# Three-Dimensional PEM Fuel Cells Modeling using COMSOL Multiphysics

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**ABSTRACT**
Proton Exchange Membrane Fuel Cell (PEMFC) has become one of the most promising energy technologies at the present time. Several factors are driving the growing interest in this technology. Modeling different phenomena occurring in PEMFC plays an important role in this development and performance. The performance of a Proton Exchange Membrane Fuel Cell (PEMFC) depends on the characteristics of the membrane, gas diffusion layer (GDL), catalyst and operating parameters such as operating pressure, cell operation temperature, relative humidity, and mass flow rate of feed gases, channel geometries and design of the stack. Recent studies on the compilation of factors affecting durability and performance of PEMFC indicate that the performance of fuel cell strongly depends on the performance of its membrane. In this paper, a three-dimensional PEM fuel Cell model has been developed and is used to investigate the effects of geometry membrane on cell performance. The numerical results indicated that a thinner membrane corresponds to the higher current density, the hydrogen and oxygen consumption and, accordingly water production is high. Finally, the numerical results of the proposed CFD model are compared with the available experimental data and that represent good agreement.

## 1. INTRODUCTION

The proton exchange membrane (PEM) fuel cell converts chemical energy into electricity using an electrochemical cell, and it could be used as efficient power sources, offering high power density and low environmental impact [1-4]. Within the last couple of years [5-6], so many improvements have been made for PEMFCs in design, materials, manufacturing and application. Up to now, cost, durability, hydrogen storage and performance are the major barriers facing the full commercialization of PEMFC. The performance of PEMFC depends strongly on the characteristics of the membrane, gas diffusion layer (GDL), catalyst and operating parameters such as operating temperature, pressure, humidity, and mass flow rate of feed gases, channel geometries and design of the stack [7-16]. Membrane is the most important component of PEMFC [17]; it is a proton conductor between two electrode anode and cathode and yet pushes the electron to flow through the external circuit to produce useful electricity. It also a physical barrier between the anode and the cathode by stopping penetration of fuel from cathode side to anode side or opposite. According to previous studies by the authors [1] on the compilation of factors affecting durability and performance

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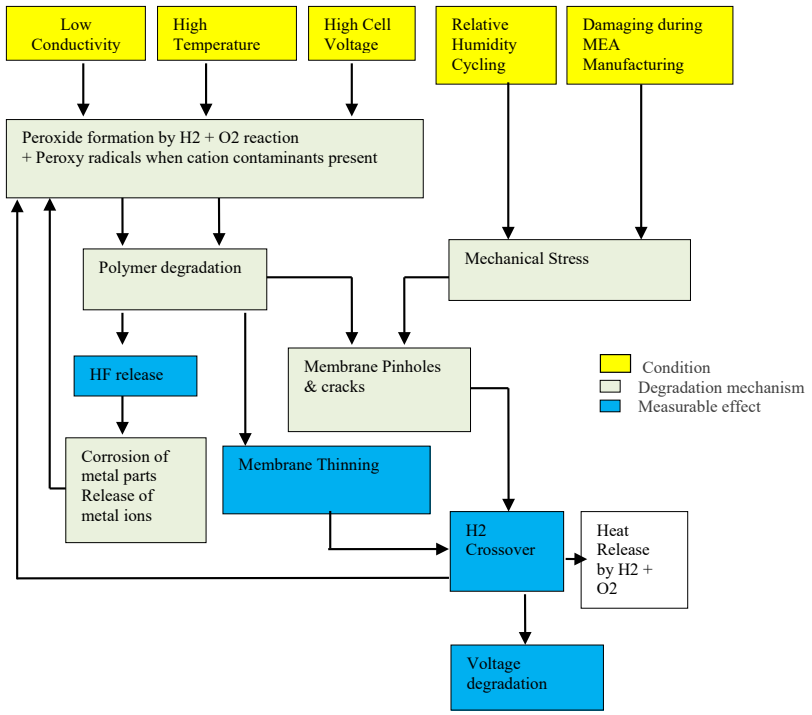


