

Original Article

# Modelling and Simulation of Polymer Electrolyte Fuel Cell with Cylindrical Architecture

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**Abstract** - In the last decade, constant innovation and research have been done in the field of clean energy generation. Researchers are in search of feasible options for clean energy generation methods. Polymer electrolyte membrane fuel cell is one of those methods, but it should be compact, have less weight, and be cost-efficient to be acceptable for various applications. In such scenarios cylindrical architecture of a PEM Fuel cell becomes a feasible option to be considered. Because it is designed to eliminate the cost of bipolar plates and precisely machined flow channels, which reduces the overall cost, it makes it lighter in weight and compact in size. It possesses high volumetric and gravimetric power density compared to the planar fuel cell. This paper presents the electrical analysis and modelling of the cylindrical architecture of the PEM fuel cell, where the results obtained are compared with those of the planer PEM fuel cell.

**Keywords** - Fuel cell, Cylindrical, Membrane, PEMFC, Bipolar plates.

## 1. Introduction

In the era of global development and industrialization, the demands for global energy are getting higher daily. The giant economies in the world are growing day by day, increasing production in their state, and the first raw material for the production is energy. According to the World Energy Council, if the predicted pattern of the global economy's growth comes true, the global energy demand will increase by 45% - 60%. In order to fulfil these huge demands, the primary source is fossil fuels, but fossil fuels result in degradation and disruption of the environment [1].

Researchers have been researching sustainable methods other than renewable energy sources to fulfil this global energy demand for the last 2-3 decades. In such a scenario, a fuel cell becomes one of the feasible options to be considered. A device that converts the chemical energy in the fuel by means of an electrochemical process into electric energy is known as a fuel cell. This process is carried out by supplying fuel, an oxidising agent, to get electricity as the output. The substance capable of chemical oxidation can be supplied as fuel to the fuel cell. This fuel is burned galvanically at the anode, and the oxidising agent is supplied at the cathode, where the reduction process occurs [2]. In such a scenario, hydrogen, the simplest form of all molecules, becomes a feasible option that is contemplated as a fuel for the fuel cell when the proton exchange membrane fuel cell is considered.

Because of its weight, hydrogen has the highest energy content of any fuel. Hydrogen becomes a feasible option because it is easily available in the atmosphere and mainly creates zero emissions, an important point to consider in today's environmental conditions [3].

Hydrogen is a concentrated energy source, so it can conveniently be used as fuel for proton exchange in membrane fuel cells; as it is an inexhaustible source of energy, availability of fuel will be inserted, and it can be generated easily from liquid (water) by means of the electrolysis process. The important parameter that makes hydrogen a proper fuel that is commercially accepted is the higher gravimetric energy density of the hydrogen [4]. The hydrogen fuel cell commercially used generally has a planar structure consisting of components such as anode and cathode current collector, the membrane electrode assembly, and one more component, bipolar plates [5].

The costing model of the fuel cell proposed by Direct Technologies, Inc (DTI) stated that the overall cost distribution of fuel cells among every component shows 29% of the total cost contributed by the bipolar plates [6]. According to the study report by Jayakumar et al. [8]. The oral cost contribution of bipolar plates after considering two different types of graphite plates is 13 -42% in 1Kw of stack. The bipolar plates also increase the overall weight of the fuel



cell. The study by Xiong et al. [9] stated that the bipolar plate comprises two materials: graphite and metal. Graphite is considered because of its high chemical stability and anti-corrosiveness as well as high electrical conductivity, but because of its brittleness, it becomes difficult to manufacture, which increases the cost of the bipolar plates because of the precise manufacturing requirement [7]. In the second case, metal is considered because of the high electric conductivity and ease of machine, but metal is corrosive in nature, and precious metals like titanium and platinum are to be used. So, in such cases, the overall cost of the bipolar plate is higher.

An important area of research is the dearth of thorough modeling and comparative analysis of cylindrical PEM fuel cells. With little assessment of the advantages and disadvantages of cylindrical structures, the majority of research focuses on planar systems. The goal of this research is to develop a fuel cell construction that improves electrochemical performance, mechanical stability, and heat distribution. A computer model to simulate the performance of cylindrical PEM fuel cells' performance is developed to close this gap. Through a methodical comparison of cylindrical and planar buildings, this study emphasizes cylindrical designs' useful benefits and compromises. Using sophisticated simulations to measure the effects of design changes on stability and efficiency is innovative and advances fuel cell technology.

