SINGLE PHASE MODELLING OF A PEM FUEL CELL USING COMSOL MULTIPHYSICS 5.5

Submitted by

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in partial fulfilment for the award of the degree

Of

BACHELOR OF ENGINEERING

IN

MECHANICAL ENGINEERING

PSG INSTITUTE OF TECHNOLOGY AND APPLIED RESEARCH, COIMBATORE

ANNA UNIVERSITY: CHENNAI 600 025

AUGUST 2021

BONAFIDE CERTIFICATE

Certified that this project report **"Single Phase Modelling of a PEM Fuel Cell using COMSOL MULTIPHYSICS 5.5."** is the bonafide work of **CHANDRABOSE N S, NARESH G, SAI SUBRAMANIAN P and VISHNU VARDHAN JANA** who carried out the project work under my guidance.

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INTERNAL EXAMINER   **EXTERNAL EXAMINER**

ACKNOWLEDGEMENT

ABSTRACT

This project presents a study on Single Phase three dimensional Isothermal model of a Proton Exchange Membrane Fuel Cell (PEMFC). The domain has been restricted to understanding the flow and distribution of reactants such as hydrogen and oxygen in the anode and cathode respectively. This study is also done to understand the formation and distribution of the water formed as a by-product. The current density distribution over the catalyst layers has been studied. It has been observed that the concentration of the reactant gases decrease and the concentration of water is been increased as we move along the channel. Considering the computational resources available the scope has been restricted to modelling a single phase 3D model with a single channel and a single phase 3D model with multichannel (2 passes) .The modelling and analysis of the component was done using the COMSOL MULTIPHYSICS 5.5 software. Simulations employing the single-phase model are performed on a single channel section of a complete cell including the anode and cathode flow channels. The power density obtained in this model is 0.426 W/cm^2 at a voltage of 0.4 V. The results obtained for the simulation has been presented and have been validated using experiments presented in literature.

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CHAPTER 1

INTRODUCTION

1.1 Overview

In the current era, the need for using renewable energy is increasing due to the depletion of non renewable resources and its associated environmental pollution. Non renewable resources like coals and fossil fuels are used extensively to meet the energy demands. Though they serve as the best resource to obtain energy they get depleted over time and cause significant level of pollution. The urge to reduce the pollution caused by the fossil fuels and its depletion over time were the main reasons for the development of new alternate source of energy that are renewable and pollution free. One such renewable energy is the fuel cell. Fuel cells help in producing clean energy. They use hydrogen and oxygen as their inputs to generate electricity. The hydrogen and oxygen chemically react in the fuel cell to produce an electron. The electron produced is allowed to move in an external circuit to generate current and the water is obtained as a by-product. Among the many fuel cells that have been developed the proton exchange membrane (PEM) fuel cells have served as the best.

In the past decade researches have focussed their attention on the following aspects like operation conditions, transport phenomena of the gases and water, the kinetics of chemical reactions, membrane electrode assembly and geometry

of bipolar plates. Among the critical factors, PEM fuel cell's bipolar plate pattern geometry are gaining more importance as they provide one of the most important issues regarding the performance of stack, the homogeneous distribution of reactive gases all over the catalyst surface and bipolar plates areas through the flow channels: physical flow patterns or paths fabricated on the bipolar plate's surface to guide the gases all along the Bipolar plate for correct distribution.

1.1.1 WHAT IS A FUEL CELL ?

A fuel cell is a device that generates electrical power through a chemical reaction by converting a fuel (hydrogen) into electricity. Although fuel cells and batteries are both considered electrochemical cells and consist of similar structure, fuel cells require a continuous source of fuel and oxygen to run; similar to how an internal combustion engine needs a continuous flow of gasoline or diesel.

1.2 PRINCIPLE OF OPERATION

A fuel cell needs three main components to create the chemical reaction: an **anode**, **cathode** and an **electrolyte**. First, a hydrogen fuel is channelled to the anode via **flow fields**. Hydrogen atoms become ionized (stripped of electrons), and now carry only a positive charge. Then, oxygen enters the fuel cell at the cathode, where it combines with electrons returning from the electrical circuit and the ionized hydrogen atoms. Next, after the oxygen atom picks up the electrons,

it then travels through the electrolyte to combine with the hydrogen ion. The combination of oxygen and ionized hydrogen serve as the basis for the chemical reaction.

A polymer electrolyte membrane permits the appropriate ions to pass between the anode and the cathode. If the electrolyte gave free control for all electrons or ions to pass freely, it would disrupt the chemical reaction. At the end of the process the positively charged hydrogen atoms react with the oxygen to form both water and heat while creating an electrical charge.

1.3 TYPES OF FUEL CELLS

- Polymer exchange membrane fuel cell (PEMFC) – Study of interest

- Solid oxide fuel cell (SOFC)

- Alkaline fuel cell (AFC)

- Molten-carbonate fuel cell (MCFC)

- Phosphoric-acid fuel cell (PAFC)

- Direct-methanol fuel cell (DMFC)

1.4 CONSTRUCTION

The PEMFC mainly consists of two components (a) the bipolar plates (b) the Membrane Electrode Assembly (MEA).

1.4.1 Bipolar Plates (Study of interest) : These are plates that have channels through which the reactants hydrogen and oxygen. The gases from here diffuse to the Membrane Electrode Assembly (MEA).

1.4.2 Membrane Electrode Assembly (MEA): The membrane electrode assembly consists of 3 components the Proton Exchange Membrane sandwiched between the catalysts for the redox reaction to take place at the anode and cathode.

1.4.2.1 Anode : It is the negative post of the fuel cell. It conducts the electrons that are freed from the hydrogen molecules so that they can be used in an external circuit. It has channels etched into it that disperse the hydrogen gas equally over the surface of the catalyst.

1.4.2.2 Cathode: It is the positive post of the fuel cell, has channels etched into it that distribute the oxygen to the surface of the catalyst. It also conducts the electrons back from the external circuit to the catalyst, where they can recombine with the hydrogen ions and oxygen to form water.

1.4.2.3 Electrolyte: In PEMFC a Proton Exchange Membrane acts as the electrolyte. The membrane is very thin in nature having a thickness around

0.033μm to 3μm.This membrane is generally made of Nafion .This specially treated membrane, only conducts positively charged ions. The membrane blocks electrons. For a PEMFC, the membrane must be hydrated in order to function and remain stable.

1.4.2.4 Catalyst: It is a special material that facilitates the reaction of oxygen and hydrogen. It is usually made of platinum nano particles very thinly coated onto carbon paper or cloth. The catalyst is rough and porous so that the maximum surface area of platinum can be exposed to the hydrogen or oxygen. The platinum-coated side of the catalyst faces the PEM.

1.4.2.5 Proton-Exchange Membrane It is also called as polymer-electrolyte membrane (PEM). It is a semi-permeable membrane which is commonly made from ionomers and modelled to conduct protons and also to act as an electronic insulator or a reactant barrier. The main function of PEM when integrated into an assembly PEMFC is the dissolution of reactants and transport of protons while obstructing a direct electronic path through the membrane.

1.4.2.6 Gas-Diffusion Layer It is a significant supporting part of the Membrane Electrode Assembly (MEA). It is a porous material composed of a dense matrix of carbon fibre, which provides an electrically conductive pathway for current passage. It plays a major role of electronic contact between the bipolar plate and channel-land structure and to the electrode.

1.5 WORKING

At the anode, the pressurised H_2 gas enters the fuel cell on the anode side. This gas is forced through the catalyst by the pressure. When an H_2 molecule comes in contact with the platinum on the catalyst, it splits into two H^+ ions and two electrons (e^-). The electrons are conducted through the anode, where they make their way through the external circuit (doing useful work such as turning a motor) and return to the cathode side of the fuel cell.

$$H_2 \longrightarrow 2H^+ + 2e^- \qquad\qquad (1.1)$$

At the cathode, the oxygen gas (O_2) is being forced through the catalyst, where it forms two oxygen atoms. Each of these atoms has a strong negative charge. This negative charge attracts the two H^+ ions through the membrane, where they combine with an oxygen atom and two of the electrons from the external circuit to form a water molecule (H_2O).

$$\tfrac{1}{2} O_2 + 2H^+ + 2e^- \longrightarrow H_2O \qquad\qquad (1.2)$$

The overall Reaction in a PEM fuel cell can be written as:

$$H_2 + \tfrac{1}{2} O_2 \longrightarrow H_2O \qquad\qquad (1.3)$$

This reaction in a single fuel cell produces only about 0.7 volts. To get this voltage up to a reasonable level, many separate fuel cells must be combined to form

a **fuel-cell stack**. **Bipolar plates** are used to connect one fuel cell to another and are subjected to both **oxidizing** and **reducing** conditions and potentials.

A big issue with bipolar plates is stability. Metallic bipolar plates can corrode, and the byproducts of corrosion (iron and chromium ions) can decrease the effectiveness of fuel cell membranes and electrodes. Low- temperature fuel cells use light weight metals, graphite and carbon/thermoset composites (thermoset is a kind of plastic that remains rigid even when subjected to high temperatures) as a bipolar plate material.

1.6 Bipolar Plates

The proton exchange membrane fuel cell offers an exceptional potential for a clean, efficient, and reliable power source. The bipolar plate is a key component in this device, as it connects each cell electrically, supplies reactant gases to both anode and cathode, and removes reaction products from the cell. Bipolar plates have been fabricated primarily from high-density graphite, but in recent years, much attention has been paid to developing cost-effective and feasible alternative materials. Two different classes of materials have attracted attention: metals and composites.

The practical operating voltage from a single cell—also known as a membrane-electrode assembly (MEA)—is about 0.7 V. Desired voltages are obtained by connecting cells in series; this is accomplished by inserting a highly conductive

material (e.g., a bipolar plate) between two parallel MEAs. Such plates are by volume, weight, and cost the most critical component of a fuel cell stack and account for more than 40% of the total stack cost and about 80% of the total weight As a result, there have been significant activities in the past few years to lower their cost, reduce their size, and improve their performance and lifetime.