Figure 1. Factors affecting performance of membrane

of PEMFC (Fig.1), we observed that the performance of fuel cell PEM depends mainly on the performance of membrane, which is measured by the degree of its conductivity. So, we can notice that the thickness of membrane is related to his conductivity [18-22]; In fact, when we increase the thickness, the conductivity is decreased. Thickness of membrane is among the key factors in increasing the performance of a PEM fuel cell. In literature [23-26], several modeling and experimental studies have been investigated to understand the effect of membrane on the fuel cell performance. Atifi et al [23] present the effect of internal current, fuel crossover, and membrane thickness on a PEMFC performance. The results obtained show that the internal currents and fuel crossover can be reduced by using thicker membrane and that the activation over potential increases as temperature increases. Ionescu et al [24] present a two-dimensional model for PEMFC with different width dimensions of PEM membrane: 50µm, 100µm and 200 µm. The 50µm of thickness cell model showed the smallest ohmic loses by registering smallest voltage drop (of 6.9mV) across the electrolyte membrane and also the smallest over potential drop along the cell length. But there is no validation with the experimental study. Belkhiri et al [25] presented a model for a two-dimensional which analyses of the effect of temperature and water content on proton conductivity of the membrane. Results shows that the electrochemical performance of a fuel cell will be strongly depend temperature and water content. The conductivity of the membrane ($\sigma m$) increases with increasing temperature and leads to greater diffusion of

hydrogen protons within the membrane, so the resistance of the membrane which means higher temperatures, the electrochemical reaction is faster, increases the production of water in the cathode and hydrates better membrane, and thus the ionic resistance is reduced. Khazaee et al [26] investigated the effects of gas diffusion layer and membrane properties in an annular proton exchange membrane fuel cell. The results show that by increasing the thickness and decreasing the porosity of GDL the performance of the cell enhances that it is different with planner PEM fuel cell. Also the results show that by decreasing the thickness of the membrane the performance of the cell increases. In this paper, a mathematical model for analysis of proton exchange membrane (PEM) fuel cell is proposed. The proposed model is simulated in the COMSOL and studied the effects of thickness of membrane on the performance of the PEM fuel cell. Theoretical model shows that the performance of PEM fuel cell improves as thickness is scaling down towards nanoscale. The model has been validated with the experimental results trends and comparisons shows there is good agreement between the experimental data trends and the proposed model.

## 2. MATHEMATICAL MODELING

### 2.1. Geometric model

Fig.2 illustrates a 3D model of the single channel of PEMFC. The model is composed of seven zones which are anode channel, anode GDL, Anode Electrode, Membrane, Cathode Electrode, Cathode GDL, and Cathode Channel. The geometric parameters of model are listed in (Table1) and are taken from the experimental study published by Bates and Alex Martin [27].

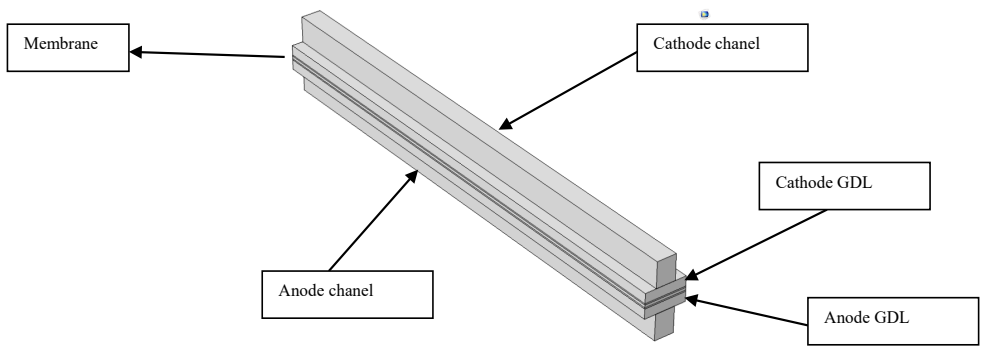


Figure 2. Geometry Model

Table1. Design parameters

| Description | | Value |
|---|---|---|
| Cell length | L | 0.01 m |
| Channel height | H_ch | 1.1e-3 m |
| Channel width | W_ch | 1.1e-3 m |
| Rib width | Wrib | 0.90932e-3 m |
| GDL width | H_gdl | 380e-6 m |
| Electrode thickness | Hel | 50e-6 m |
| Membrane thickness | Hm | 100e-6 m |

### 2.2. Basic Assumptions

For our model, the following assumptions were employed:

- 3D domain
- Cell temperature is held constant
- Flow is laminar everywhere
- Stationary model
- The membrane is impermeable for the gas
- Membrane and electrodes are isotropic and homogeneous
- The GDL is porous
- Ideal gas
- The fluid is incompressible