The cylindrical (Cy.) architecture of the fuel cell Kelly eliminates the bipolar plates, solving the above-stated problems. In the study by P. Sapkot et al. [10], a cylindrical geometry of the fuel cell reduces the overall mass cost. It makes the fuel cell self-breathing, which means no external energy or system is needed to supply an oxidising agent (oxygen), as shown in Figure 1.

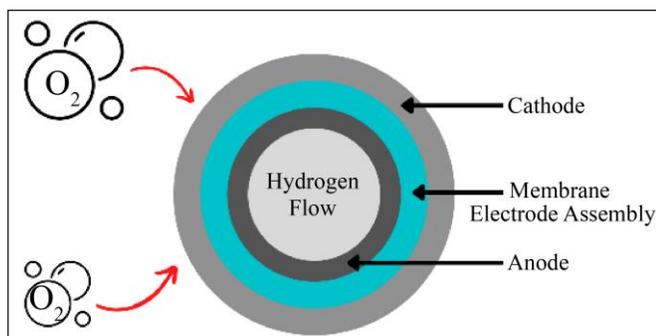


Fig. 1 Cut section view of cylinder fuel cell

In the study by A. Bhosale et al. [11], Higher gravimetric and volumetric power densities were offered in cylindrical fuel cells compared to the planer fuel cell. This paper focuses on modelling the cylindrical polymer electrolyte membrane fuel cell with slotted anode and cathode structure by considerable design assumptions and calculations. The performance analysis of the fuel cells is done on the analysing

software ANSYS®, where electric output is represented graphically by I-V graphs and compared to the planar structure output.

Bipolar plates are the primary cause of the problems with conventional planar PEM fuel cells, which include difficult production, uneven temperature distribution, and expensive material prices. Because they do not require bipolar plates, are lighter and less expensive, and have better mechanical stability and temperature control, cylindrical PEM fuel cells provide a revolutionary substitute. Higher gravimetric and volumetric power densities are reported by A. Bhosale et al. [11], while studies by P. Sapkot et al. [10] demonstrate that cylindrical designs allow self-breathing operation, improving efficiency. A thorough computational comparison with planar structures is still lacking, though. In order to close that gap, this work models and analyzes cylindrical PEM fuel cells using ANSYS®. Next-generation fuel cell technology is advanced by the comparative assessment offered by the I-V characteristic graphs, which emphasize cost savings, structural enhancements, and efficiency advances.

The information presented in the paper provides a comprehensive overview of the latest research and developments in Proton Exchange Membrane Fuel Cells (PEMFCs). Several studies have been referenced, highlighting various aspects of PEMFC technology, such as cost reduction, technical challenges, material improvements, performance optimization, and environmental considerations. There is a good overview of ongoing efforts to improve PEMFCs, including reducing platinum use, enhancing efficiency, and addressing issues related to fuel storage and manufacturing. Key research, such as advancements in materials (e.g., carbon nanotubes and novel cathode current collectors), manufacturing processes, and optimization algorithms, is well-presented. The studies also consider the environmental impact of PEMFCs and their potential in sectors like electric vehicles and renewable energy, creating a comprehensive background on the topic.

The primary objective is to generate energy through sustainable methods. This includes addressing the weight issue in the current PEMFC models, removing the integrated oxygen supply system, and improving heat dissipation and management. Additionally, efforts aim to enhance water management within the cell, eliminate the need for bipolar plates, and reduce the overall size of the cell for increased compactness. The focus is also on improving the fuel cell's efficiency while lowering its overall cost.

The study of Polymer Electrolyte Fuel Cells (PEMFC) with Cylindrical Architecture might benefit from case studies from various sectors. For example, cylindrical fuel cell stacks maximize efficiency and space in hydrogen-powered electric vehicles such as Hyundai's NEXO and Toyota's Mirai. PEMFCs are used for remote energy solutions and grid

stability in renewable energy, and nations like Germany use them to store excess energy from renewable sources. Cylindrical PEMFCs are also utilized in critical infrastructure backup power systems and portable power generators, including those employed in disaster assistance. They also contribute to the aircraft and marine sectors, where weight and space efficiency depend heavily on compact designs. Case studies from organizations and research centers such as Plug Power, Ballard Power Systems, and ZeroAvia demonstrate the various real-world applications of PEMFC technology. These actual cases illustrate the viability of PEMFC developments and provide light on the difficulties and advantages of this technology.

