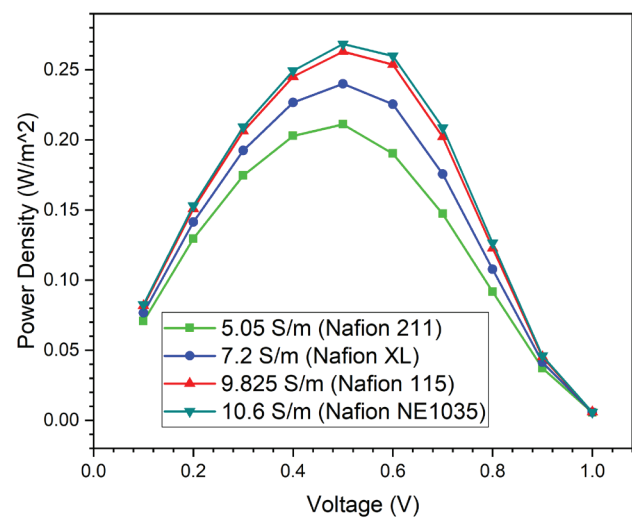


Figure 15. Power density curve for the effect of membrane conductivity.

without the need for intensive thermal regulation. This stability is advantageous for practical applications, where maintaining precise temperature control may be challenging, reinforcing the robustness of PEMFCs in various operating environments.

Effect of Electrolyte Conductivity

The variation of current density with voltage of different Nafion membranes is typically analyzed to realize the dependence of ionic conductivity on fuel cell effectiveness. The conductivity of Nafion membranes is a critical factor because it influences the ionic transport of protons from positive electrode to negative electrode, a key process in

fuel cell operation. Higher conductivity means better proton conductivity, which allows for more efficient charge transfer and improved fuel cell performance. The comparison of the Nafion membranes shows a clear trend depicted in Figure 14 and Figure 15. Higher ionic conductivity leads to better fuel cell performance. The fuel cell demonstrates improved performance as conductivity increases, due to enhanced proton mobility that reduces internal resistance and improves power output. This trend is consistent with findings [11,12,14]. Therefore, selecting a membrane with higher conductivity is essential for optimizing fuel cell efficiency, especially in applications requiring high power densities.

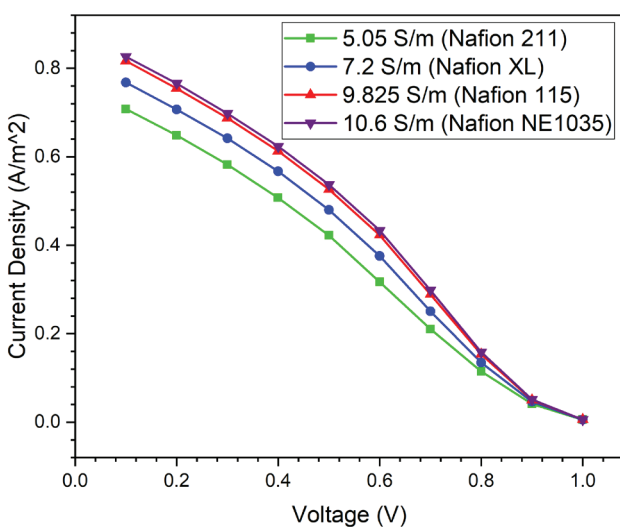


Figure 14. Polarization graph for the effect of membrane conductivity.

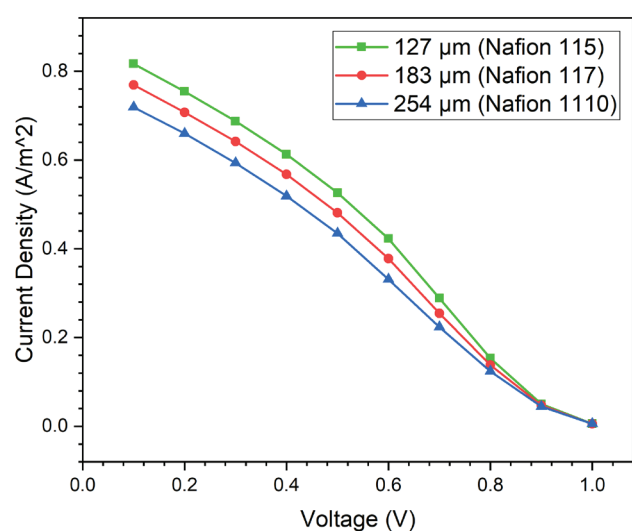


Figure 16. Polarization graph for the effect of membrane thickness.

Effect of Electrolyte Thickness

The performance characteristics demonstrated in Figure 16 show that thinner electrolytes provide better fuel cell performance and the same trend was observed by Kösters et al. [13]. Because an increase in thickness causes an increase in resistivity, a barrier is formed against flow of protons from the positive electrode to negative electrode. Thus the effectiveness of the cell decreases.