### 2.3. Governing equations

#### 2.3.1 Thermofluid Model

The form of mathematical equations of Continuity, momentum, energy, species and charge can be summarized as follows [28]:

Continuity equation:

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla.(\varepsilon\rho U) = 0 \tag{1}$$

Momentum Conservation:

$$\frac{\partial(\varepsilon\rho\bar{U})}{\partial t} + \nabla.(\varepsilon\rho\bar{U}\bar{U}) = -\varepsilon\nabla p + \varepsilon\bar{F} + \nabla.(\varepsilon\bar{\tau}) + \frac{\varepsilon^2\mu}{k}\bar{U} \tag{2}$$

Conversation of energy equation:

$$\nabla.(\rho U C_p T) = \nabla.(K^{eff}\nabla T) + S_T \tag{3}$$

Species conservation equation:

$$\frac{\partial(\varepsilon\rho X_i)}{\partial t} + \nabla.(\varepsilon\rho U X_i) = \nabla.N_i + S_i \tag{4}$$

Where:

$\varepsilon$ : The porosity for a porous medium

$\rho$ : The density of the liquid

$U$ : The floating speed vector when the liquid in the porous medium

$p$ : The pressure

$F$ : The floating mass vector
$\tau$ : The stress tensor
$\mu$ : The liquid viscidity degree
$k$ : The permeate ratio of the liquid through the porous medium
Cp: represent the specific heat capacity at constant pressure
$K^{eff}$: The effective thermal conductivity of gas mixture in porous medium
ST: energy source term which represents the rate of increase or decrease of energy due to heat generations or consumptions
$X_i$: is the mass fraction of specy i
$S_i$: is the produce speed of specy i adapt to the electrochemistry reaction

### 2.3.2 Electrochimic Model

The electrochemical model of a single cell of the proton exchange membrane fuel cell is modeled by the following equations [29]:

$$V_{cell} = E - V_{activation} - V_{ahmic} - V_{concentration} \tag{5}$$

Where:
$V_{cell}$: Fuel cell voltage
E: Reversible voltage
$V_{activation}$: Activation voltage
$V_{ohmic}$: Ohmic voltage
$V_{concentration}$: Concentration voltage

$$E = \frac{\Delta G}{2F} + \frac{\Delta S}{2F}\left(T - T_{ref}\right) + \frac{RT}{2F}\left[\ln\left(P_{H_2}\right) + \frac{1}{2}\ln\left(P_{O_2}\right)\right] \tag{6}$$

Using the standard pressure and temperature values for ΔG, ΔS and $T_{ref}$, Eq. (6) can be simplified to [30]:

$$E = 1.229 - 0.85\times10^{-3}\left(T - 298.15\right) + 4.31\times10^{-5}T\left[\ln\left(P_{H_2}\right) + \frac{1}{2}\ln\left(P_{O_2}\right)\right] \tag{7}$$

$$V_{activation} = \frac{RT}{2\Omega T}\ln\left(\frac{i}{i_0}\right) \tag{8}$$

$$V_{ohmic} = i\left(r_{ion} + r_{el}\right) \tag{9}$$

$$V_{con} = -b.\ln\left(1 - \frac{j}{j_{\max}}\right) \tag{10}$$

Where:
ΔG: is the change in the Gibbs free energy
F: is the constant of Faraday
ΔS: is the change of the entropy
R: is the universal constant of the gases
PH2 and PO2: are the partial pressures of hydrogen and oxygen
T: is the cell operation temperature
$T_{ref}$: is the reference temperature
$\Omega$: is electron transfer coefficient.
i: is the cell's current density,
$i_0$: is exchange current density.
b:is a parametric coefficient.
J: represents the actual current density of the cell ($A/cm^2$)

## 2.4. Boundary conditions

The boundary conditions and inlet parameters for the numerical model are summarized in table2:

Table2. Boundary conditions

| **Domain** | **Temp.T [K]** | **Mass flow [kg/mol]** | **Electric potential [V]** | | |
|---|---|---|---|---|---|
| Inlet-a (anode) | 333 | 0.002 | - | O2 mass fraction<br>H2 mass fraction<br>H2O mass fraction | 0<br>0.743<br>0 |
| Inlet-c (Cathode) | 333 | 0.032 | - | O2 mass fraction<br>H2 mass fraction<br>H2O mass fraction | 0.228<br>0<br>0.023 |
| Outlet-a | 333 | - | - | - | - |
| Outlet-c | 333 | - | - | - | - |
| Terminal-a | 353 | - | 0 | - | - |
| Terminal-c | 333 | - | 0.75 | - | - |