## 2. First Computer-Aided Design (CAD) Modelling

The planar architecture of the PEMFC consists of anode and cathode current collector and membrane electrode assembly along with bipolar plates. This cylindrical architecture eliminates the bipolar plates and forms PEMFC by layers of cathode current collector PEM assembly and innermost anode current collector, making it easy to operate [9]. The anode acts as a pipe through which hydrogen flows from inside. The anode has to perform two important roles in working the cell: first is hydrogen supply without any leakages and second is to collect the current produced due to the process. In such cases, the material used for the anode must contain certain properties to carry out its role, like endurance to the high compression, because the internal pressure between each layer of PEMFC must be high in order to avoid contact resistance. If the contact resistance is high, then the overall output will be affected. So, to tackle this, the material needs to endure high compression [10]. The material should be convenient for fabrication as slots are to be machined on an anode current collector, as shown in Figure 2, so the hydrogen can be passed easily to the PEM Assembly. So, the anode must be perforated. The material must possess good electrical and thermal conductivity, as the final output is electricity, which is collected by an anode; the material needs to be electrically conductive [11]. The overall process generates heat that needs to be transferred to the outermost layer of PEMFC so that it gets dissipated into the atmosphere. In that case, the material should be thermally conductive [12].

According to all of the above requirements, brass becomes the feasible option to be considered. The anode and cathode both play a similar role in collecting the electrons formed during the chemical reaction in PEMFC. So, the cathode is also made up of brass. But the thickness of the cathode as compared to the anode is less as it is not directly subjected to the pressure of hydrogen flow, and in order to keep the overall volume of the cell low, the thickness is kept smaller but permissible to the compression for low contact resistance [13, 14]. Along with anode and cathode to proton exchange, membrane assembly is also one of the important

components of PEMFC. It is the heart of the whole system as the chemical reaction between hydrogen and oxygen happens to add a proton exchange membrane [15].

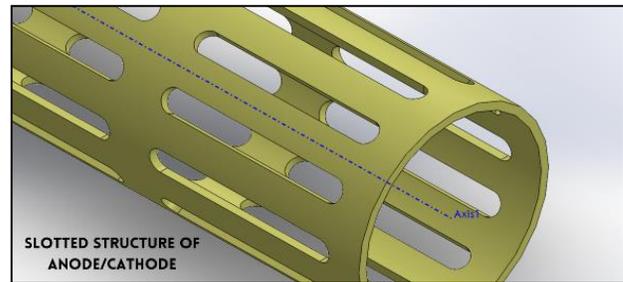


Fig. 2 Slotted structure of anode and cathode current collectors

So, the PEM Assembly consists of two catalyst layers between the membranes present, forming a sandwich-like structure of catalysts in the membrane. The catalyst fastens up reactions that take place between hydrogen and oxygen, resulting in greater outputs [16]. Generally, the catalysts used in PEMFC are of three types: platinum-based catalysts, non-platinum-based catalysts and organometallic complexes. The catalyst must possess high activity ability, high durability under special conditions, and cost efficiency. According to the requirements, the modified platinum-based catalysts named platinum ruthenium combination catalysts are used commercially. It is considered because of lower overpotential and cathodic activities higher for oxidation and reduction reaction of hydrogen and oxygen, respectively. Hence, a chemical reaction takes place inside the fuel cell; the inside environment is generally acidic, so this modified platinum-based catalyst possesses the ability to withstand it [17-19].

Other than catalyst and polymer electrolyte membrane, the gas diffusion layer is also present on the inner and outer sides of the membrane electrode assembly. The GDL carry out the role of supplying physical aid to the structure, transportation of fuel in the direction of the catalyst layer at the same time, and water vapour to the membrane in order to improve the ionic conductivity of the cell, as well as GDL ensures low humidity at the membrane [20, 21]. As water is one of the by-products of the PEMFC, its overall percentage in cells must be maintained. GDL ensures the drain out of excessive water present in this cell in order to avoid electrode flooding [20, 22]. GDL is mainly made of carbon fibre, carbon cloth or polytetrafluoroethylene. Among these, carbon fibre is commercially acceptable as it has a macroporous substrate that acts as a gas distributor and corrects current. It also has a Microporous Layer (MPL) that manages its two-phase water flow. Carbon fibre fulfils the core ability of GDL, namely hydrophobicity, high conductivity, and mechanical strength [23, 24].

