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Numerical Investigation of Mass Transfer in PEM Fuel Cell with Straight Gas Flow Channels using CFD

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Abstract: ***Interest in PEM fuel cells has grown rapidly in recent years because of its possible applications. The performance of PEM fuel cells is strongly affected by various physical factors, such as the flow of reactant gas, thermal management and water management. The performance and characteristics of a PEM fuel cell have been analysed through the development of a 3D model and numerical simulation. The result obtained from the computational model shows details of species movement, charge Transport and mass transfer phenomena. This paper also investigates the influence of input parameters on the output of the PEM fuel cell model. The result from the analytical study is compared with experimental results to check the accuracy of the model.***

Keywords: PEM fuel cell, CFD Simulation, Mass Transfer, Computational Model, Polarization Curve.

I. INTRODUCTION

The impact of continuous growth in the world's population and economy has been seen in the sales of automotive vehicles. Consequently, the demand for automotive vehicles is projected to increase. It is important to look beyond conventional heat engines for powering automobiles. Clean energy for vehicle transportation is one of the greatest challenges in this situation. Fuel cell technology is likely to play a major role in the future green energy-based economy. Among various types of fuel cell, the proton-exchange membrane (PEM) fuel cell is best suited for automobile applications [1]. High efficiency, high energy density, quick start-up, and low operating temperature are the main advantages of PEM fuel cells [2-3].

The structure of PEM fuel cell can be divided into three parts: anode, cathode, and electrolyte membrane. The PEM fuel cell consists of components such as flow channel, gas diffusion layer (GDL), catalyst layer (CL), membrane and bipolar plate, etc. PEM fuel cells undergo a number of complex dynamic processes including gas flow and thermal phenomena for conversion of chemical energy into electrical energy. The process descriptive diagram of the PEM fuel cell is shown in figure 1. Hydrogen and oxygen are used as reactant gas for the PEM fuel cell system. Hydrogen at the anode and oxygen at the cathode are supplied in the flow channel. The GDL is the porous region that allows the transport of the gases to the CL. As a result of the reaction at anode CL, the electron and proton are released. Electrons follow an external circuit to reach the cathode region. The hydrated membrane ensures the flow of proton ions. Proton ions combine with electrons and oxygen at the cathode catalyst layer to produce water and heat.

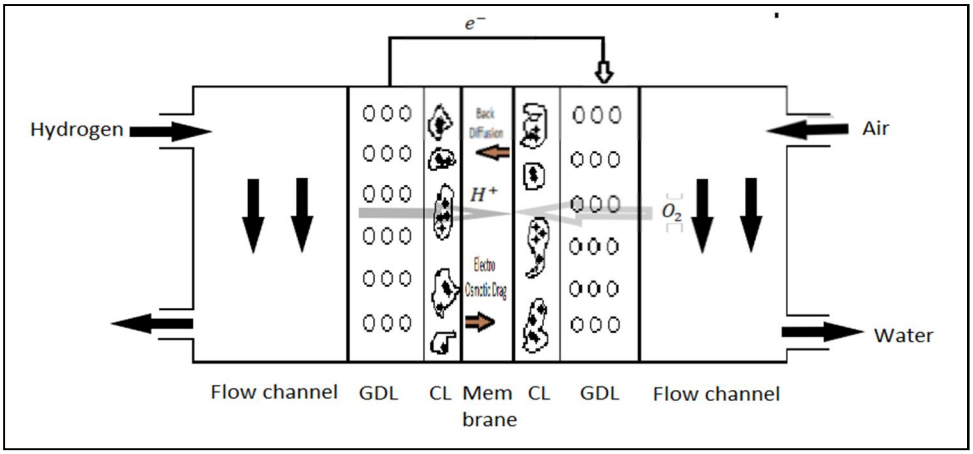


Fig. 1 PEM fuel cell descriptive diagram

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The performance of PEM fuel cells depends on the presence of water content in the membrane [4], transport phenomena, and electrochemical kinetics. In the early 1990s, Bernardi and Verbrugge [5] developed a steady-state, constant temperature PEM fuel cell model to evaluate water management in the membrane. Dutta et al. [6] developed a three-dimensional fuel cell model for the investigation of species concentrations and serpentine flow field effect. Nguyen et al. [7] considered a single-phase, serpentine flow field model of PEM fuel cell, they computed mass transfer using the Stefan–Maxwell equation and the Bruggeman correlation. Recently many computational models have been investigated by researchers to enhance performance. Most of these models are based on the CFD approach. The purpose of this work is to develop a three-dimensional straight flow model of PEM fuel cell. Phenomena taken into account for model development:

1) Electrochemical kinetics
2) Mass and momentum transfer
3) Heat transfer
4) Potential

II. MODEL DEVELOPMENT

Computational models are a time-saving option to create three-dimensional flow simulations and design studies. To reduce computational time and complexity only one cell domain of fuel stack was picked for the solution of CFD simulation. The computational domain consists of current collector, flow channel, GDL, CL, and membrane. The following assumptions have been taken for model development:

1) The model operates at steady-state conditions.
2) Isothermal condition.
3) Reactant gas flow is laminar.
4) The membrane's proton conductivity is fixed.
5) The reactant gas is treated as an ideal gas.
6) Butler Volmer equation is used for electrochemical reactions.