## 3. Numerical procedure

The model geometry is meshed with a structured grid (Fig.03) by the Comsol 5.0. The complete mesh which consists of 6880 domain elements, 3516 boundary elements and 628 edge elements. The governing equations are solved using Comsol boundary conditions with a simple algorithm based on the finite element technique. Calculation time took 51 min 47 s in order to show the study diagrams.

The model operated at a constant temperature of 333K, and with reference pressure 101e3 (Pa). The geometry of cell model is listed in (Table 1). The physicochemical parameters values that used in this modeling are listed in (Table 3).

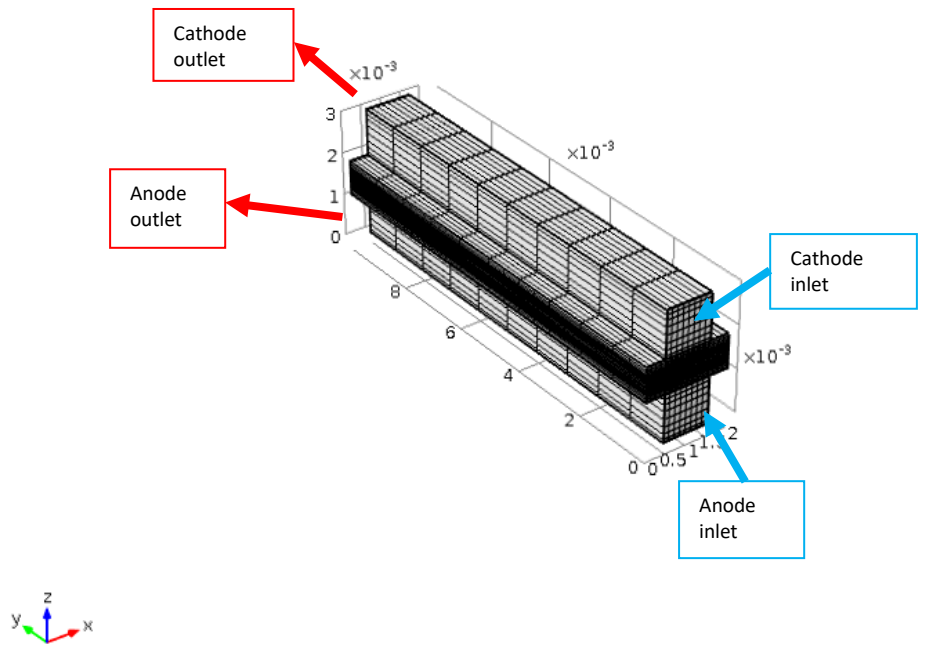


Figure 3: Structure after meshing

Table 3. Operating parameters

| Parameter | Value |
|---|---|
| GDL porosity | 0.4 |
| GDL permeability ( e -11 m2 ) | 1.18 |
| GDL electric conductivity ( S/m) | 222 |
| Inlet H2 mass fraction (anode) | 0.743 |
| Inlet H2O mass fraction (cathode) | 0.023 |
| Inlet oxygen mass fraction (cathode) | 0.228 |
| Anode inlet flow velocity m/s | 0.4 |
| Cathode inlet flow velocity m/s | 0.7 |
| Anode viscosity (e-5 Pa.s) | 1.19 |
| Cathode viscosity (e-5 Pa.s) | 2.46 |
| 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 |
| H2-H2O Binary diffusion coefficient (e-4 m2/s) | 1.55 |
| N2-H2O Binary diffusion coefficient (e-5 m2/s) | 2.95 |
| O2-N2 binary diffusion coefficient (e-5 m2/s) | 2.75 |
| O2-H2O binary diffusion coefficient (e-5 m2/s) | 3.23 |
| Cell temperature (K) | 333 |
| Reference pressure (Pa) | 101e3 |
| Cell voltage V | 0.9 |
| Oxygen reference concentration (mol/m$^3$) | 40.88 |
| Hydrogen reference concentration (mol/m$^3$) | 40.88 |
| Membrane conductivity (S/m) | 9.82 |