In PEMFC, the polymer electrolyte membrane is the middle layer; generally, PEMFC has solid polymer electrolyte. The electrolyte must be structurally stronger to

withstand the compression pressure; at the same time, it must be durable and flexible. Most importantly, it should possess high proton conductivity to fulfil its role in the fuel cell. Generally, thinner membranes are used for hydrogen and oxygen fuel cells to avoid ohmic losses [25, 26]. Material developed in 1996 by Dr. Walther Grot named Nafion has been commercially used. As it possesses high conductivity, it moderately swells water and can be used in applications where the operating temperature is up to 190 degrees celsius. The water in the fuel cell positively affects nafion and conductivity. It controls the formation of connectivity of the proton pathway in nafion and results in a higher proton transfer rate [27-29]. The working of cylindrical PEMFC is shown in Figure 3, where hydrogen passes from inside the cell while oxygen passes over the cell. The closed chamber is for analysis purposes, but the cell is open to the ambient air in real working conditions.

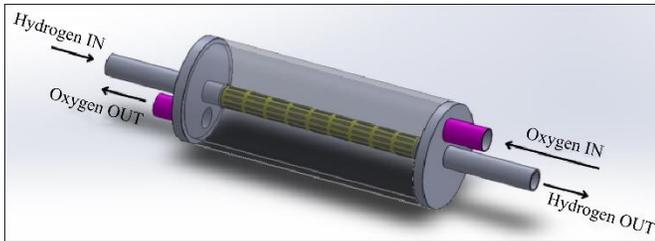


Fig. 3 Working of cylinder PEMFC

### 3. Design Calculations

#### 3.1. Design Assumptions

1. Mass flow rate of hydrogen {Q} -  $7.25 \times 10^{-4}$  m<sup>3</sup>/min
2. Velocity of hydrogen {V} - 12 m/min

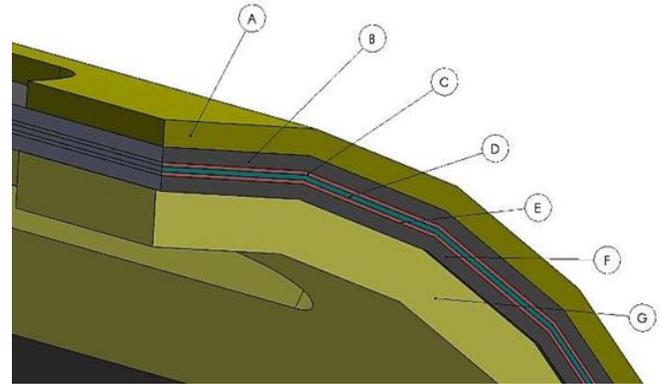
$$3. \text{ Inner diameter of anode } \{D\} - 1.13 \sqrt{\frac{Q}{V}} \quad [30]$$

Therefore, the internal diameter of the anode is 8.78mm.

#### 3.2. Thickness of Each Layer of Cylinder PEMFC

The design of the components in a tubular Proton Exchange Membrane (PEM) Fuel Cell (PEMFC) is shown in Figure 4. The anode layer's thickness range is 600  $\mu\text{m}$  to 800  $\mu\text{m}$ , and the average thickness is considered 700  $\mu\text{m}$ , which is 0.7mm. For Gas Diffusion Layers (GDL), the thickness range is 150  $\mu\text{m}$  to 250  $\mu\text{m}$ , and the average thickness considered is 200  $\mu\text{m}$ , which is 0.2mm. The catalyst layer for anode has a range of thickness from 20  $\mu\text{m}$  to 80  $\mu\text{m}$ , and the average thickness considered is 50  $\mu\text{m}$ , which is 0.05mm.