A. Model Equations

Continuity, conservation of species transport, and momentum equations etc, have been opted as governing equations for the model.

1) Continuity Equation

$$\rho\vec{v} = S_c \quad (1)$$

Where ρ is density and S_c source term for continuity equation

2) Momentum Equation

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

Where μ, p and S_P are viscosity, pressure and momentum source term respectively.

3) Mass Transfer Equation

$$\nabla.(\rho\varepsilon\vec{v}y_i) = \nabla.\left(\rho\varepsilon D_{ij}^{eff}\nabla y_i\right) + S_i \quad (3)$$

Equation 3 is valid within porous electrode. The meaning of terms y_i is mass fraction, D_{ij} diffusivity of species i and j and ε is porosity.

4) Conservation of energy

$$\nabla\left(\rho\, c_p\vec{v}\, T\right) = \nabla(k^{eff}\nabla T) + S_h \quad (4)$$

Where c_p is the specific heat, k^{eff} is the thermal conductivity of the fluid and S_h is source term for the energy equation.

5) Electrochemical Model

Equation for electron and proton transport:

$$\nabla.(\sigma_s\,\nabla\Phi_s) + R_s = 0 \quad (5)$$

$$\nabla.(\sigma_m\,\nabla\Phi_m) + R_m = 0 \quad (6)$$

Where σ_s is electric conductivity of electrode and σ_m is Electrical conductivity of membrane, R is transfer current and Φ is cell potential.

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6) Water Transport in the Membrane

The two-major transport process in the membrane are electro osmotic drag and back diffusion coefficient [8].

$$\lambda = 0.043 + 17.81a - 39.85a^2 + 36a^3 \qquad 0 \le a \le 1 \qquad (7)$$

$$\lambda = 14 + 1.4(a - 1) \qquad 1 < a \le 3 \qquad (8)$$

Where a is water activity and λ is water content of membrane**.**

III. GEOMETRY AND MESH GENERATION

Three-dimensional parts of PEM fuel cell components are created. Individual components are designed separately and assembled. The geometry of the PEM fuel cell is axis-symmetric. The geometry of the PEM fuel cell system is shown in the figure 2. Anode and cathode both the side consist current collector, gas diffusion layer, catalyst layer. A polymer electrolyte membrane separates anode and cathode side. The GDL, CL, membrane is rectangular in shape. The second step after geometry creation is meshing. For further solution created geometry is divided into a smaller number of nodes and elements. For this PEM fuel cell model, automatic mesh was generated in Ansys 19 R3 Fluent software.

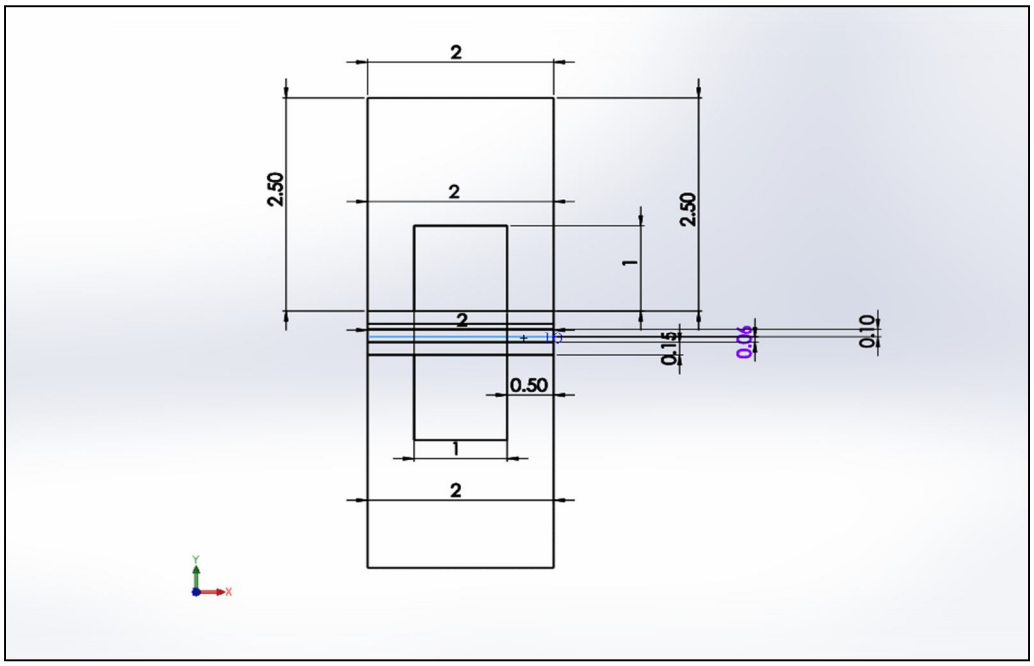


Fig. 2 Geometry of PEM fuel cell model (all dimensions are in mm)