## 4. RESULTS AND DISCUSSION

### 4.1. Model validation

In order to validate our model, the numerical study obtained from the present model is compared with experimental study measured by Bates and Alex Martin which their model including thickness membrane of 100e$^{-6}$ m [7] (Fig. 04). In the activation and the ohmic area of the polarization curve, our results by using Comsol are in a good match with the experimental study, with deviation at 0.5 A/cm$^2$ (Fig. 04). As we see, the model is unable to reproduce the experimental data at high current densities, maybe caused by the presence of liquid water in the catalyst layers and the gas diffusions layers.

### 4.2. Simulation results

Based on the results above, it is now possible to consider a reference case and investigate its performance behavior under different membrane thickness. Cell geometry and flow conditions for the reference case are listed in Table 1 and 2.

Fig.05 shows the overall full cell performance in terms of polarization obtained under the four operating membrane thickness. In fact, we choose two thicknesses under Bates and Alex thickness and one above it and this just to understand the performance of PEMFC by choosing thinner or larger membrane thickness. According to the comparison we see that the PEMFC has the highest cell potential at 50 e-6m, especially in the high current density region. A low ohmic loss and a high concentration loss are observed at 125e-6m. Ohmic loss is found to

increase with temperature and the loss is due to the higher temperatures. In the following, the results of modeling will be used to explore the transport phenomena inside the fuel cell and the effects of membrane on fuel cell performance. All the following results are generated with a constant cell voltage of 0.9V.

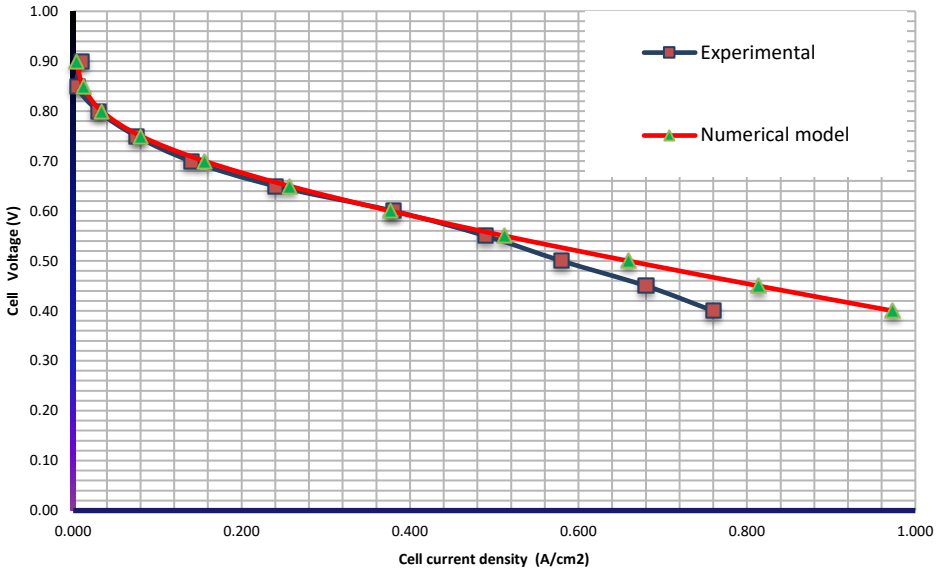


Figure 4. Comparison between experimental data and the current modeling results.