For the catalyst layer of the cathode, the average thickness remains the same as for the anode, which is 0.05mm. The thickness range for the Proton Exchange Membrane (PEM) is between 60  $\mu\text{m}$  and 80  $\mu\text{m}$ , and the average thickness considered is about 0.07mm. The outermost layer of the fuel cell, which is the cathode, has a thickness range from 250  $\mu\text{m}$  to 450  $\mu\text{m}$ , and the average thickness considered is about 0.35mm.



(A- Cathode, B- GDL for O<sub>2</sub>, C and E- Catalyst, D- PEM, F - GDL for H<sub>2</sub>, G- Anode)

Fig. 4 Layers of T-PEMFC

The image of the model of the cylinder PEMFC is shown in Figure 5. This model is prepared using modelling software named SOLIDWORKS® as per the design calculations and thickness stated above.

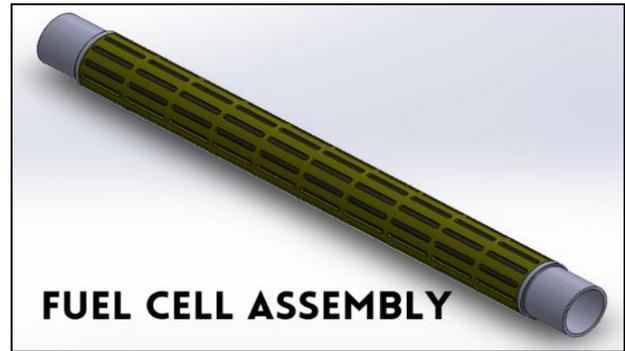


Fig. 5 Cylindrical fuel cell

#### 3.3. Design Analysis

Studying Tubular Proton Exchange Membrane Fuel Cells (T-PEMFCs) is essential to comprehending their properties and modes of operation. In this study, we analyzed the T-PEMFC model using Computational Fluid Dynamics (CFD) methods, with an emphasis on electrochemical processes, species transport, and fluid flow under different operating circumstances. Using SolidWorks, we produced a comprehensive three-dimensional model of the fuel cell, including all its vital parts, such as the flow channels, catalyst layers, gas diffusion layers, and proton exchange membrane. The analysis process involves simulation setup, mesh creation, and CFD simulation.

The Tubular Proton Exchange Membrane Fuel Cell (T-PEMFC) was first modelled geometrically in SolidWorks, shown in Figure 6 and then imported into ANSYS Workbench to start the analytical process. The model had essential elements such as the hydrogen and oxygen flow channels, catalyst layers, gas diffusion layers, and proton exchange membranes. Following the geometry import, we established

solid zones for the membrane and catalyst layers and fluid zones for the reactant channels. We then named each component's solid zones (like the proton exchange membrane and catalyst layers) and fluid zones (like the hydrogen and oxygen flow channels). This simplified the simulation setup and enabled application of boundary conditions and material properties effectively.

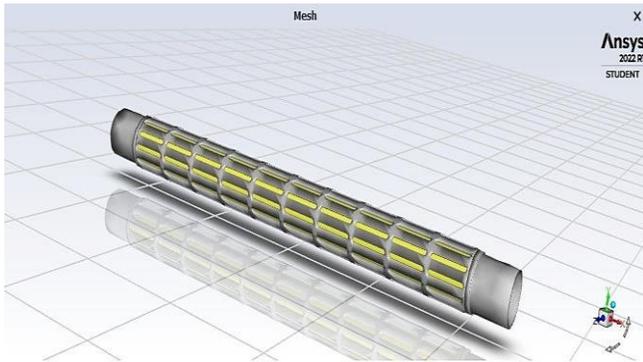


Fig. 6 Fuel Cell Assembly Imported In ANSYS Workbench

We used ANSYS Workbench to generate the mesh after defining fluid and solid zones and identifying the T-PEMFC model's components. The geometry was broken up into smaller components, places that needed more precision and had finer divisions. Using a finer mesh to capture velocity gradients and boundary layer effects, the fuel cell was meshed using tetrahedral elements with particular emphasis paid to the boundary layers close to the walls shown in Figure 7.