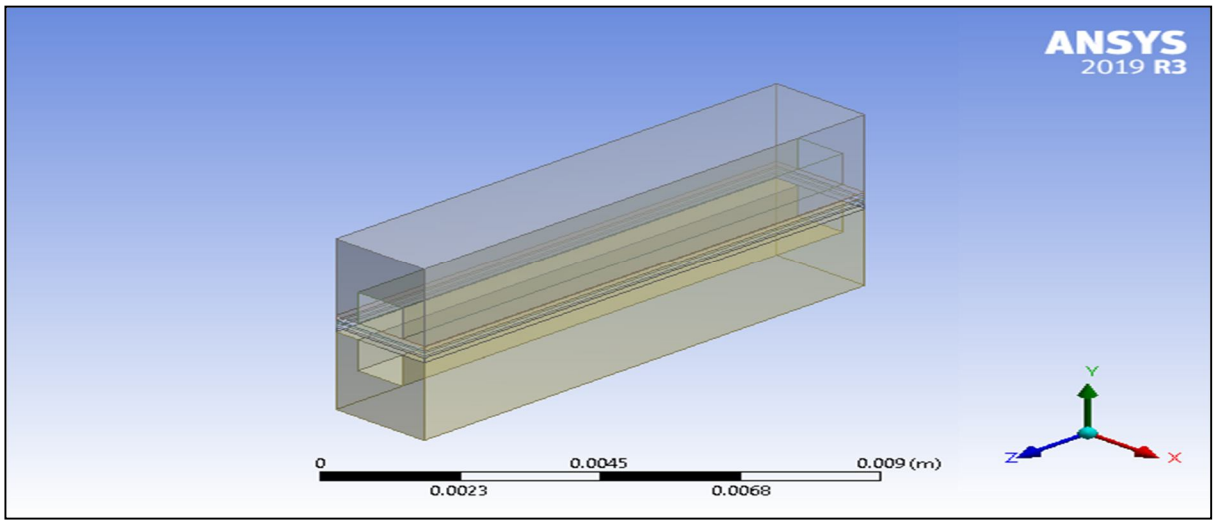


Fig. 3 Isometric view of PEM fuel cell model

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IV. BOUNDARY CONDITIONS

Boundary conditions were defined for different zones. Mass fraction of reactant gas at the inlet of the anode and cathode flow channel are prescribed. The value of pressure at the inlet and outlet are defined. Temperature is set to the same for all the components of the PEM fuel cell. No-slip condition is applied at the interface of solid fluids.

TABLE I
BOUNDARY CONDITIONS AT INLET ANODE

Inlet Anode	Value	Unit
Velocity [9]	2	m/s
Pressure [9]	3	atm
Temperature	343	K
H_2	0.6	–
H_2O	0.4	–

TABLE II
BOUNDARY CONDITIONS AT INLET CATHODE

Inlet Cathode	Value	Unit
Velocity	1	m/s
Pressure	3	atm
Temperature	343	K
O_2	0.21	–
H_2O	0.25	–

TABLE III
OTHER VALUES

Parameter	Value	Unit
Cell voltage	0.7	V
Cell Temperature	343	K
Open Circuit Voltage	1.1	V
Membrane Equivalent Weight	1100	$kg/kmol$
Protonic Conduction Coefficient	1	–
Membrane Thickness	0.10	mm
Faraday's Constant	96485	$C\ mol^{-1}$
Gas Constant	8.3144	$mol^{-1}K^{-1}$

V. SOLUTION PROCEDURE

The Ansys 19 Fluent R3 was used to undertake the simulation of the PEM fuel cell model. The PEM fuel cell add-on module is loaded into Fluent via the text user interface. A finite-volume-based approach is used for the representation of equations. The governing equations were solved using the SIMPLE algorithm. Intel Core(TM) i5-6600K CPU @ 3.50GHz processor with 8 GB RAM was used to solve the problem.

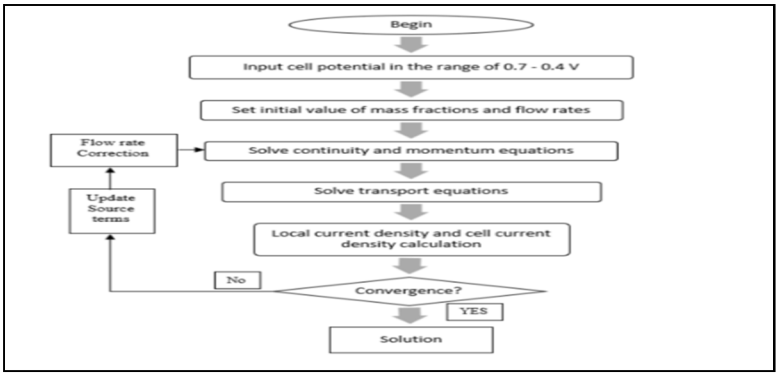


Fig. 4 PEM fuel cell modelling solution procedure

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VI. RESULT AND DISCUSSION

The developed model simulation results were compared in terms of polarization curve with experiment result of wang et al. [10]. The model showed good agreement with the experiment result.