Bipolar plates perform a number of critical functions simultaneously in a fuel cell stack to ensure acceptable levels of power output and a long stack lifetime. They act as a current conductor between adjacent MEAs, provide pathways for reactant gases (hydrogen and oxygen or air), facilitate water and heat management throughout the stack, and provide structural support for the whole stack.

Accordingly, they must exhibit excellent electrical and thermal conductivity, corrosion resistance, mechanical and chemical stability, and very low gas permeability. Furthermore, raw materials must be widely available at reasonable cost and be amenable to rapid and cost-effective fabrication methods and processes.

1.7 Fuel Cell Thermodynamics
1.7.1 Free-Energy Change of Chemical Reaction

Electrochemical energy conversion is the transformation of the free-energy change related to a chemical reaction directly into electrical energy.

The free-energy change accompanied to a chemical reaction is a measure of the maximum work obtained from the reaction. It equals the enthalpy change of the reaction only if the entropy change ($\Delta\delta$) is zero.

$$\Delta g = \Delta h - T\Delta S \tag{1.4}$$

In a chemical reaction, if the number of moles of gaseous products and reactants are equal in magnitude, the net entropy change of this reaction is zero.

Since the number of moles of the molecule on the right-hand side of equation 1.3 is lower than that on the left hand or the reactant side, the gross entropy change inside the PEM Fuel Cell will be negative. This means that the quantity of energy that can be obtained from the enthalpy is decreased.

The standard Gibbs free enthalpy for the entire reaction in a PEM Fuel Cell is given as $\Delta g^\circ = -237.3 \times 10^3 \, J \,/\, mol$ if the byproduct or water obtained is in liquid phase.

$$\alpha A + B \rightarrow \gamma C + \delta D \tag{1.5}$$
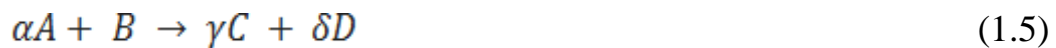
The standard free energy of reaction:

$$\mu_i = \left(\frac{\delta g}{\delta n}\right)_{T,p,n} \tag{1.6}$$

The chemical potential of any substance can be expressed by:

$$\mu = \mu^\circ + RT\ln a \tag{1.7}$$

where a is the activity of the substance and has the value μ° when a is unity

$$\Delta g^{-0} = \gamma \mu_C^0 + \delta \mu_D^0 - \alpha \mu_A^0 - \beta^0 \mu_B \tag{1.8}$$

Substituting eq 1.6 and 1.7 in 1.8, we get

$$\Delta g^- = \Delta g^{-0} + RTln\frac{a_C^\gamma * a_D^\delta}{a_A^\alpha * a_B^\beta} \tag{1.9}$$

Once Δg^{-o} is determined, Δg^- is calculated for any given reaction composition. The sign of Δg^- indicates the feasibility of a reaction. If it is positive, a reaction will not occur for the given composition of reactants and byproducts. If the value is negative, then a reaction can occur.

1.7.2 The Nernst Equation

Nernst equation is used to convert the free energy to cell potential. This is obtained by applying first law of thermodynamics or an isothermal open system:

$$0 = n^{\cdot}{}_{H_2} h^-{}_{H_2} + n^{\cdot}{}_{O_2} h^-{}_{O_2} - n^{\cdot}{}_{H_2O} h^-{}_{H_2O} + Q^{\cdot} - W^{\cdot} \tag{1.10}$$

wheren_i is the molar flow rate in [mol / s] and $\hat{h}$ is the molar enthalpy expressed in J/mol . Q represents the heat given to the system and W represents net work done by the system.

Here, we recall the entire fuel cell reaction:

$$2H_2 + O_2 \rightarrow 2H_2O \tag{1.11}$$

Substituting the coefficients in eq 1.10, we get :

$$0 = h^-_{H_2} + \left(\frac{1}{2}\right)h^-_{O_2} - \left(\frac{1}{2}\right)h^-_{H_2O} + \frac{Q^\cdot}{n^\cdot_{H_2}} + \frac{W^\cdot}{n^\cdot_{H_2}} \qquad (1.12)$$

Herein, the second law of thermodynamics is applied, which gives:

$$s^-_{out} - s^-_{in} - \left(\frac{\frac{Q^\cdot}{n^\cdot_{H_2}}}{T}\right) \geq 0 \qquad (1.13)$$

If we consider the first and second law of thermodynamics, an expression for the work for the reversible process which has the maximum work that can be obtained per mole of hydrogen as :

$$\frac{W^\cdot_{rev}}{n^\cdot_{H_2}} = h^-_{in} - h^-_{out} - T(s^-_{in} - s^-_{out}) \qquad (1.14)$$

The reversible work done in a fuel cell is the electrical work done in transferring the charges along the circuit from the anode to the cathode side and these are represented by the variables $v_{rev,a}$, $v_{rev,c}$ respectively

$$\frac{W^\cdot_{rev}}{n^\cdot_{H_2}} = ne(V_{rev,c} - V_{rev,a}) \qquad (1.15)$$

In order to convert the value into molar quantities, we need to multiply by the Avogadro number (6.022×10^{23} mol^{-1}). Since the product of unit electric charge (e = 1.602×10^{-19} C) and the Avogadro's number, we get Faraday's constant F(96485 C mol^{-1}), we get:

$$\frac{\dot{W}_{rev}}{\dot{n}_{H_2}} = nF(V_{rev,c} - V_{rev,a}) \tag{1.16}$$

Gibbs energy definition states that:

$$\frac{\dot{W}_{rev}}{\dot{n}_{H_2}} = \bar{g}_{in} - \bar{g}_{out} = -\Delta\bar{g} \tag{1.17}$$

Combining eq 1.16 and 1.17, we get:

$$\Delta\bar{g} = -nF(V_{rev,c} - V_{rev,a}) \tag{1.18}$$

Relating ΔV, we get

$$\Delta\bar{g} = -nFE_{rev} \tag{1.19}$$

where E is the electromotive force (EMF) of the cell.

Given the reactants and products are in their standard states, we obtain :

$$\Delta\bar{g}^{-0} = -nFE_{rev}^0 \tag{1.20}$$

Combining the above equation with eq 1.9, we obtain:

$$E_{rev} = E_{rev}^0 - \left(\frac{RT}{2F}\right)\ln\frac{a_{H_2O}}{a_{H_2} * a_{O_2}^{\frac{1}{2}}} \tag{1.21}$$

This equation obtained is the so-called Nernst equation specific for the H_2 - O_2 fuel cell.

1.7.3 Continuity Equation:

$$\partial(\rho u)/\partial x + \partial(\rho v)/\partial y + \partial(\rho w)/\partial z = -\partial\rho/\partial t \qquad (1.22)$$

where u, v and w are velocity in the x, y and z directions respectively, ρ is density of reactant gases.

Electrodes are made up of carbon cloth or carbon fiber. Therefore, electrodes are considered as a porous medium where reactant gases are distributed on the catalyst layers. With respect to porosity of electrodes (ε) and membrane, the continuity equation is written as follows

$$\partial(\rho\varepsilon u)/\partial x + \partial(\rho\varepsilon v)/\partial y + \partial(\rho\varepsilon w)/\partial z = Sm \qquad (1.23)$$

where Sm is mass sink term.

This term is assumed to be zero because there is no reaction in the flow channels and gas diffusion layers. The sink term is not zero in the catalyst layer due to reaction of reactant species and can be calculated from the following equations

$$SH_2 \text{ (kg s}^{-1}\text{ m}^{-3}) = - MH_2/2F \text{ Ran} \qquad (1.24)$$

$$SO_2 \text{ (kg s}^{-1}\text{ m}^{-3}) = - MO_2/4F \text{ Rcat} \qquad (1.25)$$

$$SH_2O \text{ (kg s}^{-1}\text{ m}^{-3}) = MH_2O/2F \text{ Rcat} \qquad (1.26)$$

where F is the Faraday constant and M is the molecular weight (kg/mol) of the species.

1.7.4 MOMENTUM EQUATION:

The Navier strokes equation can be used for Newtonian fluid.

$$\nabla.(\rho \overrightarrow{v}\, \overrightarrow{v}\,) = -\nabla p + \nabla\tau + S_{mom} \qquad (1.27)$$

For porous electrodes momentum equation may be written as

$$\nabla.(\varepsilon\rho \, \overrightarrow{v} \, \overrightarrow{v}) = -\varepsilon\nabla p + \nabla\varepsilon\tau + S_{mom}. \tag{1.28}$$

This equation is applied in x, y and z directions

$$u\frac{\partial(\rho u)}{\partial x} + v\frac{\partial(\rho u)}{\partial y} + \omega\frac{\partial(\rho u)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right) + S_{mom,x}$$

$$\tag{1.29}$$

where p, τ, μ and S_{mom} are velocity vector, pressure, shear tensor, viscosity and momentum sink term respectively. The equations for y and z directions are the same. Momentum sink term is assumed zero in the flow channels and in the porous media is considered as following

$$S_{mom,x} = -\frac{\mu u}{\beta_x} \tag{1.30}$$

where β is the permeability of electrodes. β_x, β_y and β_z have a value of 10^{-12} m^2.

The momentum sinks term for the y and z directions are the same.

1.7.5 MASS TRANSFER EQUATIONS:

The continuity equation in steady state is

$$\nabla.(\rho\overrightarrow{v}\,y_i) = -\nabla.\overrightarrow{j}_i + S_i \tag{1.31}$$

where y_i and j_i are mass fraction and diffusional mass flux vector respectively.

Si is mass sink term which is zero in the flow channels and gas diffusion layers because of non-reactive flow. The sink term in the catalyst layers is calculated from Eqs. (1.24) - (1.26)

Using Fick's law we can calculate diffusional mass flux vector

$$\overrightarrow{j}_i = -\sum_{j=1}^{N-1}\rho D_{ij}\nabla\overrightarrow{y_i} \tag{1.32}$$

where D_{ij} is diffusivity of species i inside j.

