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Thermal Modeling and Performance Investigation of Proton Exchange Membrane (PEM) Fuel Cell

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Abstract This research paper presents analysis of heat generation problem in Proton Exchange Membrane (PEM) fuel cell using COMSOL Multiphysics software.PEM fuel cells are widely recognized for their high electrical power output and environmental sustainability. However, in a PEM fuel cell around 50 to 60 % of energy generated from chemical reactions is dissipated as heat energy. To address this issue PEM fuel cell stack model is designed and thermal modeling is carried out to evaluate its performance. Based on thermal modeling of surface temperature distribution of cell it is found that the cathode side of PEM fuel cell is warmer and generates more heat as compared to other parts due to the exothermic reactions,slow reaction rate,joule heating effect and material properties. Moreover, it is also found that there is uniform temperature distribution across the cell due to rapid heat conduction from cathode side to the surface of the cell.The results of this study show that due to more heat generation on cathode side temperature will tend to increase.This increasing temperature enhances the average cell current density but as the average cell current density increases it reduces the average cell voltage thus declining the efficiency of PEM fuel cell. Hence ,there should be an optimal temperature range between 60 to 80°C for the better performance of a PEM fuel cell. Findings of this study can serve as a valuable resource for understanding heat generation process in PEM fuel cell for the development of efficient and reliable fuel cell technology in future.

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1 Introduction

World is facing serious environmental and resources problems, and more attention is being paid to develop the sustainable energy resources for energy applications.Over last couple of years in all developed and developing countries electrical energy requirement has become inevitable. In future, this demand will increase exponentially so it is important to develop clean and sustainable energy sources [11].Moreover,in near future traditional mineral energy resources such as fossil fuels will be depleted and it will put great pressure on the economic growth [17] .Meanwhile, scientists around the world are exploring renewable energy resources such as solar,wind,biomass and fuel cell technology to meet the increasing power demands [2] .Fuel cell is a renewable energy technology because electricity or energy generated through it is obtained from the chemical reaction of two elements hydrogen and oxygen which are abundantly available in nature [9].

Fuel cells are devices that work on electro-chemical principle, putting it in simple words fuel cell uses processed hydrogen gas as prime source of fuel and oxygen from air as an oxidizing agent and produces electrical power along with water drops and waste heat (thermal) energy as other by-products [13].While operating a PEM Fuel cell produces zero emissions and green house gases (GHG) thus eliminating diverse effect of climate change and environmental pollution[16] .

Fuel cell working system involves the process of electrolysis which uses different types of electrolytic solutions .These electrolytic solutions determines the operating temperatures of fuel cells. According to the electrolytic solutions fuel cells are classified in six different types which are known as Alkaline, Molten Carbonate, Phosphoric Acid, Solid Oxide, Direct Methanol and Proton Exchange Membrane (PEM) Fuel Cell[1].The PEM fuel cell is considered more beneficial when compared to other fuel cell technologies because of net- zero emissions, high electrical power density, low operating temperature, high conversion efficiency and long stack life [18]. The PEM fuel cell could further be divided in Active and Passive PEM fuel cells. The main difference between these fuel cells is that active fuel cells need fans, pumps and other auxiliary equipments to provide fuel, oxidant and to extract heat dissipated from the reactions.Whereas, in Passive fuel cell neither the hydrogen feeding in anode and nor oxygen feeding in cathode rely on circulating pumps and heat is also removed by the passive cooling mechanisms [5].

Fuel cell technology is not mature yet, it is under development stage so it possess many challenges and issues. Fuel cells have high initial cost of installation because electrodes and catalyst materials are expensive [3]. Another issue for fuel cell is lack of dedicated infrastructure for safe handling of hydrogen production, transportation and storage [27]. Furthermore, excessive heat generation is a major challenge for a PEM fuel cell technology. When a PEM fuel cell device operates it generates significant amount of excessive thermal (heat) energy along with electricity production and water as by-product. This heat energy has adverse impact on the fuel cell performance and reduces electrical efficiency. Furthermore, generated heat energy also influences the stability of fuel cell stack and temperature curve along the cell [20].This waste heat is generated due to improper electro-chemical reactions, resistance provided by conductive materials like Joules heating and Ohmic resistance [19]. Overall 50 to 60 % heat is produced due to entropy change or enthalpy change , phase change like condensation and hydration which occurs in membrane [8].This heat energy changes temperature uniformity which leads to significant impact on current density and voltage of the cell [6].Most important aspect of PEM fuel cell is that it performs with best efficiency under appropriate temperature range (60-80°C) [26]. High proton conductivity could be achieved if temperature range bounds to 80°C and if temperature range goes below 60°C this may lead to water condensation and flooding of metal electrodes resulting in voltage drop [22].Moreover,ohmic losses are also a challenge for fuel cell technology. These losses occur due to resistance in the path of proton flow in the electrolytic membrane and also conduction resistance in anode and cathode electrodes which reduces electric power efficiency of PEM fuel cell [24].