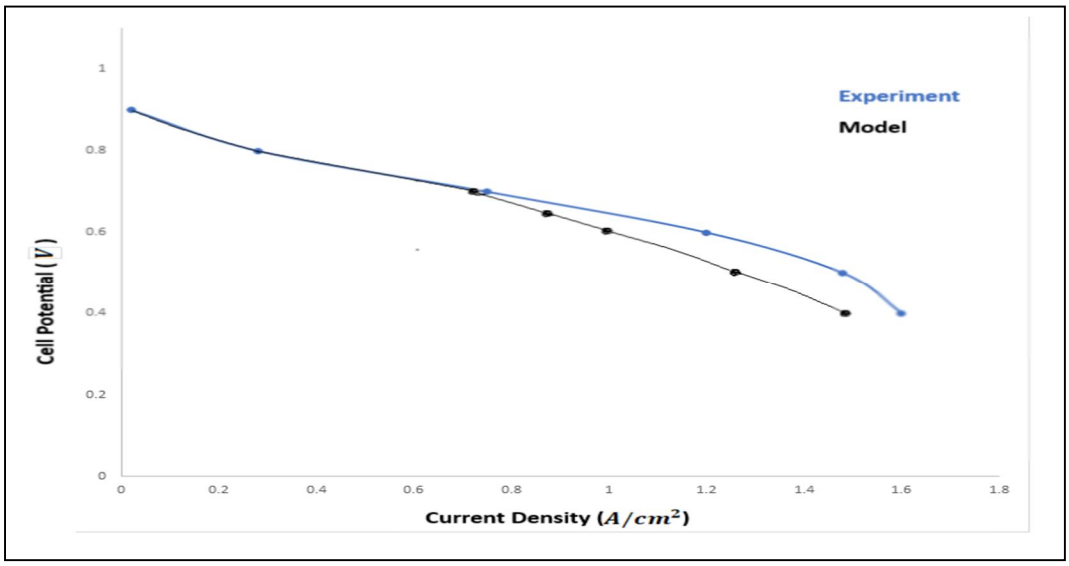


Fig. 5 Model validation via polarization curve

The hydrogen transport plays a significant role in increasing the performance of the PEM fuel cell model. The mass fraction of hydrogen at the anode section is shown in figure 6 & 7. Figure represents the hydrogen mass fraction distribution at 343 K, 0.7 V and 0.6 V respectively. The maximum value of the mass fraction of hydrogen found in the gas flow channel for both the voltage. Hydrogen concentration decreases if moving in the direction of the Y-axis downward. For gas diffusion layer, catalyst layer, and membrane result shows hydrogen concentration increase at lower voltages.