Within porous electrodes mass transfer equation may be written as:

$$\nabla.(\rho\varepsilon\vec{v}y_i) = \nabla.(\rho\varepsilon D_{ij}^{eff}\nabla y_i) + S_i.$$ (1.33)

Within porous media, diffusivity is estimated from the modified Brueggemann equation

$$D_{ij}^{eff} = D_{ij} \times \varepsilon^{1.5}.$$ (1.34)

Therefore, mass transfer equations for hydrogen, oxygen and water are as follows:

$$u\frac{\partial(\rho y_i)}{\partial x} + v\frac{\partial(\rho y_i)}{\partial y} + w\frac{\partial(\rho y_i)}{\partial z} = \frac{\partial(j_{x,i})}{\partial x} + \frac{\partial(j_{y,i})}{\partial y} + \frac{\partial(j_{z,i})}{\partial z} + S_i$$ (1.35)

CHAPTER 2

LITERATURE REVIEW

Computational model of 3D, non isothermal PEMFC is done and various critical parameters such as mass and energy movement, heat movement and electrode kinetics and many such parameters were considered. The over potential is kept constant in cathode and anode activation. Better current density and temperature are obtained from Serpentine flow pattern. The construction, elements involved and working of a PEMFC are known.[1]

A serpentine flow path is created to find the mass flow channels in a PEMFC by computational model. Navier Strokes method with multi species mix is used to solve. Control volumes are used to model the mass source using electro chemical reactions. Mass utilization patterns influence the flow in anode and cathode channels of membrane electrode assembly. Except overall pressure drop, All other parameters are less in straight channel flow. Polymer electrolyte membrane fuel cells work at low temperatures when compared to other fuel cells and they are the future generation automobiles. [2]

Different design and operating parameters such as are examined analytically to enhance the performance of the PEMFC. Some of them are temperature, gas flow rates, electrode thickness etc. To increase the performance of PEMFC thinner electrode thickness and smaller porosity is preferred. The temperature is maintained at 100 degree celsius to maintain liquid water in nafion membrane. [3]

Cell performance at various flow rates of both hydrogen and relative humidity are critical parameters for a better performance. Studies shows that hydrogen air flow rate and relative humidity is critical for current density, membrane dry out and electrode flooding. Thermal management and fuel cell life are critical when

uniform current density flows along the channel. The computational cost is less and can be extended to fuel cell stack easily.[4]

The PEMFC need better thermal management system to attain maximum efficiency. Two dimensional model of water and thermal management model was created and the effect of various operating parameters are observed by trial and error method. The humidification of cathode and anode is very important for the performance of PEMFC. [5]

The life and efficiency of the fuel cell is one of the most important factors to take into account. If the temperature is increased, the voltage and current density is increased but the transportation of the fluid is difficult resulting in dehydration of the nafion membrane and reducing the thickness of the electrode, thereby decreasing the life of fuel cell [6]

The presence of humidity is the most important parameter of the fuel cell performance. The water which is produced as a by product can be used for internal humidification and it is proved that internal humidification is effective than external humidification.[7]

An experiment on the effect of inlet velocity and proton conductivity of acid doped PBI membrane are performed on High Temperature PEMFC. The best results were obtained when hydrogen velocity is one tenth the velocity of air and proton conductivity of 14 S/m. [8]

As the temperature increases the performance of the fuel cell increases with some effects. So a two phase and cell agglomerate model will be useful to find the best optimum temperature to get the maximum efficiency of the fuel cell.[9]

A minimum amount of hydration is required for a proper operation of the proton exchange membrane to attain minimum degradation of membrane. But the same amount of humidification in Cathode and anode side resulted in uneven characteristics, so the anode was fully humidified and the cathode was kept dry

to attain maximum performance of the fuel cell. But the cathode cannot be left dry so an intermediate humidity is maintained.[10]

For same operating parameters such as air flow rates and relative humidity interdigitated flow design is more effective than normal flow design. The Relative humidity is the key parameter which decides the performance of the fuel cell.[11]

A one dimensional proton exchange membrane fuel cell is a good model for verifying the varying characteristics parameters [12]

In the fuel cell the catalytic layer and the membrane are considered as separate entities. The current density and voltage varies based on critical parameters such as porosity, Relative Humidity, pressure, Temperature etc. [13]

To enhance the performance of the fuel cell the water balance of fuel cell should be well understood and monitored. The flow characteristics and the cell efficiencies are determined by the humidification on the cathode and anode side. The cell efficiency is based on the humidification that is in direct relation with the current density and temperature difference. The efficiency is increased by anode humidification.[14]

The performance of the fuel cell is affected by the humidity and water on the cathode side. The water produced in the reaction enters the pores due to shear force of gas flow and capillary action which affects the function of fuel cell.[15]

CHAPTER 3

## A Three-Dimensional, Single-Phase Model of a PEM Fuel Cell

3.1 Modelling of PEM Fuel Cell

The modelling of membrane electrode assembly along with the gas diffusion layer, cathode and the anode channel was done in COMSOL MULTIPHYSICS 5.5 for single and multipass. The mass transport analysis comprising of the flow of hydrogen and oxygen in the anode and cathode respectively and the formation of water molecules in the anode and cathode compartments are studied using the COMSOL MULTIPHYSICS 5.5 software. The polarisation plot (Cell Voltage Vs Cell average current density) and contours such as the ionic current in the centre of membrane, molar concentration of Hydrogen in the anode channel, molar concentration oxygen in the cathode channel and water concentration in the anode and cathode channels were generated.

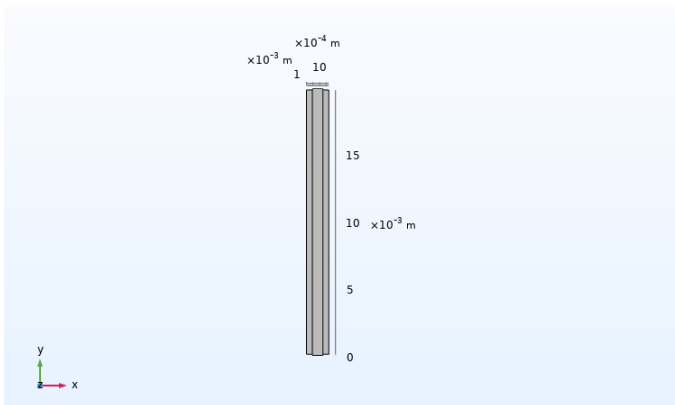### 3.1.1 Modelling Geometry of Single Pass
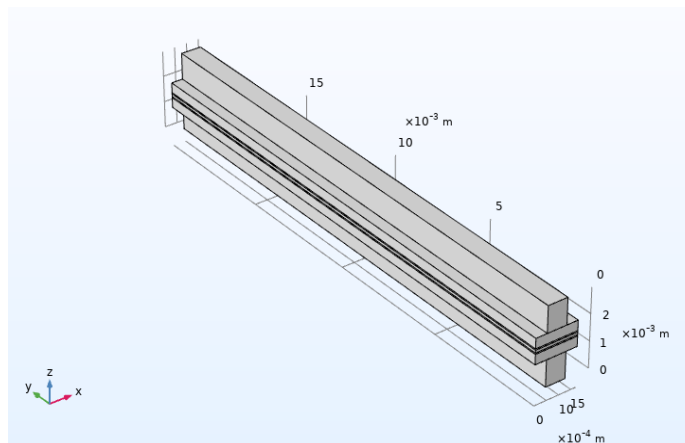
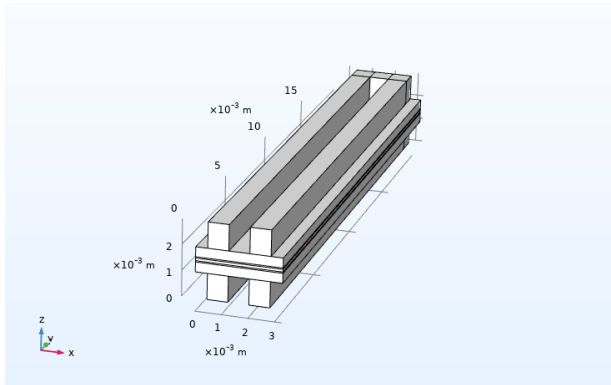Isometric view
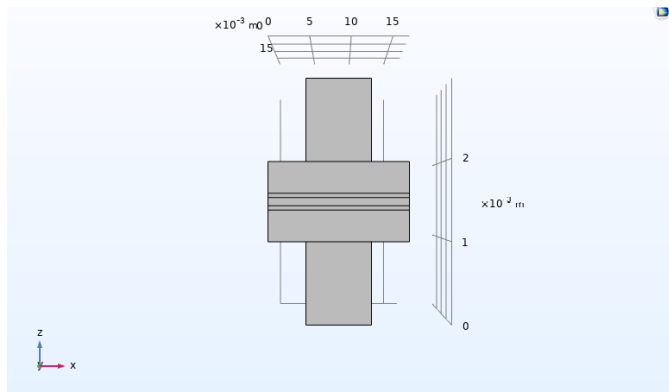
Front View
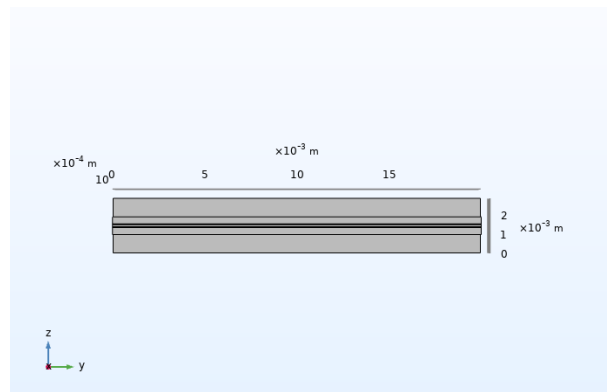
Left Hand Side View