Fuel cells devices could be used for vast applications such as stationary power systems, transportation, portable devices and space applications. Stationary power systems include residential applications, combined heat and power systems (CHP) and distributed power generations. Transportation consists of electric cars, motorcycles, buses, aero-planes and trains etc. Portable devices are mobile phones,laptops and UPS systems. In space applications, fuel cells are mainly used for heating and cooling purposes [10].

Pakistan is a developing country and it has always been under energy crises due to lack of electricity production and distribution. However, Pakistan could use its renewable energy potential to produce green hydrogen and use it in fuel cell technology to produce electricity [23].Thus,fuel cell technology could help Pakistan to reduce environmental degradation and cut the costs of power production [15].

There are many system control and modeling techniques available for the fuel cell technology. But best featuring and parameter oriented tools include COMSOL Multi-physics software, MATLAB and ANSYS FLUENT etc. These modeling tools reduce high computational cost and provide access to real time controlling of electrical and thermal models of PEM fuel cell [4]. Meanwhile, above cited research publications have attempted to cater the heat generation problem in fuel cell technology using different technical tools, however, this study will focus on the gap of simulation and modeling techniques using COMSOL Multiphysics software. Hence, performance investigation of proton exchange membrane (PEM) fuel cell is carried out by studying fuel cell stack model,simulating surface temperature distribution, uniform temperature distribution, average cell current density and average cell voltage.

2 Modeling of Proton Exchange Membrane (PEM) fuel cell

2.1 Modeling assumptions

Following assumptions are made to simplify the modeling and simulations.

(1) In a PEM fuel cell individual cells perform similarly so all cells are lumped as stack.
(2) Hydrogen and oxygen gases are considered ideal.
(3) Pure hydrogen is assumed
(4) Pressure is considered constant in the gas flow channels
(5) Temperature of the hydrogen and oxygen gases inside the stack is the same as the stack temperature.
(6) The by-product of chemical reactions is only liquid water.

2.2 Modeling input parameters and materials

Modeling input parameters and materials for proposed design of PEM fuel cell stack are provided in Table No:01 and Table No:02 respectively [12] .

Table 01: PEM fuel cell modeling parameters

Parameter Name	**Expression**	**Value**	**Description**
L	10 cm	0.1 m	Length of cell
D	2cm	0.02 m	Width of cell
H-film	0.035mm	3.5×10^{-5} m	Cu film thickness
H-GDL	0.3mm	3×10^{-4} m	GDL thickness
H-membrane	0.02mm	2×10^{-5} m	Membrane thickness
H-plate	0.5mm	5×10^{-4} m	Steel plate thickness
r-film	2mm	0.002 m	Hole radius in Cu film
r-plate	4mm	0.004 m	Hole radius in steel plate
d-gde	0.0000001m	1×10^{-7} m	Thin GDE Thickness
V-cell	1[V]	1 V	Cell voltage
T-amb	25[degC]	298.15 K	Ambient temperature
xH2O	0.02	0.02	Mole fraction of water, cathode
xN2	0.79	0.79	Mole fraction of nitrogen, cathode
i0-refa	1000[A/m^2]	1000 [A/m^2]	Reference exchange current density, anode
i0-refc	10[A/m^2]	10 [A/m^2]	Reference exchange current density, cathode
Av	$1\times10^7[1/m]$	$1\times10^7[1/m]$	Active specific surface area of thin GDEs
htc	50[W/m^2/K]	50 [W/m^2/K]	Heat transfer coefficient

Table 02: PEM fuel cell modeling materials

Component	**Material**
Proton Exchange Membrane (PEM)	Typically made of Nafion
Catalyst	Platinum or platinum alloy
Gas diffusion layer (GDL)	Carbon cloth or paper
Bipolar plate	Carbon-fiber reinforced polymer (CFRP) or metal Steel AISI4340
Gasket	Elastomeric material
Endplate	Metal
Current collector	Metal (Copper)