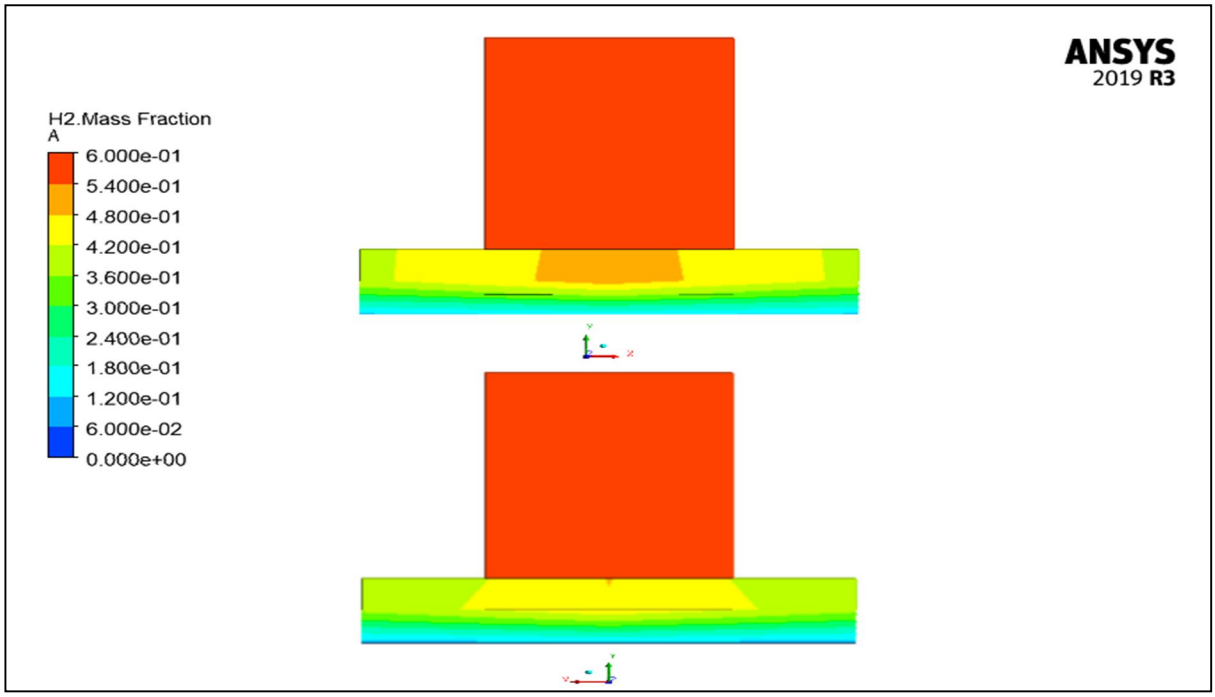


Fig. 6 Hydrogen mass fraction distribution in PEM fuel cell for 0.7 V

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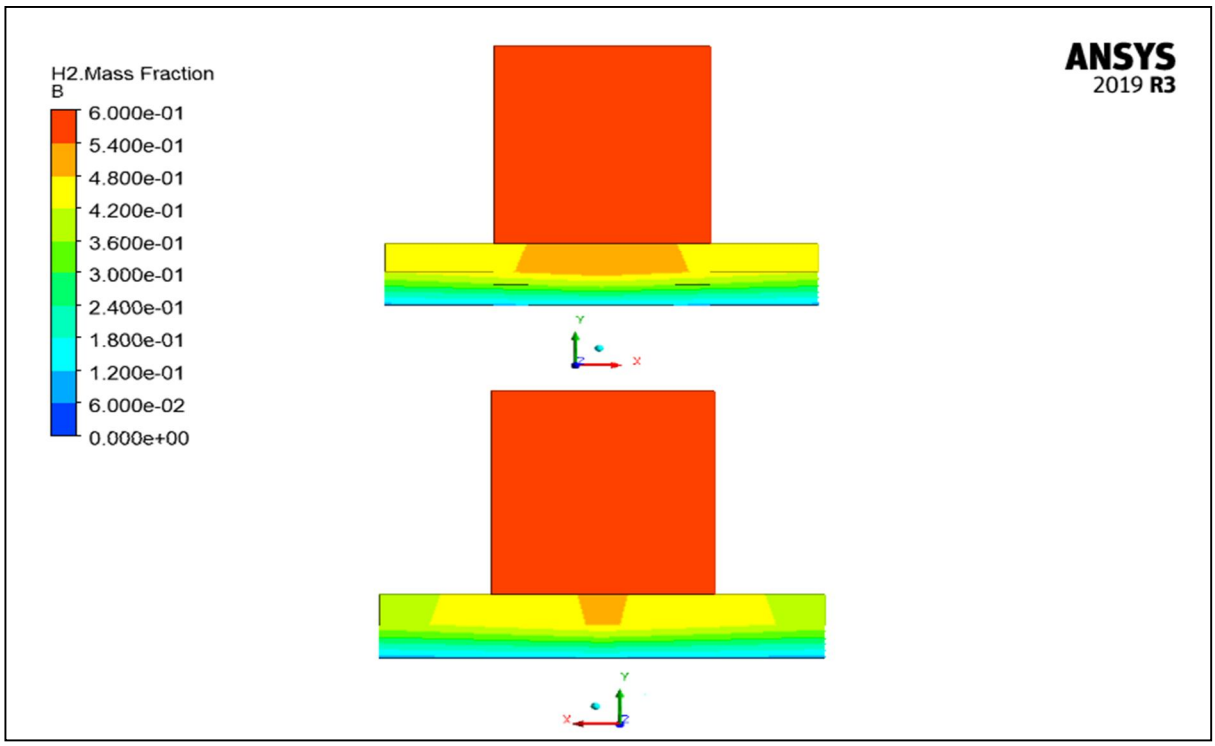


Fig. 7 Hydrogen mass fraction distribution in PEM fuel cell for 0.6 V

Since oxygen concentration is concerned with describing current density distribution the analysis of oxygen mass fraction is significant. The oxygen is reduced at the interface of the catalyst layer. The oxygen distribution is limited only at the cathode side. The comparison of oxygen mass fraction at the cathode section for 343 K, 0.7 V, and 0.6 V is shown in figure 8 & 9. The highest value of oxygen mass fraction found in the flow channel. However, the gradual decreases between the inlet and outlet of the flow channel are visible at lower voltages. The oxygen mass fraction in GDL, CL, and membrane decreases at lower voltages.