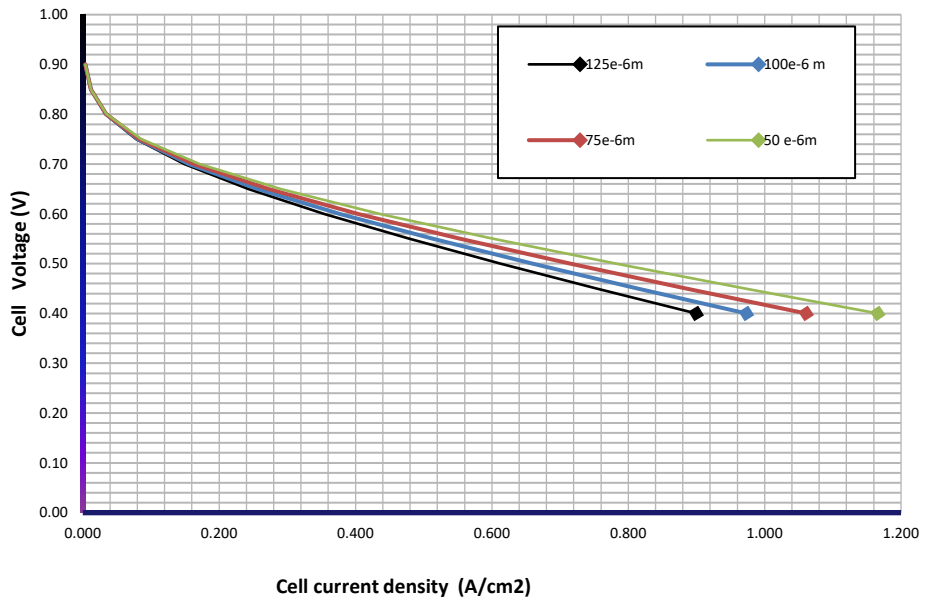


Figure 5. Comparison of polarization curves by PEMFC at different membrane thickness.