2.3 PEM fuel cell single cell modeling

The basic model of a Proton Exchange Membrane (PEM) fuel cell consists of a single cell.This single cell is made up of two metal electrodes anode and cathode .Furthermore, fuel cell uses a thin layer of Polymer Electrolyte Membrane (PEM) sandwiched between these two electrodes.The PEM allows to transfer the protons through it but blocks the passage electrons. Most widely used membrane in PEM fuel cell is Nafion , which is perflourinated sulfonic acid membrane [14]. Single cell models generated through COMSOL multiphysics software are shown in fig 01,02 and 03 respectively.

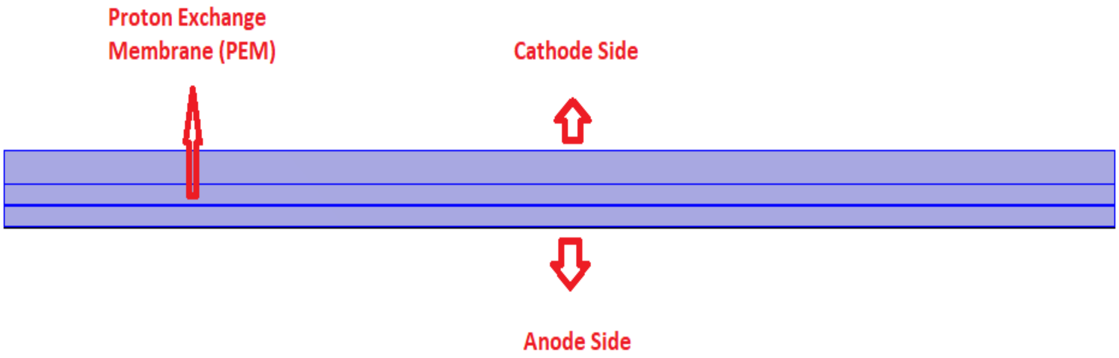

Fig 01: YZ-plane fuel cell single cell model

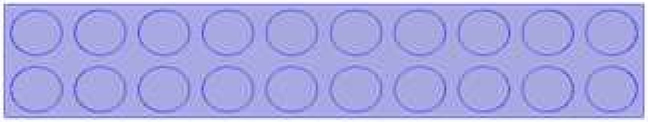

Fig 02: XY-plane fuel cell single cell model

Fig 03: XYZ-plane fuel cell single cell model

In this single cell hydrogen fuel enters through anode side (fig 04) where hydrogen oxidation reaction (HOR) gets activated.In this reaction, a catalyst called platinum converts hydrogen gas into two ions positive ions (protons) and negatively charged ions (electrons) (eq 01).

$$H_2 \rightarrow 2H^+ + 2e^- \tag{1}$$

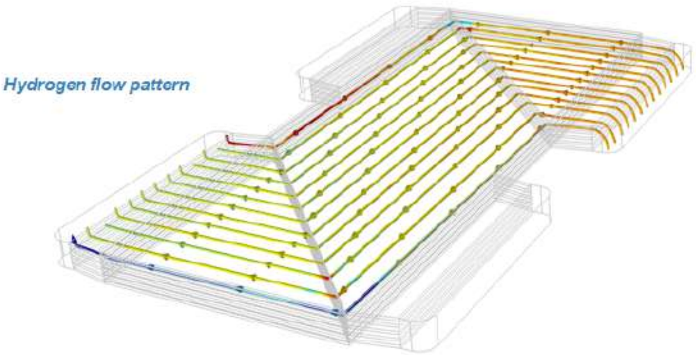

Fig 04:Hydrogen flow pattern

These newly converted protons (positive ions) can pass through proton exchange membrane (PEM) so they will move from anode to cathode but electrons can not pass through it so they will travel through external circuit to reach the cathode side .

Moreover, oxygen gas extracted from air is introduced on cathode side (fig 05).Where this pure oxygen meets with electrons and protons to start the oxygen reduction reaction (ORR).In this reaction, palladium catalyst combines oxygen with electrons and protons to produce water as by-product (eq 02).