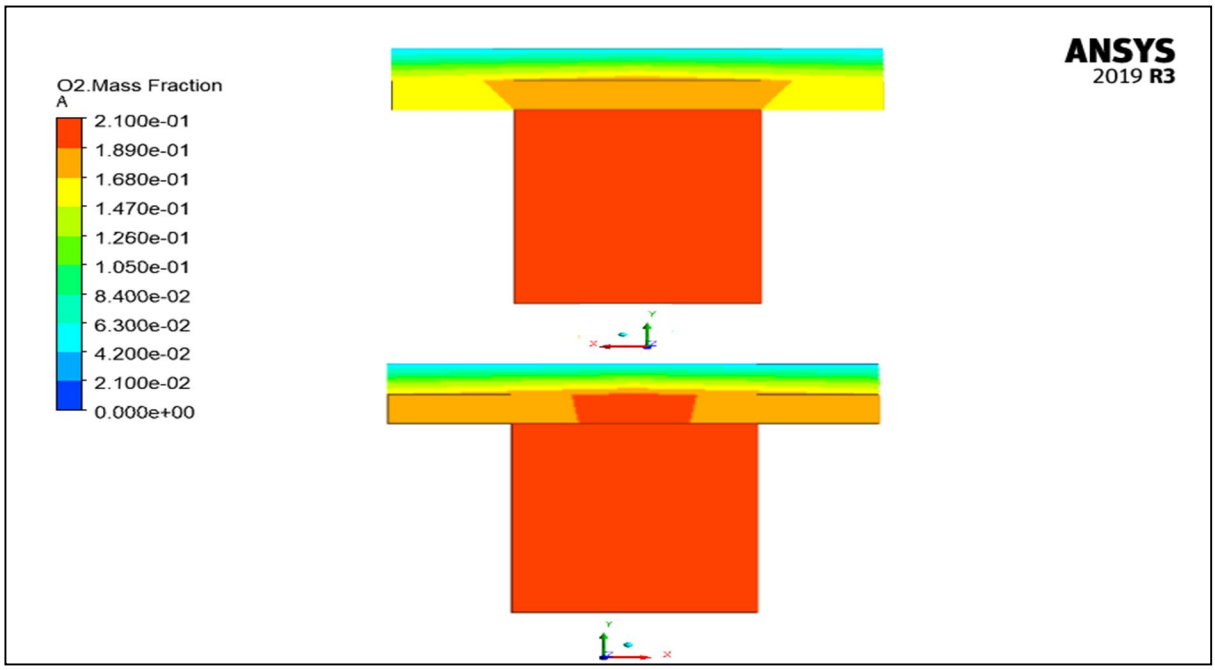


Figure 8. Oxygen mass fraction distribution in PEM fuel cell for 0.7 V

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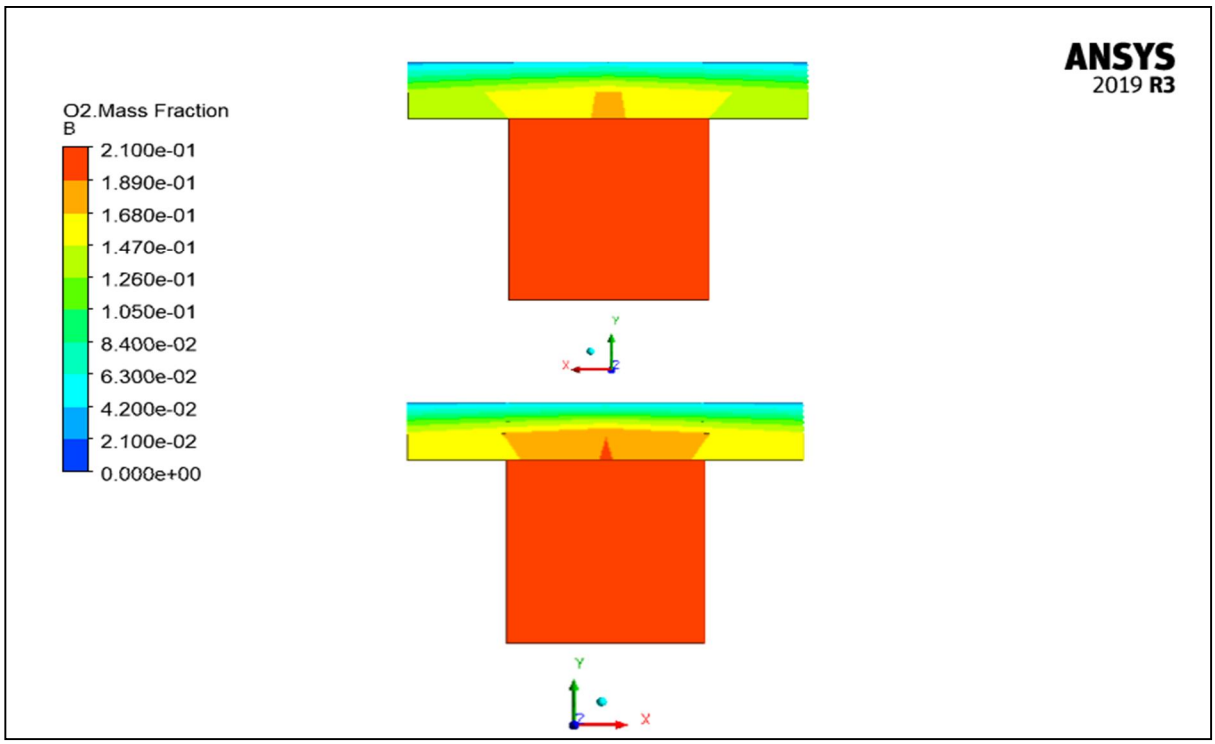


Figure 9. Oxygen mass fraction distribution in PEM fuel cell for 0.6 V

The concentration variation of water in the fuel cell system is the result of a complex electrochemical reaction that takes place inside the PEM fuel cell. Electro osmosis drags cause the liquid water migration from the anode side to the cathode side takes place. Figure 10 & 11 shows the result of water mass fraction in PEM fuel cell model for base case condition and 0.6 V.