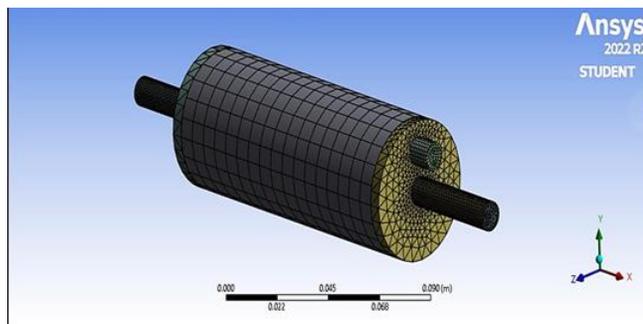


Fig. 7 Mesh Generation and Boundary Layer Refinement in the T-PEMFC Model

Quality tests were conducted to determine the integrity of the mesh, analyzing factors including aspect ratio and skewness. We imported the fine-tuned mesh into ANSYS Fluent and used a planar fuel cell model to define boundary conditions to set up the simulation. After setting up the simulation environment in ANSYS Fluent, we simulated to solve the governing equations. This step generated the results necessary for evaluating the fuel cell's performance under various operating conditions.

#### 4. Results and Discussion

So we simulated fuel cell geometry, which contained over 5,00,000 elements using ANSYS WORKBENCH®. The

initial Anode Voltage was set to 0 while Cathode voltage was set and the y-current flux density integral was calculated on the cathode terminal. The anode mass flow rate was assumed to be  $3e-7$ , and hydrogen and water mass fraction was 0.8 and 0.2, respectively. The cathode mass flow inlet was set to  $8.1e-6$  with a mass fraction of water of 0.2 and 0.02 oxygen. Temperature was set to a constant value, while all other parameters, like materials, were set to default values.

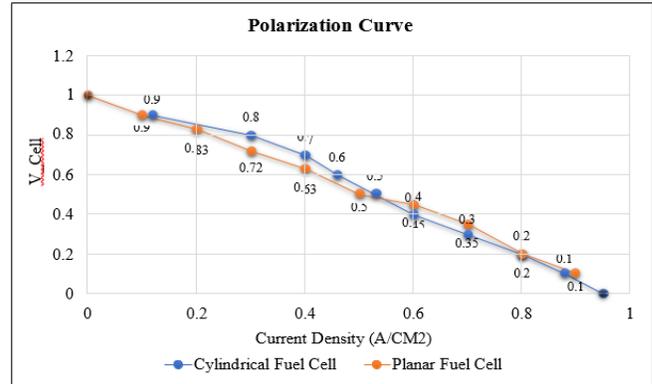


Fig. 8 Polarization curve (comparison of cylindrical and planar outputs)

The fuel cell performance can be represented by the I-V Curve, which shows the fuel cell voltage output for current density. From the graph, it is seen that it is hard to achieve high fuel cell voltage with current load due to irreversible losses [31]. The results of the Cylindrical Fuel cell were later compared with the Planar Fuel Cell, as shown in Figure 8, and our design showed the same voltage output as the planar fuel cell by eliminating the bipolar plates.

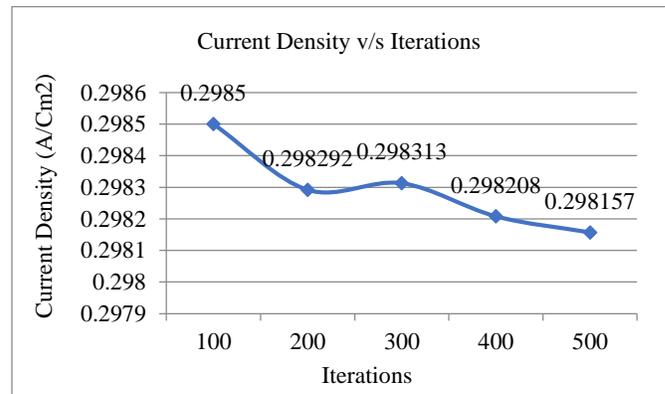


Fig. 9 Current density vs Iterations curve

An iteration sensitivity analysis was performed to determine the final behaviour of the graphs. The above graph in Figure 9 was generated at a Voltage input (Cathode) of 0.8V. The graph shows the current density values after 500 iterations. There is a slight decrease in current density as iterations are increased. The reason behind this is that the output predicted in software is always more than the real output because of thermodynamic losses.