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O \tag{2}$$

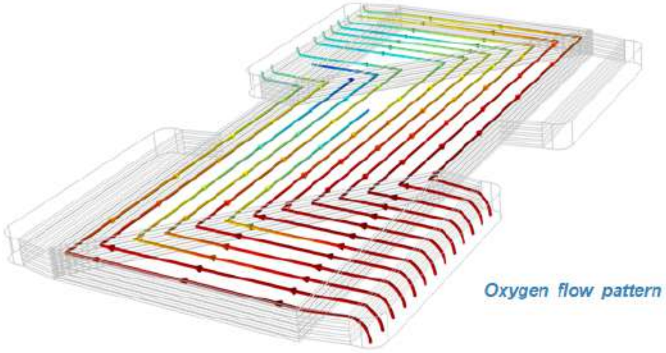

Fig 05:Oxygen flow pattern

Meanwhile,the electrons passing through the external circuit produces electric power and heat energy.Thus, over all chemical reaction of a PEM fuel cell could be written as follows (eq 03) [7].

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O + \text{Electricity} + \text{Heat} \tag{3}$$

2.4 Stack modeling

A single PEM fuel cell produces power less than 1V ,so they are connected in a series to produce higher output voltages.When these cells are combined together they form a structure called PEM fuel cell stack [21].This stack not only generates higher output voltages but it also helps to provide structural support to other components of PEM fuel cell such as gas diffusion layers (GDL),bipolar plates and gaskets [25] . A PEM fuel cell stack model developed through COMSOL Multiphysics software is shown in fig 06.

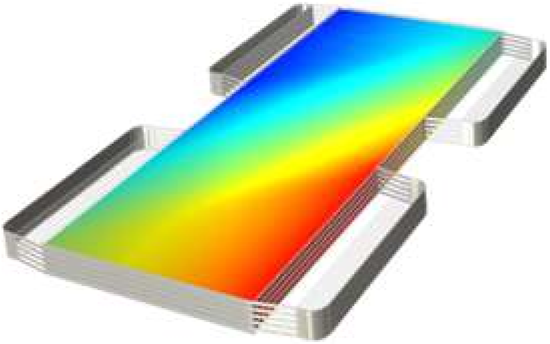

Fig 06: PEM fuel cell stack model

2.5 Thermal modeling of PEM fuel cell

Thermal modeling involves the analysis of excessive heat generation in PEM fuel cell which could be examined by temperature distribution within the fuel cell. Following sections show that thermal modeling is applied on the single cell or individual cell from the fuel cell stack to evaluate the temperature distribution on surface and centre of PEM fuel cell.

2.5.1 Surface temperature distribution in PEM fuel cell

It is important for a proton exchange membrane (PEM) fuel cell to understand the surface temperature distribution because it helps to analyse that which part or side of PEM fuel cell is generating more waste heat. Now, as thermal modeling is applied on a single cell (assumed last unit cell in stack) shows that fuel cell is warmer towards the cathode side as compared to anode side (fig 07).This thermal behavior occurs due to more heat generation on cathode side due to following reasons:

1) Exothermic Reaction: At the cathode side, oxygen, protons and electrons are combined together to produce water and release heat .Hence, due to this exothermic reaction cathode side of fuel cell becomes warmer.

2)Slow Oxygen Diffusion Rate: Fuel cell mainly works on chemical reaction between oxygen and hydrogen but when oxygen diffusion rate becomes slow it develops oxygen-rich environment on cathode side. This localized buildup of oxygen could increase heat generation on cathode side.

3) Bipolar Plates Heat Conduction: Bipolar plates transfer heat from cathode side to anode side. This can result in cathode side being warmer than anode side.

4) Joule Heating Effect: When the electrons flow through a resistive material it converts electrical energy into heat energy this effect is called Joule Heating. Joule heating effect is mainly observed on the cathode electrode due to electrical resistance, hence, increasing the capacity of heat generation on cathode side.

5) Proton Exchange Membrane Properties: Protons produced from hydrogen pass through the Proton Exchange Membrane (PEM). This membrane has different thermal conductivities on cathode and anode side which results in different heat transfer rate between these two electrodes, causing cathode side to be warmer.