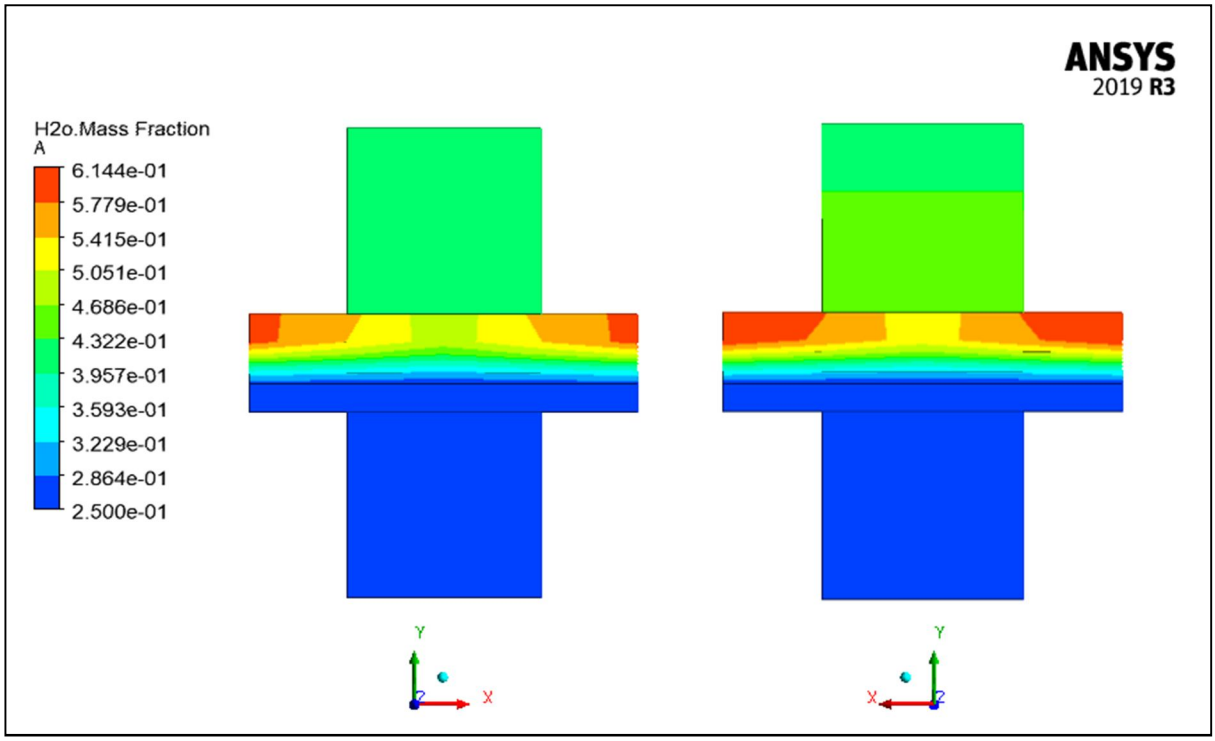


Figure 10. Water mass fraction distribution in PEM fuel cell for 0.7 V

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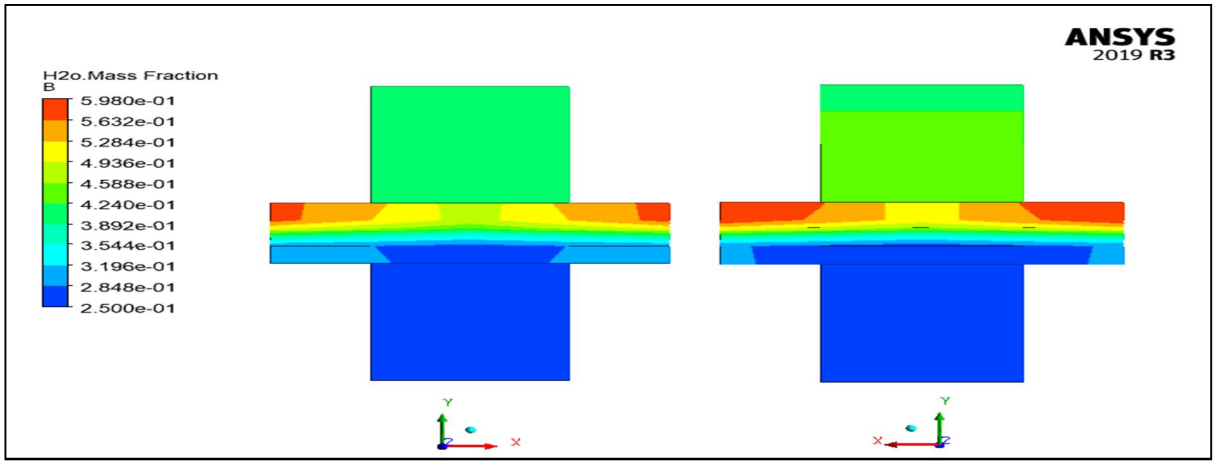


Figure 11. Water mass fraction distribution in PEM fuel cell for 0.6 V

A. Effect of Temperature

Good thermal management is necessary for high-performance and stable PEM fuel cell. Temperature change affects various phenomena inside the PEM fuel cell. For analysing the effect of temperature in this model the temperature varied from 50-80°C, while other parameters remained as base case conditions. High operating temperature affects the water balance of PEM fuel cell. The main advantages associated with high-temperature flow fields are that they help in establishing block-free flow through the domain. However, humidification of reactants becomes necessary if the fuel cell is operating at a higher temperature.