Top View

Fig 3.1 Different views of the modelled Single Pass PEMFC

The modelling was done by creating different blocks of dimensions given in the parameters table and then assembled. A single pass of the channel of the bipolar plate was used to create the assembly. The assembly consists of an anode compartment, a proton exchange membrane and a cathode compartment. The anode compartment comprises of an anode channel, a gas diffusion layer and an electrode. The cathode compartment comprises of a cathode channel, a gas diffusion layer and an electrode. The proton exchange membrane is sandwiched between the anode and the cathode compartment to form the Proton Exchange Membrane Fuel Cell.
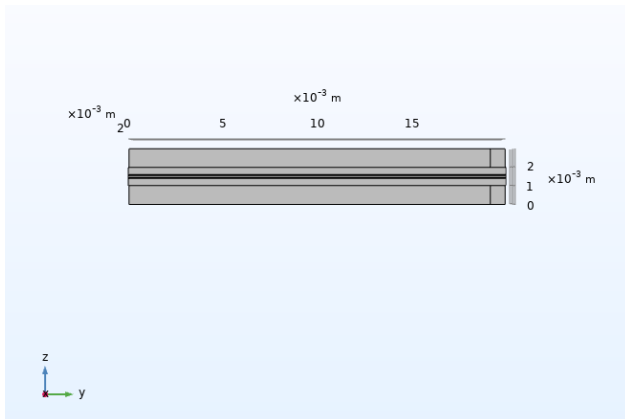
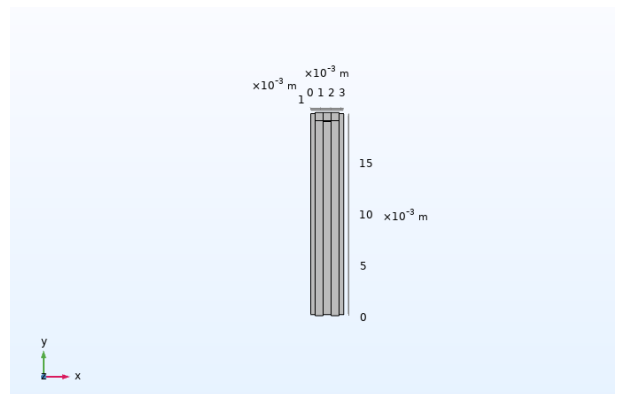## 3.1.2 Modelling Geometry of Multi Pass

Isometric View
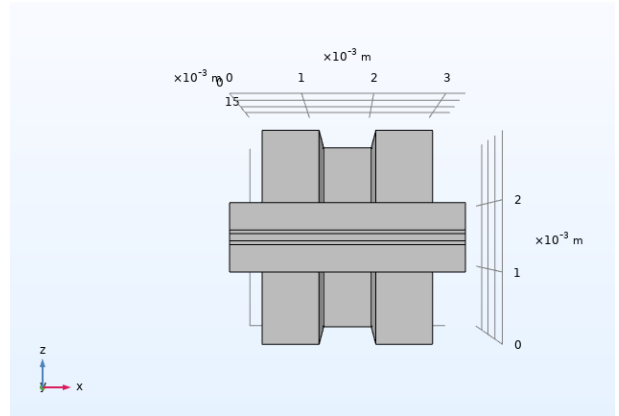
Right Side View

Front View

Top view

Fig 3.2 Different Views of Multi pass PEMFC

The modelling of the multi pass assembly was done in the same manner as that of single pass. The dimensions of the cathode and anode channel (width, height and length) were kept the same. The width of the electrodes, membrane and the gas diffusion layer were increased to fit in 2 passes. The multi pass channel was built by creating 3 blocks and then forming an union of three using the Boolean function in COMSOL MULTIPHYSICS 5.5.

3.2 Meshing

The meshing of the entire component was done in two stages. In the first stage a mapped 2D mesh was created in the plane normal to the channel direction as shown in Fig 3.3 . For this the mapped function was used .In the next stage this 2D mesh on the surface was swept along the channel length to mesh the entire component. In this step the swept function of the COMSOL MULTIPHYSICS 5.5 software was used. The 2D mesh was created by dividing the edges (edge sizing) of the front face of the component into elements. The edge sizing was done to ensure residues are properly propagated.

In acute areas such as the membrane electrode assembly the element size is kept as fine as possible and in other areas such as the gas diffusion layer and the anode and cathode channels relatively large element sizes were chosen. This has been done taking into account the time required to compute the entire geometry and the computational power of the resource available. Hence an optimized mesh was created to obtain high accuracy with the available resources for computation.
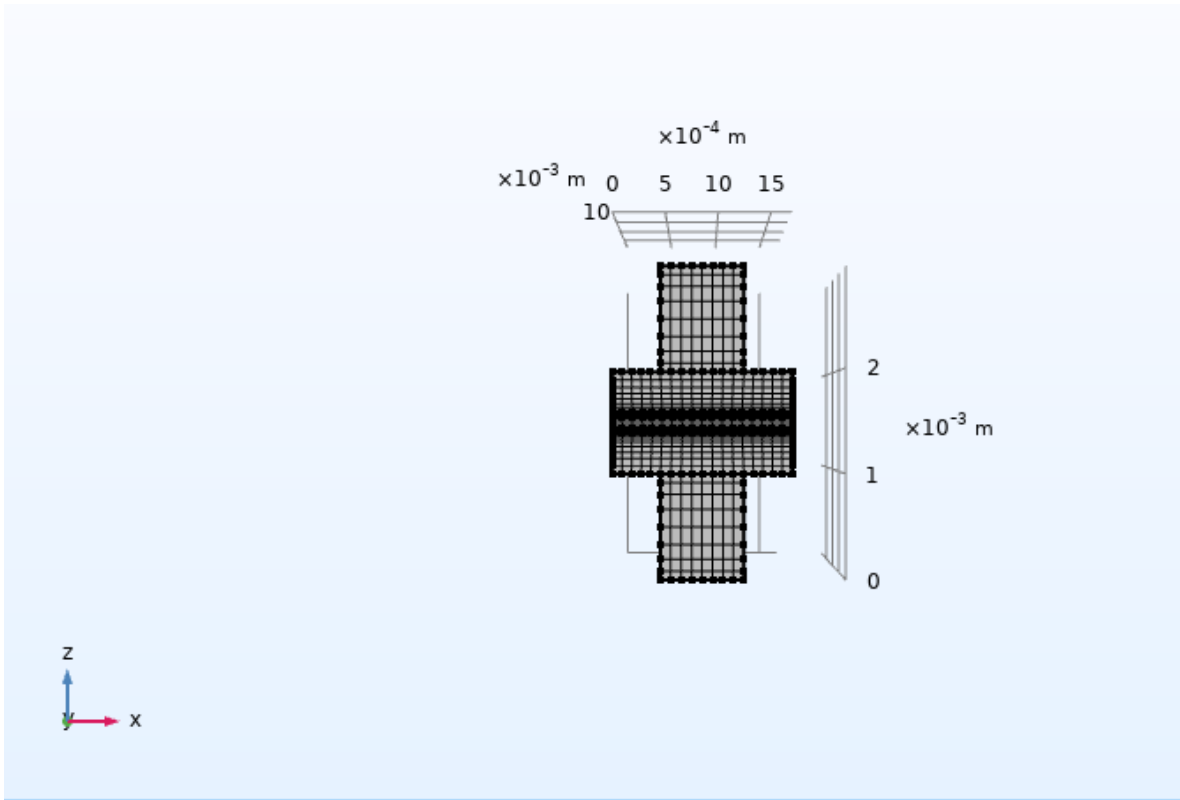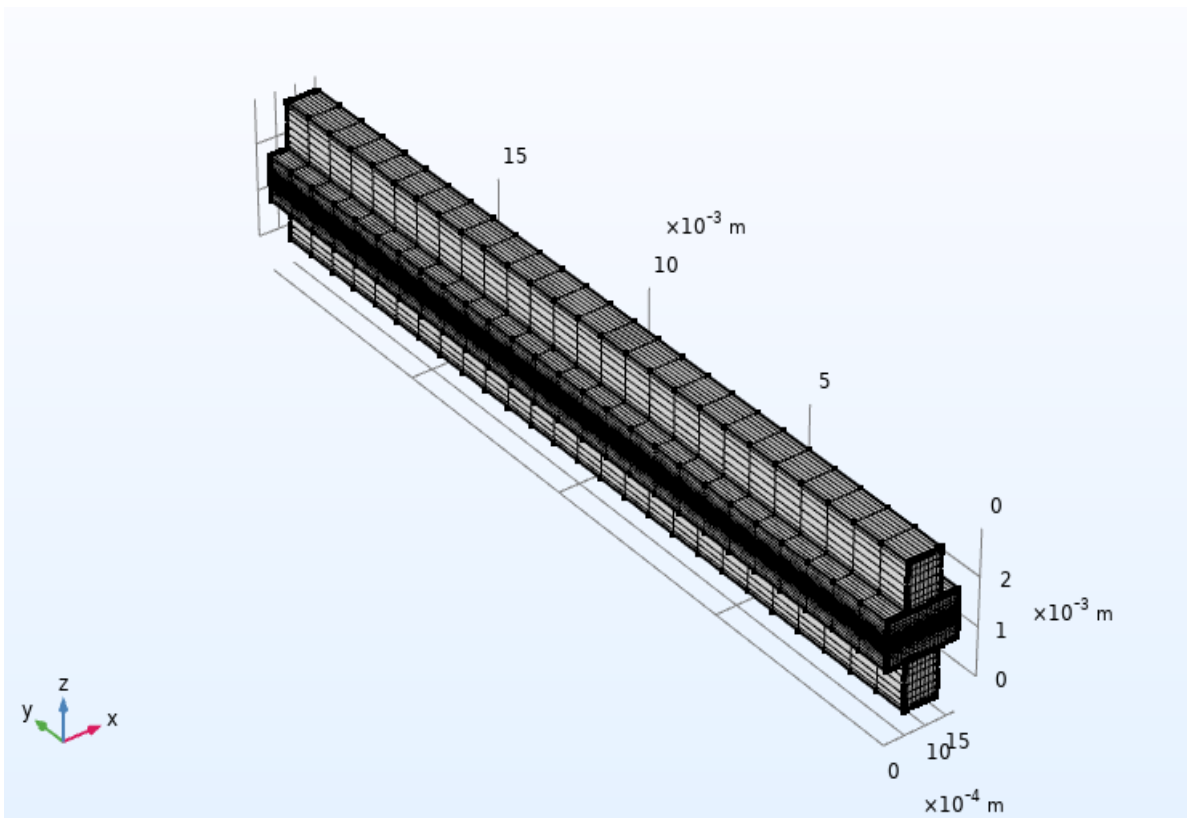
Fig 3.3 2D Mesh