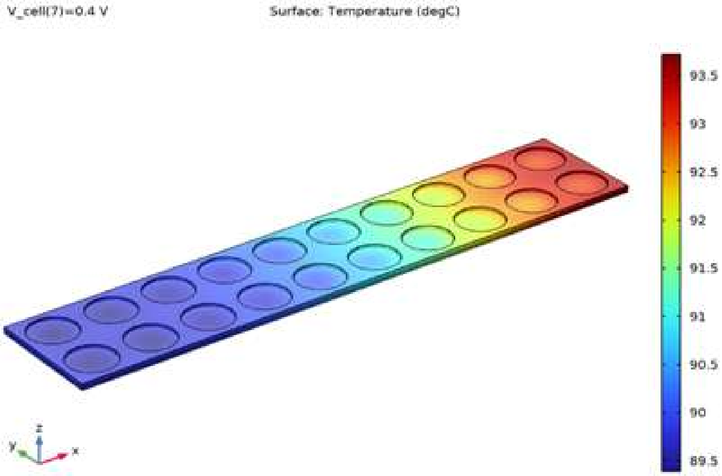

Fig 07: Surface temperature distribution of the cell

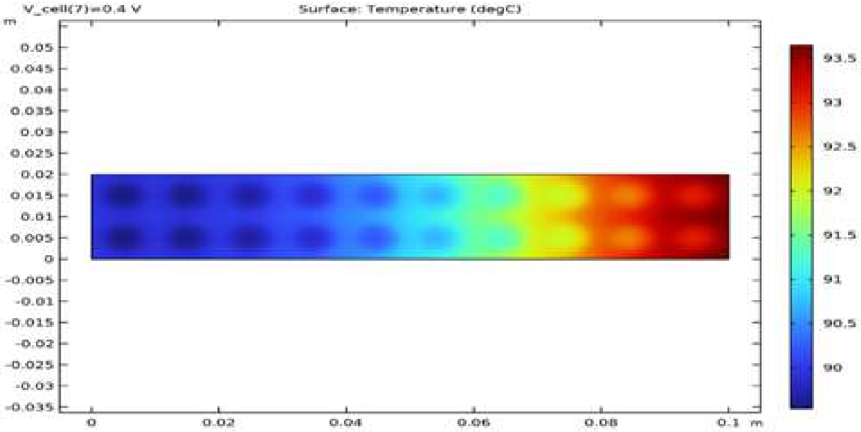

Fig 08: Temperature distribution in the centre and surface of the cell

2.5.2 Uniform (surface and centre) temperature distribution in PEM fuel cell

Modeling work shows that Temperature Distribution is uniform across the cell means it is same both in the centre and surface of the PEM fuel cell (fig 08). Now this is because, Proton Exchange Membrane used in the centre of cell works as the temperature moderator and helps to evenly distribute the heat generation in the cell. The membrane is made up of material called perfluorinated sulfonic acid polymer which has unique properties to work as good electrical and thermal insulator, hence reducing heat transfer between anode and cathode electrodes. Moreover, PEM membrane is specifically designed to conduct protons only which are key charge and thermal energy carriers, so they help to evenly distribute the heat energy across the cell. In addition with this, rate of reaction between hydrogen and oxygen is less sensitive to temperature changes which further reduce the temperature variations. The temperature at the centre of the PEM fuel cell is typically the same as the temperature at the surface of the fuel cell because the fuel cell is very thin. The heat generated by different reactions on cathode side is quickly transferred to the surface of the fuel cell by conduction.

3 Results And Discussion

3.1 Temperature distribution impact on average cell current density

Performance of proton exchange membrane (PEM) fuel cell mainly depends on the rate of the electro-chemical reactions occurring at the electrodes, and this rate is strongly influenced by the temperature variation or distribution within the cell. The relationship between Average Cathode Temperature (K) and Average Cell Current Density (A/m^2)is shown in fig 09. This figure shows that there is direct relationship between average cathode temperature and average current density.It means that as cathode temperature increases,average current density also increases and vice versa.Now this is because on cathode side hydrogen and oxygen gases react together to produce electricity but this reaction is an exothermic reaction so it also generates heat energy.Thus,this heat energy tends to increase temperature on cathode side.However, this relationship is not linear so there would be an optimal operating temperature range (60 to 80 °C) for each fuel cell design.Hence,there are two important conditions for fuel cell performance optimization one if temperature is too low or below the optimal temperature range electro-chemical reactions will occur at slower rate that will cause to reduce the average cell current density. Secondly, if temperature becomes too high or above the optimal temperature range it will enhance the average cell current density but it may cause membrane to dry out, affecting proton conductivity, damaging membrane and electrodes. Thus, maintaining optimal temperature range is essential for better performance of PEM fuel cell.