B. Effect of Pressure

Pressure regulation is the necessity of a hydrogen supply system to achieve the desired result. The density and thermal conductivity of gas depends on the pressure of the supply system. The effect of pressure on fuel cell performance is analysed by varying operating pressure from 1-3 atm, and other parameters were kept constant as base case conditions. Increasing operating pressure has a significant effect on the cathode side, also It is observed at higher pressure reaction kinetics become faster consequently better result is achieved.

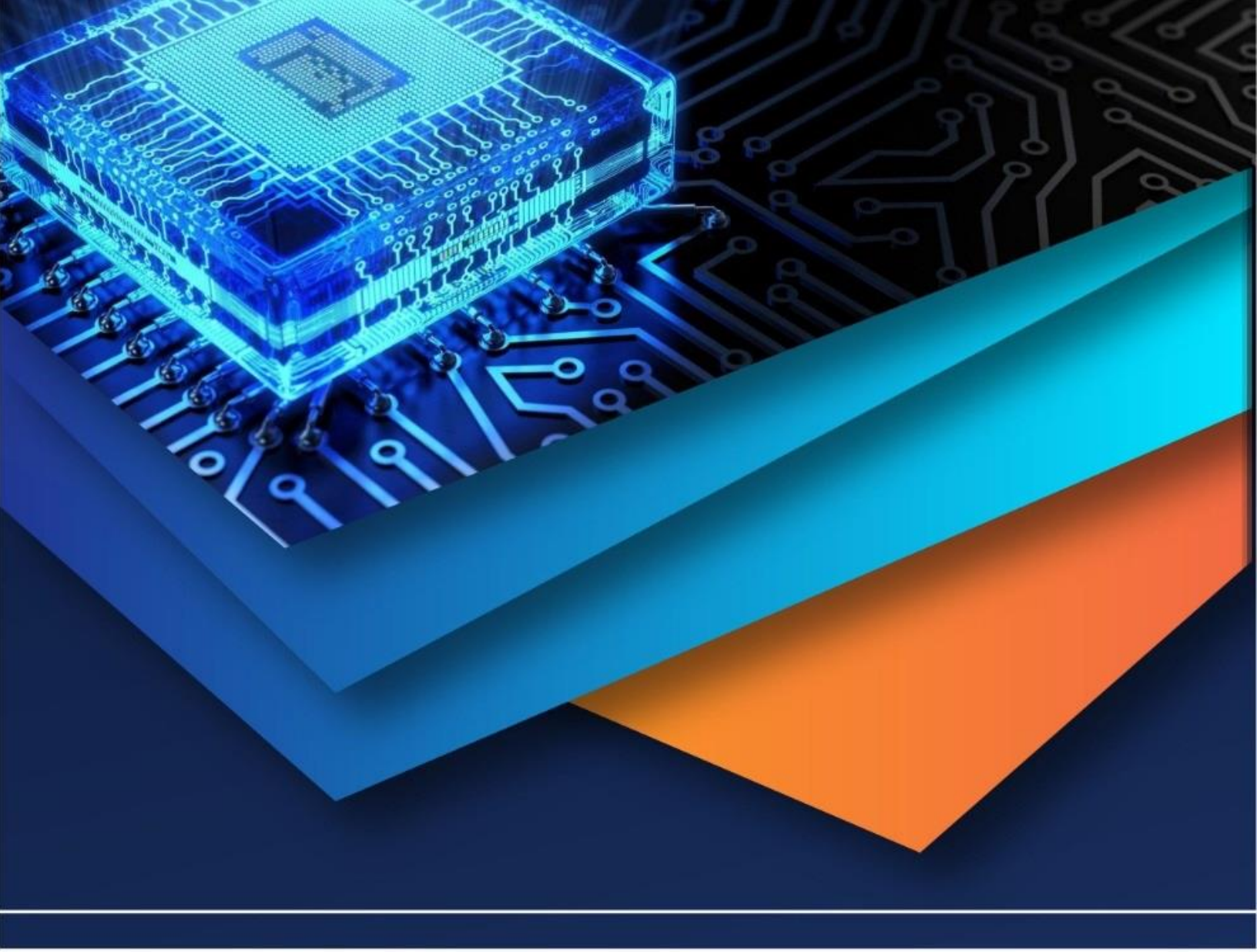
VII. CONCLUSIONS

This work presents the simulation result of the three-dimensional computational fluid dynamics model of PEM fuel cell. The model provides information about flow patterns, mass transport of reactant gas and water in the components of PEM fuel cell. Studies were undertaken for investigation of the effect of temperature and pressure on the output of the PEM fuel cell model. The result of this study shows the performance of fuel cell is better at high temperatures and pressure. The results were validated against experimental data for different values and good agreement was achieved.

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