Fig 3.3 Mesh generated along the channel length

3.3 Boundary Conditions:

The boundary conditions given for the simulation are

Region	Boundary Condition
Outlet flow channel of anode	$\partial \phi / \partial z = 0$
Outlet flow channel of cathode	$\partial \phi / \partial z = 0$
Anode terminal	$\varphi_{sol} = 0$ $\partial \varphi_{mem} / \partial y = 0$
Cathode terminal	$\varphi_{sol} = V_{cell}$ $\partial \varphi_{mem} / \partial y = 0$
Exterior boundaries	$\partial \varphi_{mem} / \partial x = 0$ $\partial \varphi_{mem} / \partial z = 0$ $\partial \varphi_{sol} / \partial x = 0$ $\partial \varphi_{sol} / \partial z = 0$

Table 3.1: Boundary conditions

3.4 INLET PARAMETERS:

The Inlet parameters for simulation of PEMFC are

Parameters	Value
Cell length (m)	0.02
Channel height (m)	0.001
Channel width (m)	0.000787
Rib width (m)	0.000909
GDL width (m)	0.00038
Porous electrode thickness (m)	5.00E-05
Membrane thickness (m)	0.0001
GDL porosity	0.4
GDL permeability (m^2)	-9.772
GDL electric conductivity (S/m)	222
Anode viscosity (Pa*s)	-2.715
Cathode viscosity (Pa*s)	-5.613
Hydrogen molar mass (kg/mol)	0.002
Nitrogen molar mass (kg/mol)	0.028
Water molar mass (kg/mol)	0.018
Oxygen molar mass (kg/mol)	0.032
H_2-H_2O Binary diffusion coefficient (m^2/s)	0.000180
N_2-H_2O Binary diffusion coefficient (m^2/s)	-11.534
O_2-N_2 binary diffusion coefficient (m^2/s)	-10.753
O_2-H_2O binary diffusion coefficient (m^2/s)	-12.638
Cell temperature (K)	453.15
Reference pressure (atm)	1

Cell voltage(V)	0.95
Electrolyte phase volume fraction	0.3
Open volume fraction for gas diffusion in porous electrodes	0.3
Permeability (porous electrode)	-21.904
Membrane conductivity (S/m)	9.825
Transfer coefficient, cathode	1
Reference equilibrium potential, anode(V)	0.1052
Reference equilibrium potential, cathode(V)	1.2362
Humidification temperature (^{o}C)	301.15
Water partial pressure (kPa)	3781.4
Reference concentrations (mg/L)	26.893
Inlet water molar fraction	0.037319
Inlet hydrogen molar fraction	0.96268
Inlet oxygen molar fraction	0.20216
Operating current for gas flow calculations	0.33934
Anode stoichiometry	1.2
Cathode stoichiometry	2
Inlet velocity, anode (m/s)	0.10352
Inlet velocity, cathode (m/s)	0.41078
Reference exchange current density, cathode (A/m^2)	0.001
Reference exchange current density, anode (A/m^2)	100
Specific surface area (m^2/m^3)	10000000

Table 3.2: Parameters and Values

CHAPTER 4

Results and Discussions

4.1 Plots and Contours for single channel

4.1.1 Polarisation Plot (Single Channel)

The polarisation plot generated after computation is presented in the figure 4.1 (A) . The cell voltage is taken in the Y-axis and the cell average current density is taken in the X-axis. This graph helps us understand the relationship between the cell voltage potential and the cell average current density developed. From Fig 4.1 (A) it can be observed that as we decrease the cell voltage of the fuel cell the average current density also decreases. This plot was also used as a reference point to validate our model with the help of journal papers. The relationship between the current density and power density can be observed from figure 4.2 (B). It can be observed that power density increases with increase in current density.
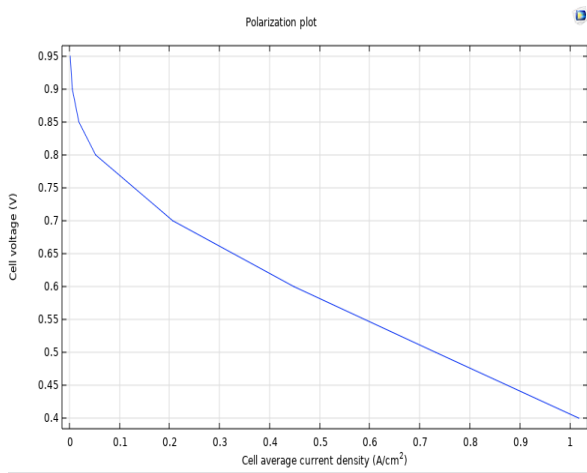

Fig 4.1 (A)   Fig 4.1 (B)

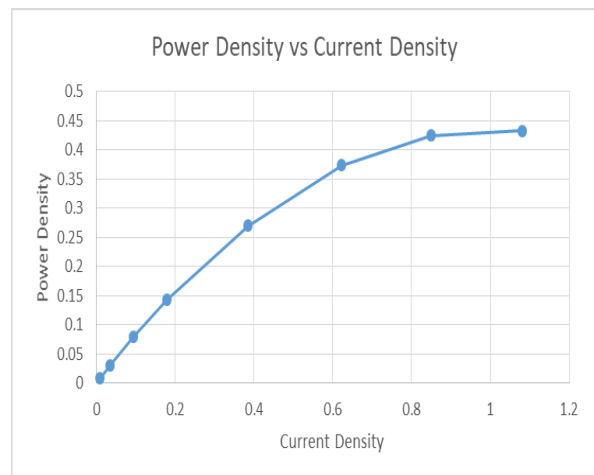Polarisation Plot   Power Density vs Current Density

4.1.2 Ionic current (z-direction) in the centre of the membrane (Single Channel)

The figure below shows the ionic current in the centre of the membrane for 0.4V. From the figure below it can be observed that in the y-direction the current density is lower towards the outlet. This is observed because the concentration of the reactants reduces towards the outlet of the channel. In x-direction it can be observed that the current density is high around the region close to the channel and decreases near the very centre of the channel. This is observed due to the Ohmic drops in the gas diffusion layers.
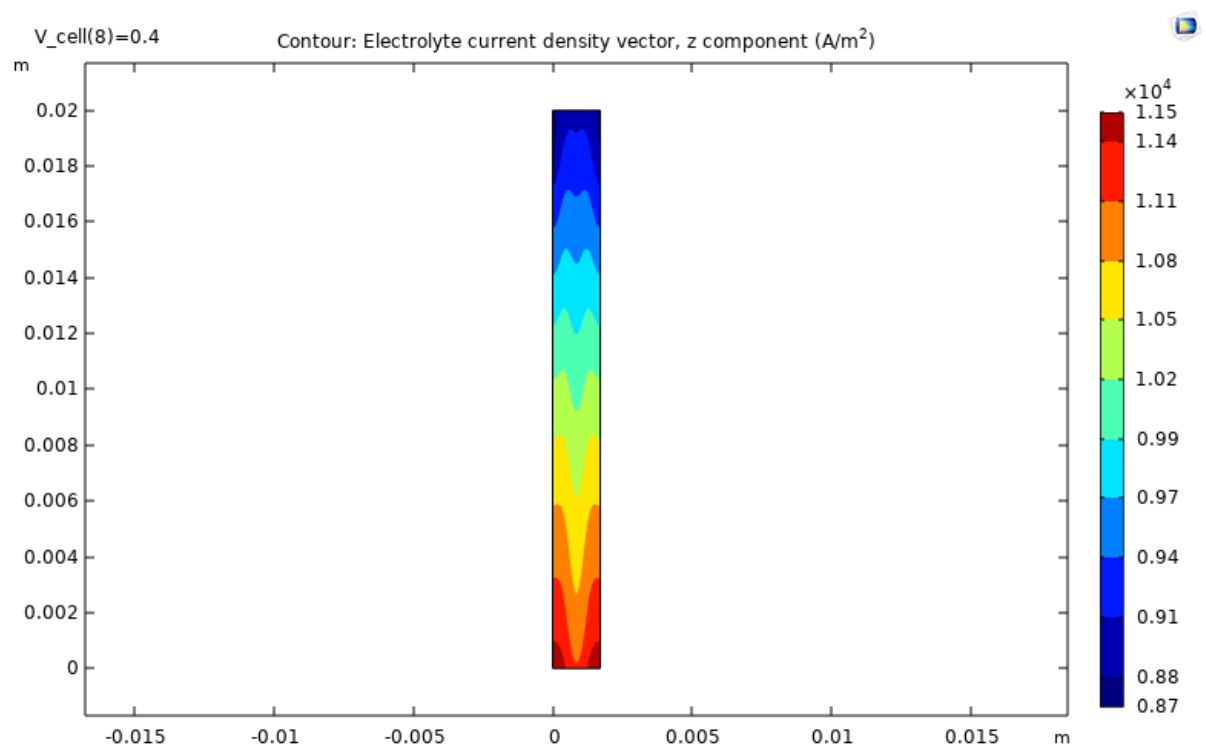

Fig 4.2 Electrolyte Current density vector (Z-component)