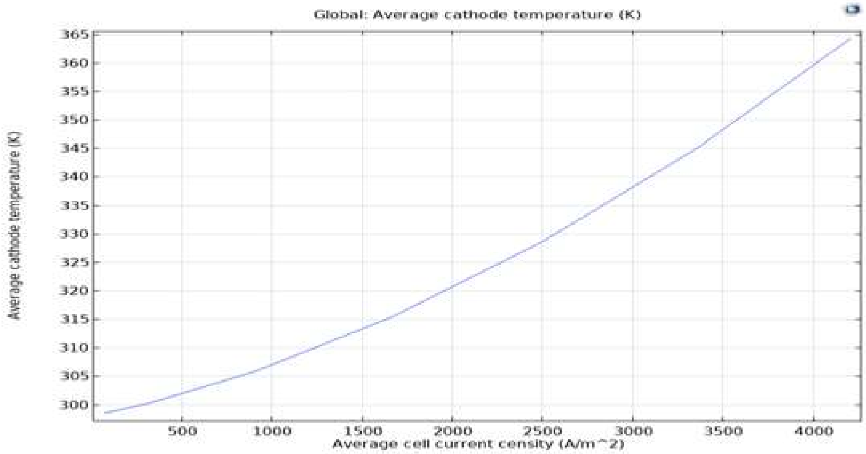

Fig 09:Average cathode temperature (K) Vs average cell current density (A/m^2)

3.2 Temperature distribution impact on average cell voltage

Polarization curve is a representation of relationship between the fuel cell voltage (V) and average cell current density (A/m^2) (fig 10). The curve shows that there is inverse relationship between average cell current density and average cell voltage.It means that as average current density increases average cell voltage drops and vice versa.Now in a PEM fuel cell, if there is less heat generation or low temperature (below the optimal range) on cathode side it will offer less resistance to electron and proton flow then average cell current density will decrease but in this case average cell voltage will increase.Furthermore, as the temperature increases (above the optimal range) average current density also increases, thus more current flows and resistance to the proton and electron increases so in this case voltage begins to decrease.

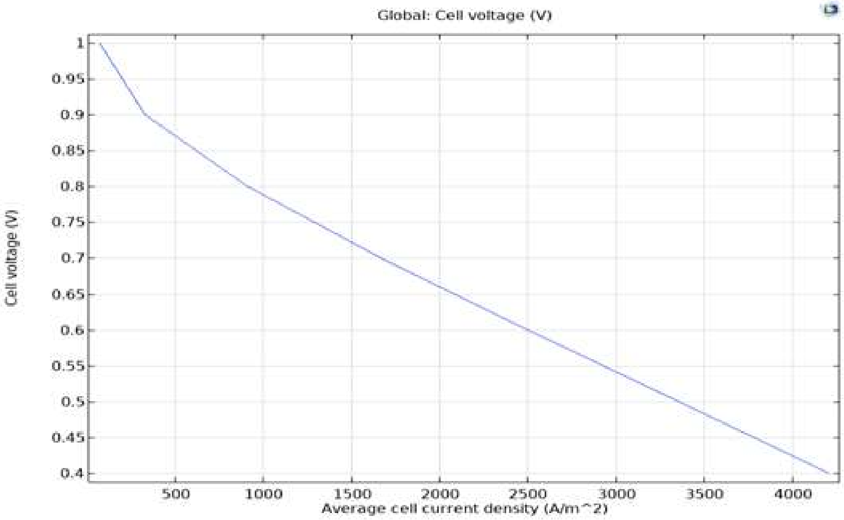

Fig 10: Polarization curve

3.3 Overall temperature distribution impact on average cell current density and average cell voltage

In a PEM fuel cell for an optimal temperature range (60 to 80°C) temperature distribution impact on average current density and average cell voltage could be summarized as in Table No 03.