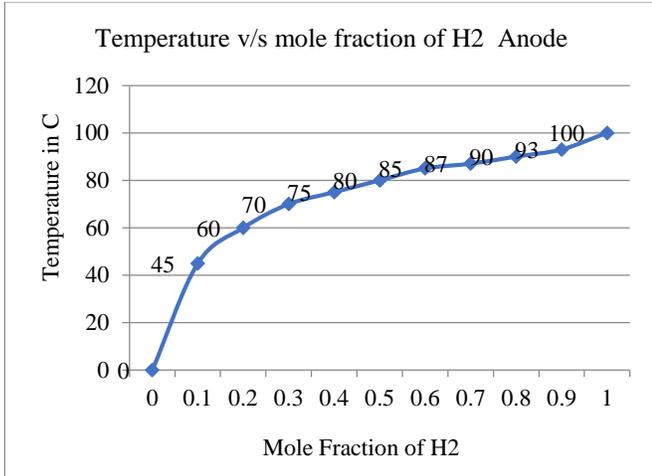


Fig. 10 Temperature of cell vs the mole fraction of H2O

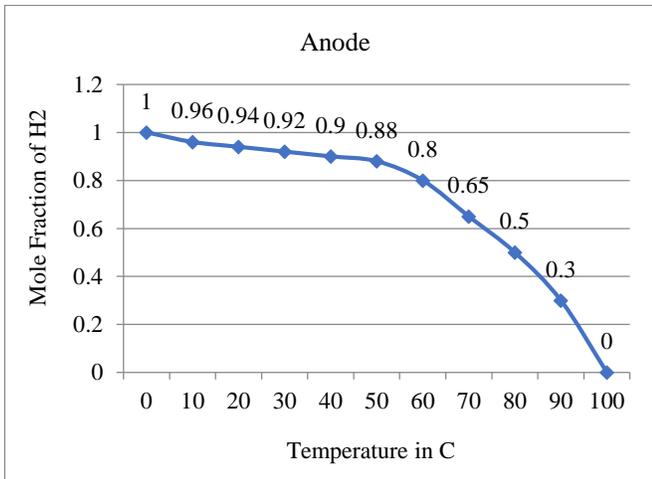


Fig. 11 Mole fraction of H2 vs Temperature of cell

The mole fraction of water vapour depends on Saturation Vapour, relative humidity and pressure. The hydrogen released to the anode inlet will have an inlet relative humidity and amount of water vapour. The effect of mole fraction for water and Hydrogen due to saturation pressure can be shown as a temperature function. Result outputs are shown in the graphs below. According to graphs, as temperature increases,

hydrogen supply will be limited. So, the optimum temperature range is between 343-353 K, as represented in Figures 10 and 11.

### 5. Conclusion

A productive design of a self-breathing PEMFC has been developed. Using the same MEA, the performance of planar and cylindrical cell designs was compared. According to the results, the cylindrical cell performs better than its planar version. The planar architecture of the fuel cell faces weight and size issues. The cylindrical architecture can overcome this limitation. The cylindrical construction makes removing water from the cathode easier during operation, while the planar configuration's flow channels make this difficult. The cylindrical architecture eliminated the bipolar plates, which decreased the weight, reduced the size, and lowered the overall cost of the fuel cell.

Additionally, the cylindrical shape improves heat dissipation and airflow to the cathode. The cylindrical PEMFC (CY-PEMFC) is lighter and smaller than the planar version, with a mass of only 1.99 g and a compact total volume of about 1985.27 mm<sup>3</sup>. Polarisation curve research showed that the cylindrical design performed better at all current densities than the planar design. At 0.6 V, the CY-PEMFC specifically obtained a current density of 0.46 A/cm<sup>2</sup>, approximately 15% greater than the 0.4 A/cm<sup>2</sup> of the planar design in the identical circumstances.

#### 5.1. Future Scope

Future studies on T-PEMFCs can concentrate on stacking cells to increase output for practical uses such as Fuel Cell Electric Vehicles (FCEVs). Creating a T-PEMFC stack that fits into the front panel of FCEVs and is modeled as a radiator is a creative way to maximize space usage.

Make use of the heat produced by the exothermic reaction of the fuel cell. This heat may be stored for use in heating systems and other purposes rather than escaping. The widespread use of fuel cells can improve efficiency and sustainability by generating green energy and functioning as a heat source.

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