4.1.3 Molar concentration of oxygen along the cathode (Single Channel)

The figure below shows the molar concentration of oxygen along the cathode channel in the fuel cell. From the contour it can be observed that the molar concentration of oxygen reduces along the channel length. This happens because

oxygen penetrates the gas diffusion layer and enters the proton exchange membrane while travelling along the channel length.
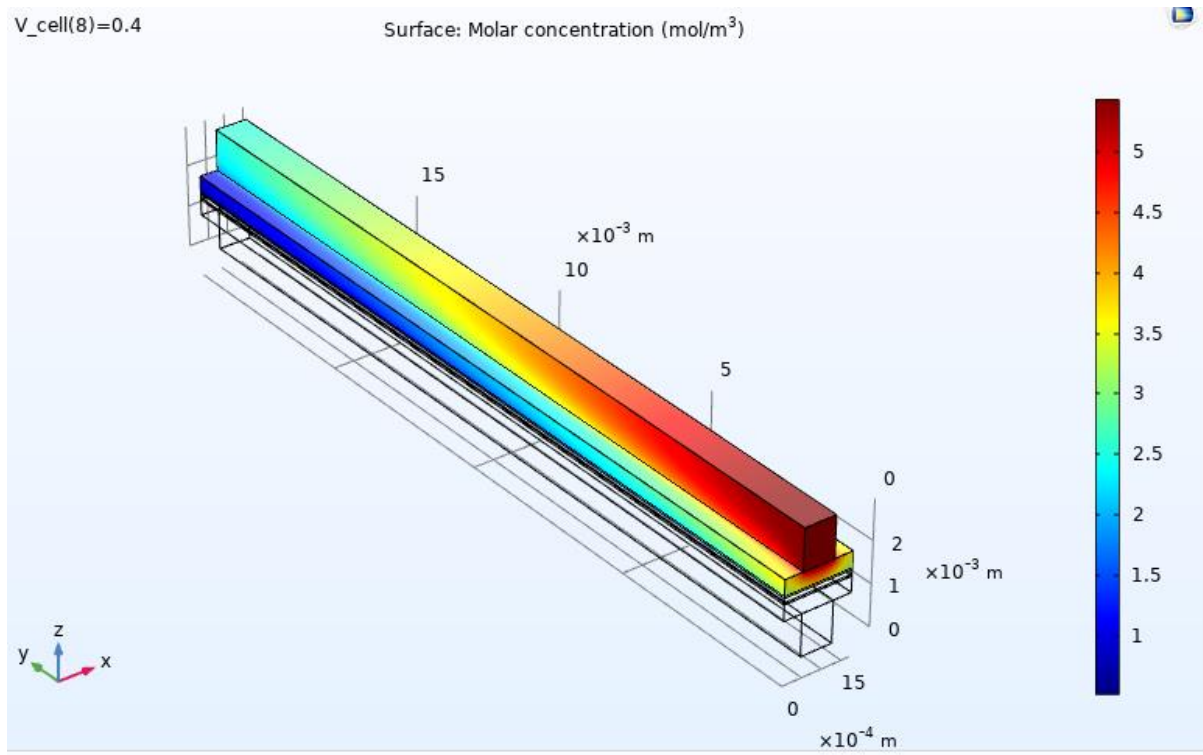

Fig 4.3 Surface Molar Concentration of oxygen in cathode

4.1.4 Molar concentration of Hydrogen along the Anode (Single channel)

The figure below shows the molar concentration of Hydrogen along the anode channel in the fuel cell. From the contour it can be observed that the molar concentration of Hydrogen reduces along the channel length. This happens because the hydrogen penetrates the gas diffusion layer and enters the proton exchange membrane while travelling along the channel length. At the same time it can be also observed that the concentration level of hydrogen in the anode is a bit more uniform when compared to the molar concentration of oxygen in the cathode
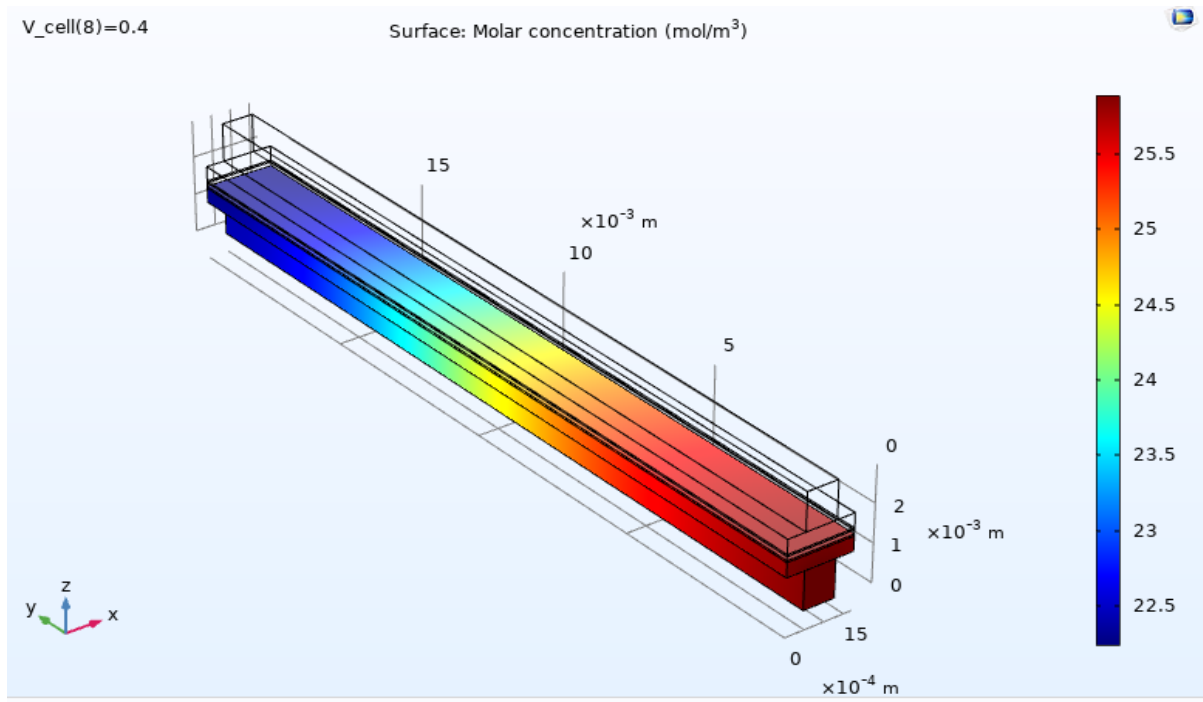
Fig 4.4 Surface Molar Concentration of hydrogen in anode

4.1.5 Water Concentration at Cathode (Single Channel)

The figure below shows the distribution of the water formed when oxygen flows in the cathode channel. From the contour given below it can be observed that the water formation in the cathode increases along the channel length. This happens because the oxygen concentration decreases along the cathode channel and towards the end of the cathode channel there is a lot of space available for the water to occupy. So the water molecules formed in the channel tends to fill these spaces. The water formed in the cathode is larger compared to that of the anode as the water formed in the anode tries to seep into the cathode compartment because of reverse diffusion.
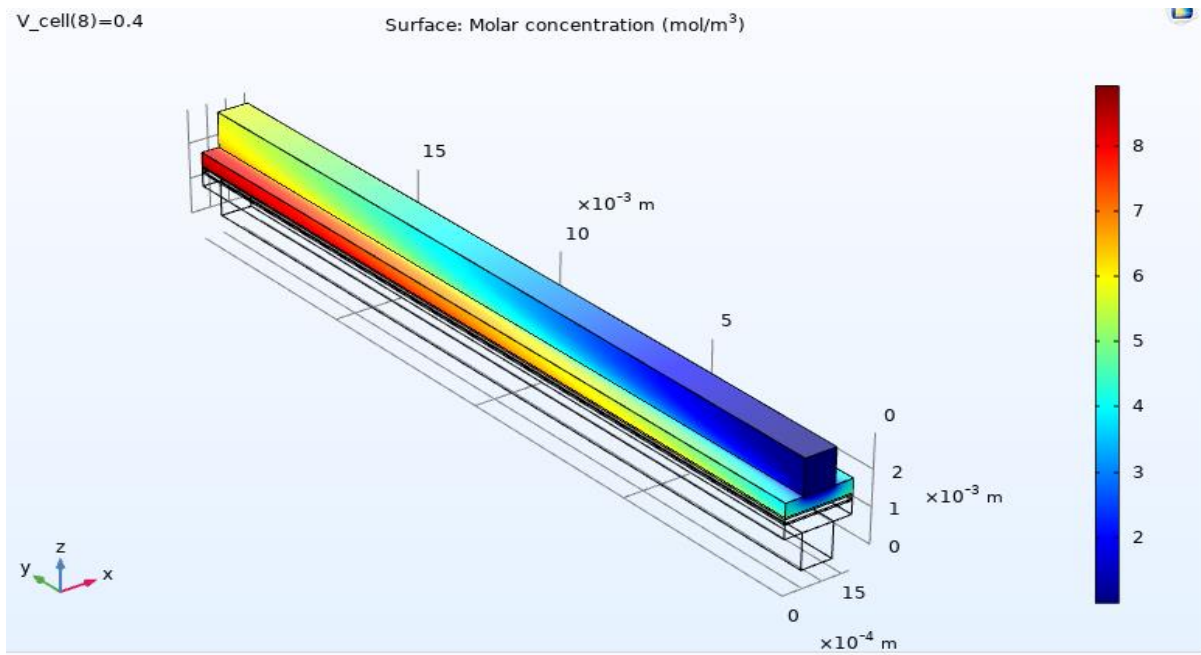
Fig 4.5 Surface Molar Concentration of water at cathode