Table 03: Temperature distribution impact on average cell current density and average cell voltage

Cathode Temperature (K)	**Average Cell Current Density** (A/m^2)	**Average Cell Voltage (V)**
High	High	Low
Low	Low	High

3.4 Performance analysis of a Proton Exchange Membrane (PEM) fuel cell

A Proton Exchange Membrane fuel cell follows the principle of electro-chemical reactions between oxygen and hydrogen, thus, generating electricity and also the waste heat energy (50%). The most important reasons behind this heat generation are exothermic reactions,slow reaction rate, joule heating effect occurring within the fuel cell.The performance of a PEM fuel cell could be analyzed from fig 11.This figure shows that there is direct relationship between average cathode temperature and average current density but inverse relationship between average cathode temperature and average voltage of the cell.Now,this is because heat energy generated on cathode side enhances chemical reaction rate which increases the temperature of the PEM fuel cell. As this temperature becomes higher the average cell current density of the fuel cell also increases.but as average current density increases average voltage of the cell drops.Meanwhile, if voltage of the cell is reduced it will decrease the power output and efficiency of the fuel cell. However, performance of a fuel cell could be improved if PEM fuel cell operates within an optimal temperature range (60 to 80°C).Moreover,optimal temperature range also helps to avoid component degradation and system failure.

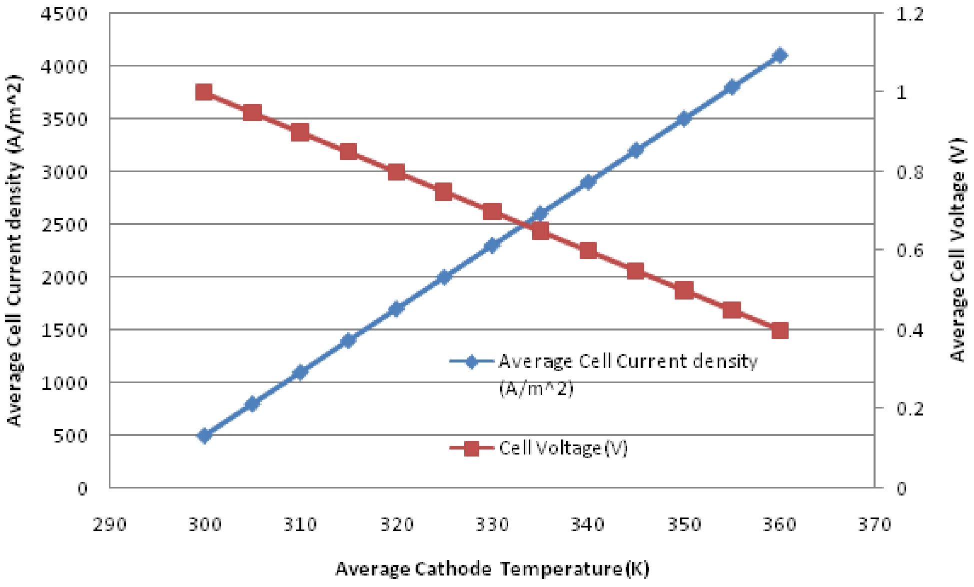

Fig 11: Average cell current density (A/m^2) and average cell voltage (V) Vs average cathode temperature (K)

4 Conclusion and Recommendations

The objective of this study was to investigate the heat generation process in Proton Exchange Membrane (PEM) fuel cell and explore the impacts of temperature distribution on average cell current density and average cell voltage. Thermal modeling was applied on a single cell from the fuel cell stack to find out the high temperature gradient or hotspot and it was found that cathode side of PEM fuel cell is warmer due to chemical reactions and restive losses.Results of this study suggests that generated heat energy tends to increase the temperature within the fuel cell which increases the average cell current density. But as the average current density increases average cell voltage drops. As voltage of the cell decreases, it reduces the power output of PEM fuel cell.However,power output could be enhanced if PEM fuel cell work under optimal temperature range 60 to 80°C.At the end, this study has opened up new avenues for future research directions such as exploring advanced cooling techniques, optimizing cell designs or studying different material properties. These directions can guide researchers towards addressing existing challenges and advancing the field of PEM fuel cell Technology.

Author Contributions

Ali Murad Jokhio : Conceptualization, Methodology, Software, Writing **Laveet Kumar:** Supervision, Software, Reviewing **Khanji Harijan:** Supervision and Validation **Hallar Parhyar :** Reviewing Editing Paper.

Compliance with Ethical Standards

It is declare that all authors don't have any conflict of interest. It is also declare that this article does not contain any studies with human participants or animals performed by any of the authors. Furthermore, informed consent was obtained from all individual participants included in the study.

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