Effect of Catalyst Layer Thickness

Figure 17 and Figure 18 depicts the characteristics curves. The thickness of the catalyst layer has very negligible effect. As a result, this is not a major parameter for improving fuel cell performance. The plot illustrates the fluctuation of current density with voltage for three different catalyst layer thicknesses of 100 μm , 80 μm and 60 μm .

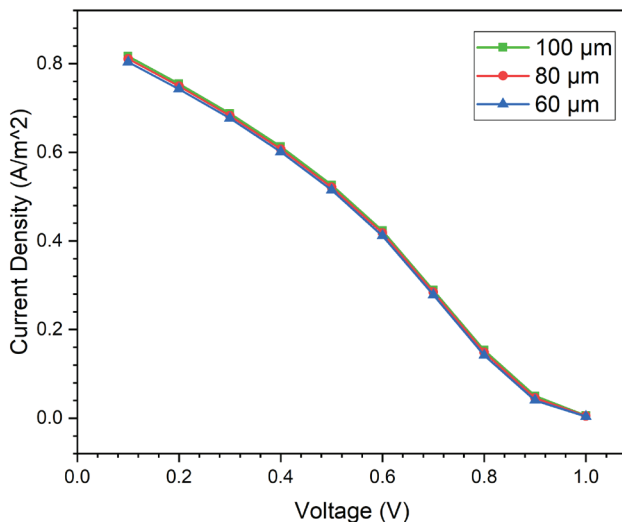


Figure 17. Catalyst layer thickness influence on V-I curve.

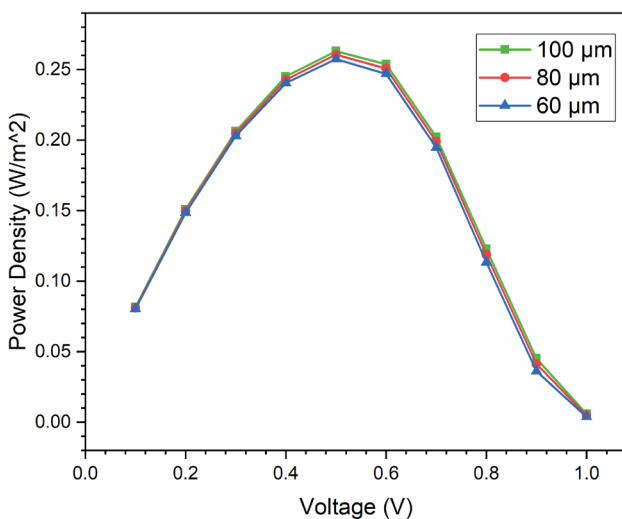


Figure 18. Variation of power density with voltage.

The present study offers some different contributions in the performance analysis of fuel cell. COMSOL Multiphysics software is employed for the systematic parametric study of fuel cell. This study provides the understandings into their specific effects on fuel cell performance. The computational analysis considered the design variables and evaluated their combined influence, which has not been extensively addressed in prior research. The results indicate that, a substantial 26.54% increase in power density with improved electrolyte conductivity, providing new insights into the optimization of fuel cell efficiency.

CONCLUSION

The following are the key conclusions from the parametric analysis of PEM fuel cell.

This research work provides valuable insights for designers, emphasizing electrolyte conductivity, thickness, and gas diffusion layer porosity as the most significant parameters for optimizing PEM fuel cell performance.

An increase in electrolyte conductivity from 5.05 to 10.6 was noticed to improve power density by 26.54%, while a decrease in electrolyte thickness from 254 μm to 127 μm resulted in a 21.19% development.

A gas diffusion layer with higher porosity is recommended to enhance fuel cell performance.

The fuel cell achieves peak performance at an operating voltage of 0.5V under all parameters studied

The operating temperature and catalyst layer thickness have a minimal impact on performance.

This study enables proton exchange membrane fuel cell in sustainable transportation, portable power systems, renewable energy integrated systems, marine and aeronautical and space applications.

This study contributes to improving PEM fuel cell performance, crucial for achieving global sustainability targets, as it encourages the adoption of clean energy technologies for efficient and pollution-free power generation.

NOMENCLATURE

L_a	Catalyst loading, mg/cm^2
m_{pt}	Mass of platinum catalyst, g
A_c	Active surface area of the platinum catalyst, mm^2
A_o	Geometric area of the catalyst layer, mm^2
d_{pt}	Diameter of the platinum particles, nm
ρ_{pt}	Density of the platinum, kg/m^3
P_t/C	Platinum to Carbon ratio

AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw

data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

STATEMENT ON THE USE OF ARTIFICIAL INTELLIGENCE

Artificial intelligence was not used in the preparation of the article

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