4.1.6 Water concentration at Anode (Single Channel)

The figure below shows the distribution of the water formed when hydrogen flows in the anode channel. From the contour given below it can be observed that the water formation in the anode increases along the channel length. This happens because the hydrogen concentration decreases along the anode channel and towards the end of the anode channel there is a lot of space available for the water to occupy. So the water molecules formed in the channel tends to fill these spaces. Water doesn't form on the anode. The water formation occurs at cathode. Due to a phenomenon called reverse diffusion we find water concentration on the anode side.
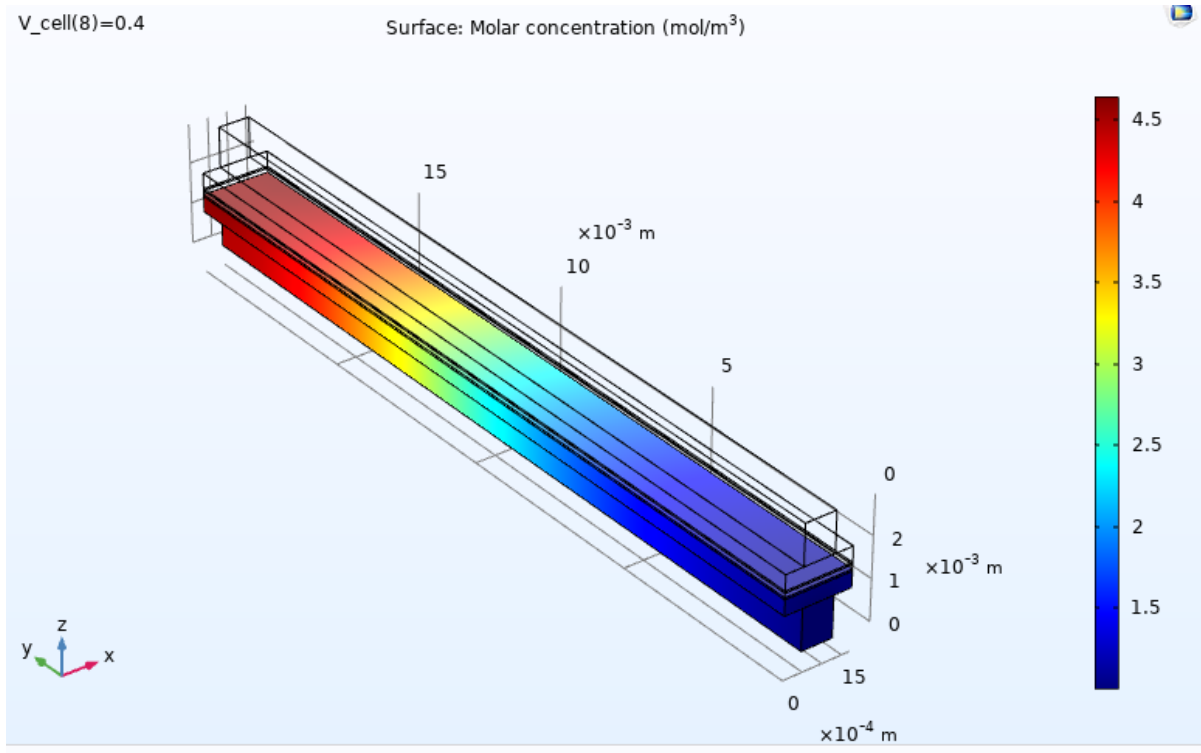
Fig 4.6 Surface Molar Concentration of water at anode

4.2 Plots and Contours for multi channel (2 channels)

The trends observed in the plots and contours of multi channel analysis were similar to that observed in single channel.
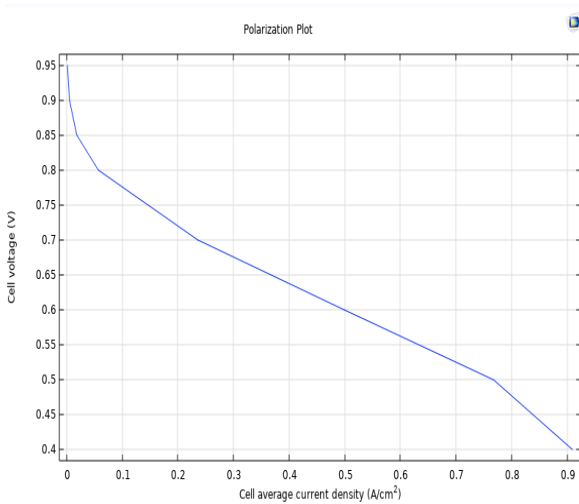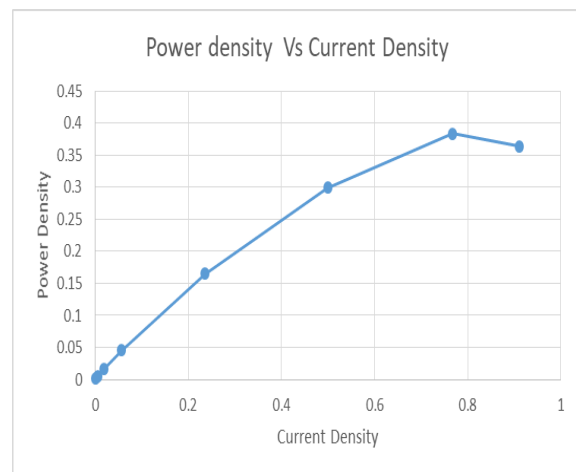

Fig 4.7(A) Polarisation plot

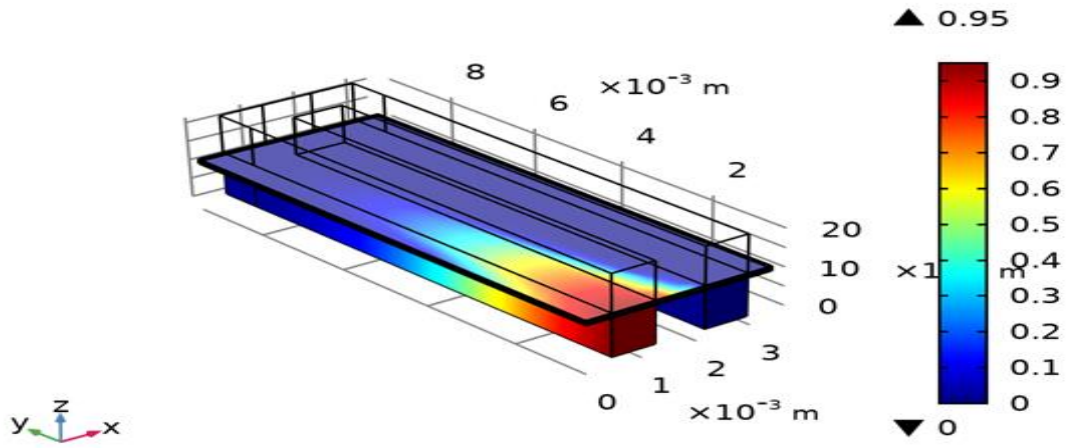Fig 4.7 (B) Power Density vs

Current Density

Fig 4.8 Surface Molar concentration of H_2 in anode
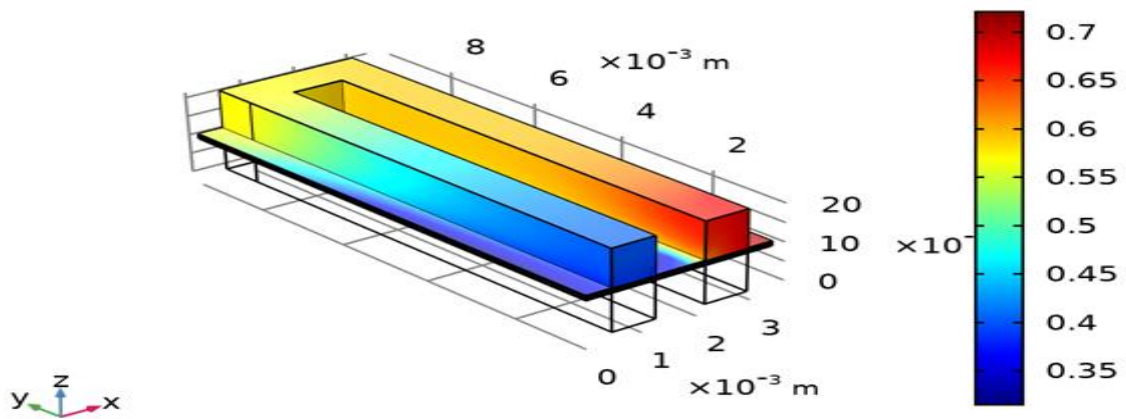

Fig 4.9 Surface Molar Concentration of o_2 in Cathode

V_cell(8)=0.4   Surface: Mole fraction (1)
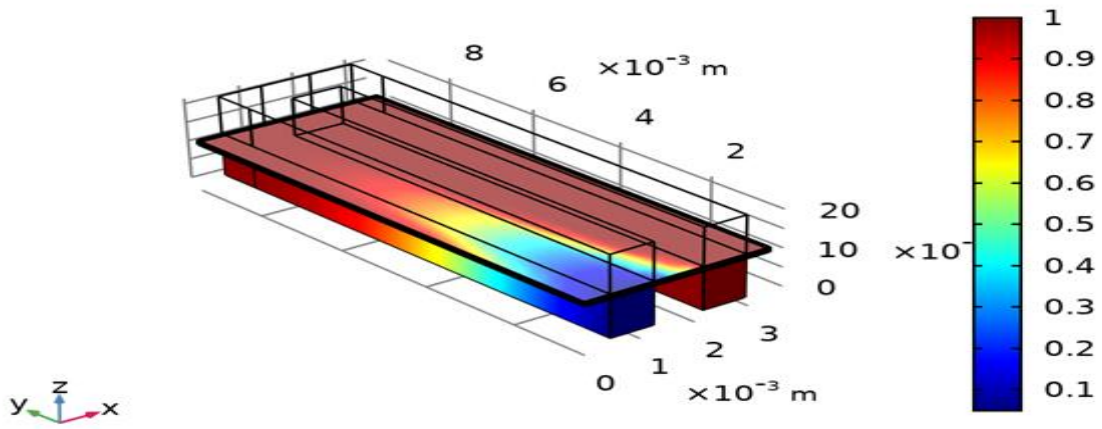
Fig 4.10 water concentration at anode
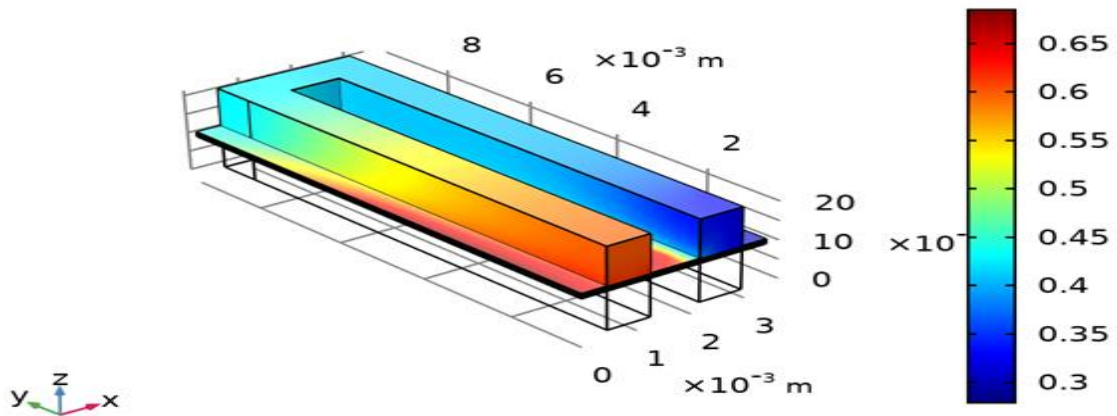

V_cell(8)=0.4   Surface: Mole fraction (1)

Fig 4.11 Water concentration at cathode

4.3 Experimental Validation:

The result obtained by the computational model is validated with the experimental values mentioned in literature. [16] and the results were compared to calculate the percentage deviation. The percentage deviation was found to be 4.76%. The Percentage deviation of current density for different voltages was found using the formula given below:

Percentage Deviation =

$$\frac{Computational\ current\ density - Experimental\ current\ density}{Experimental\ Current\ density} * 100$$

Voltage (V)	Curent Density (A/cm^2)	Experimental Current Density (A/cm^2)	Percentage Deviation (%)
0.95	0.0086985	0.0087	-0.02%
0.9	0.033984	0.034	-0.05%
0.7	0.38518	0.385	0.05%
0.6	0.62223	0.6222	0.00%
0.5	0.84886	0.9018	-5.87%
0.4	1.0809	1.0653	1.46%
Average Percentage Deviation			-0.74%

Table 4.1 Experimental validation

In the table given above the overall percentage deviation for the model created was calculated by taking the average of the individual percentage deviations for the different voltage values taken in the study.

A polarization plot was generated using the data in the table. The current density is plotted in the x axis and voltage in y axis. The current density obtained from COMSOL MULTIPHYSICS 5.5 software after applying the inputs given in the journal paper was plotted against the voltage applied. In the same graph the experimental current density was plotted for the same voltage value. This has been done to get a better understanding of the deviation between the results from the software and the experimental result mentioned in literature.
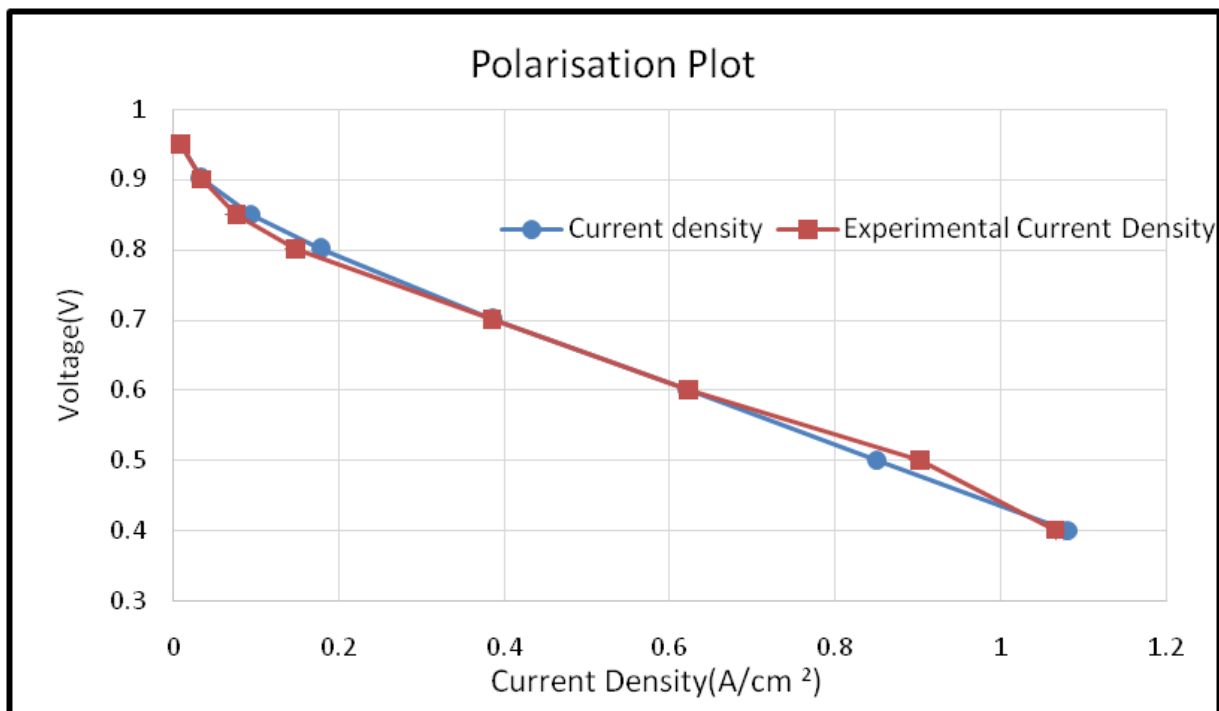

Fig 4.12 Polarisation Plot (Experimental validation)

Chapter 5

Conclusion and Scope for Future Work

In this research, a three dimensional model of the Proton Exchange Model was developed and the mass transport analysis was simulated in COMSOL MULTIPHYSICS 5.5 to understand the flow and distribution of the reactants (hydrogen and oxygen) and the by-product water formed after the reaction. The three dimensional model has been created for a single channel of the bipolar plates and the results of the simulation has been validated by applying the input parameters given in literature. A multi-channel model has also been created with 2 channels to understand the behaviour of reactants in bends. The scope has been limited to 2 channels considering the computational resources available for the computation of the model. The model is simulated by solving conservational equations for the membrane, flow channels and the electrodes.

The main objectives to run the simulations are

    a) To understand the flow and distribution of the reactants in the membrane electrode assembly

    b) To understand the relationship between the voltage applied and the current density obtained in the PEMFC

From the results it can be observed that the concentration of hydrogen and oxygen decreases along the channel length. This happens because the both the hydrogen and oxygen are being consumed while they travel along the channel. The concentration of water was found to increase along the channel. This can be attributed to the fact that the water formed in the channel tends to move to the end of the channel (outlet) as there is a lot of space available for the water molecules. These spaces are created due to the fact that a large amount of both the reactants (H_2 and O_2) get consumed near the inlet and there is a lot of free space available near the outlet.

It is evident from the results that water formed in the cathode is larger compared to that of the anode. Water doesn't form in anode but the water molecules in anode is due to a phenomenon called reverse diffusion.

The scope for future work includes modelling and simulation of multi-channel flow area with 8 to 12 passes for single phase along with experimental validation and developing multiphase model which will be able to predict the behaviour of reactants with greater accuracy and higher dependability.

References

[1]. F.Hashemi.S.rowshanzamir.M.Rezakazemi.Mathematical and Computer Modelling.55(2012) 1540-1557.

[2]. S.Dutta. S.Shimpalee. J.W.VanZee.International Journal of Heat and Mass Transfer. 44 (2001) 2029-2042.

[3]. Y.M.Ferng.A.Su.J.Hou. Energy Conversion and Management.78 (2014) 431-437.

[4]. H.G.Guvelioglu.H.G.Stenger. Journal of Power Sources.163 (2007) 882-891.

[5]. W.Haung.B.Zhou and A.Sobiesiak. International Journal of Energy. 2005.29:1051-1071.

[6]. X.Li. G.Cao. X.Zhu. Energy Conversion and Management.47 (2006) 1032–1050.

[7]. I.Tolj.D.Bezmalinovic.F.Barbir.International Journal of Hydrogen Energy.36 (2011) 13105 - 13113.

[8]Berna Sezgina,* , Dilara GulcinCaglayan a , YilserDevrim b , Thomas Steenberg c , Inci Eroglu a a

[9] L.Xing.X.Liu.T.Alaje.R.Kumar.M.Mamlouk, K.Scott .Energy.73 (2014) 618-634.

[10]K.H.Wonga.K.H.Loo.Y.M.Lai.S.C.Tan.C.K. Tse.International Journal of Hydrogen Energy.36 (2011) 11871-11885.

[11] X.D.Wang.Y.Y.Duan.W.M.Yan.F.B.Weng. Journal of Power Sources.176 (2008) 247–258.

[12]M.Tohidi.S.H.Mansouri.H.Amiri. International Journal of Hydrogen Energy.35 (2010) 9338-9348. [13] M.Sahraouia.C.Kharratb.K.Halouanib International Journal of Hydrogen Energy.34 (2009) 3091–3103.

[14] Q.Jian.G.Ma.X.Qiu.Renewable Energy. 62 (2014) 129-136.

[15] C.I,Lee.H.S.Chu. Journal of Power Sources. 161 (2006) 949–956.

[16] Hashemi, F., Rowshanzamir, S., & Rezakazemi, M. (2012). CFD simulation of PEM fuel cell performance: effect of straight and serpentine flow fields. *Mathematical and Computer Modelling*, *55*(3-4), 1540-1557.