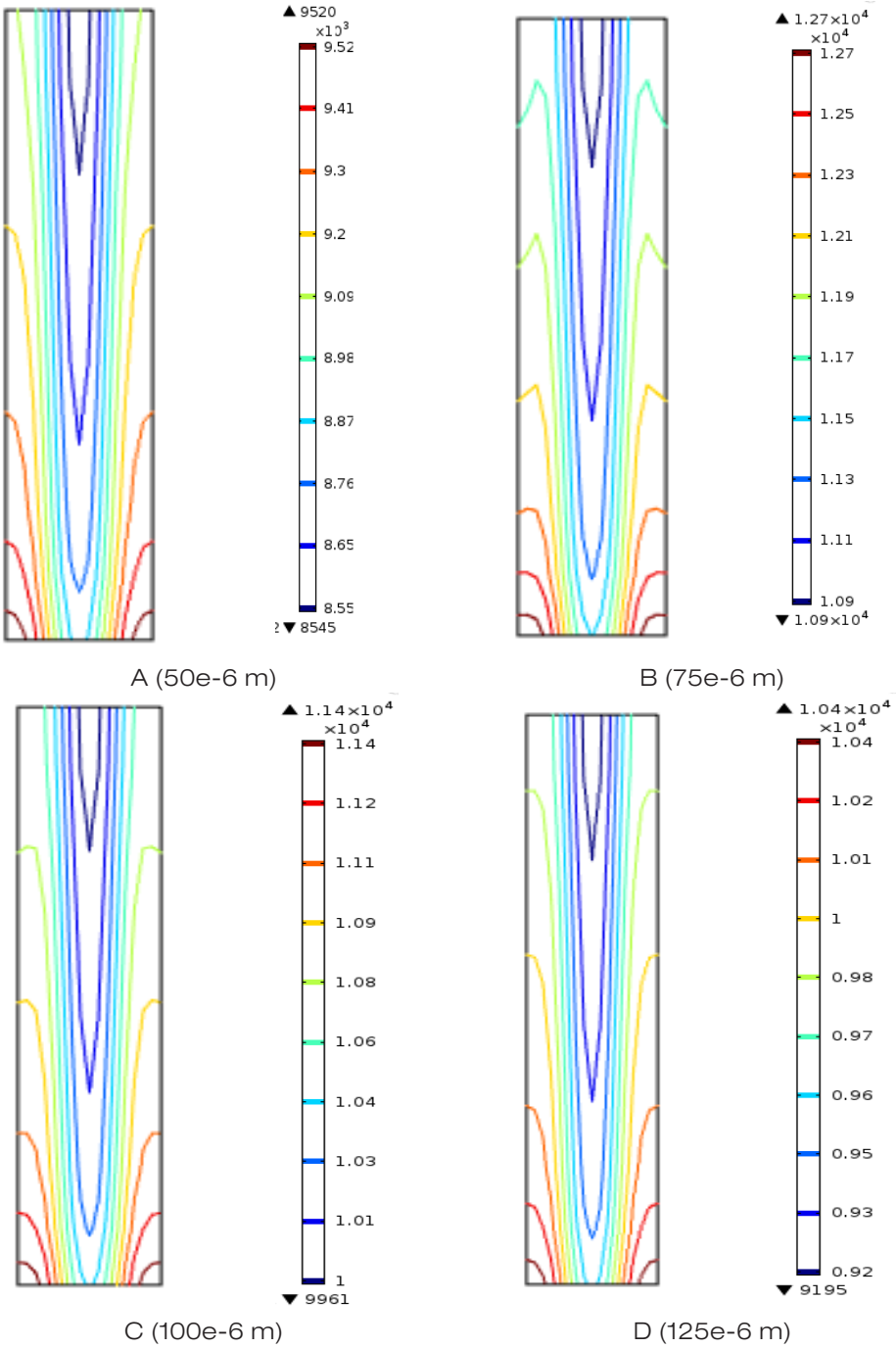


Figure 6. Current density in membrane under four thicknesses

Figure 06 shows the current density with four thickness membrane at the center of the membrane for 0.9 V. We see that the current density is lower towards the outlet of cell (due to lower reactant concentrations).As a result, the currents density is higher in the region close

to the channel, where the reactant concentrations are higher, but the current density is lower in the center of the channel because of the Ohmic drops in the GDLs. The simulation results displays that a thinner membrane corresponds to the higher current density.

Figure 7 and figure 8 show the largest water concentration in the cell at A (50e-6m) for the same voltage level. In order to increase to conductivity of membrane we must increase the temperature and this depends on thickness of membrane. So, the more thickness we have the more temperature we need, so with optimal thickness of membrane. The electrochemical reaction is faster means increases the production of water and hydrates better membrane, and thus the ionic resistance is reduced.

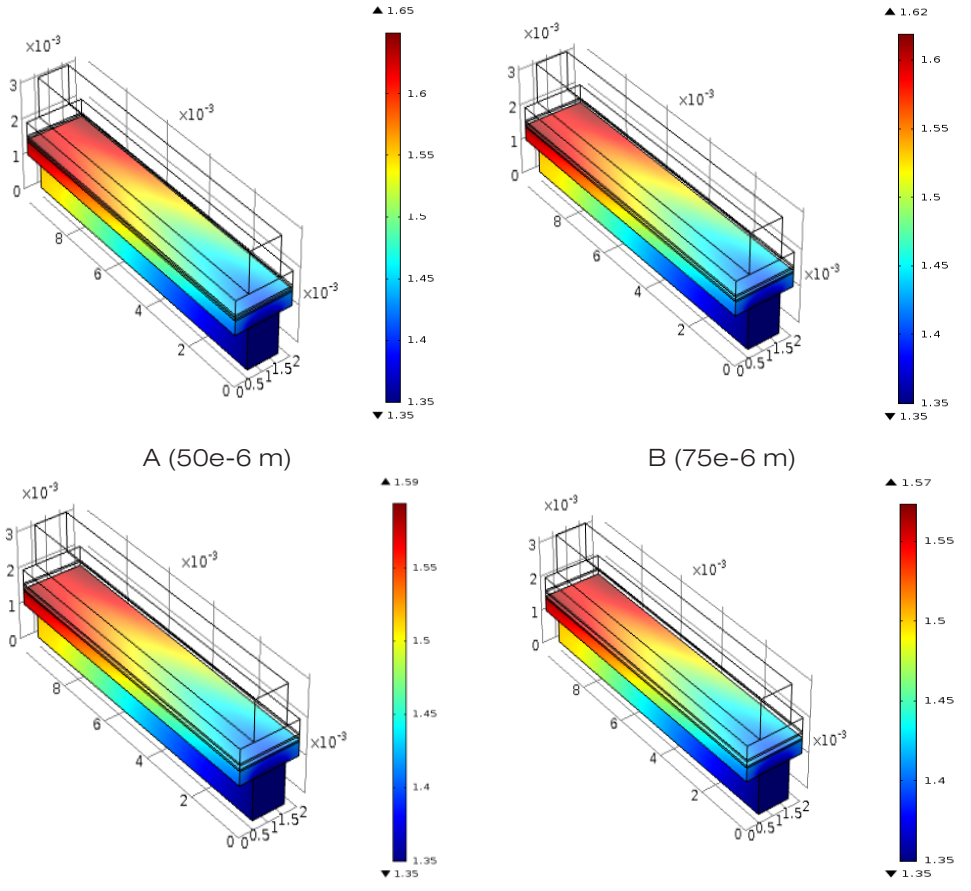


Figure 7. Anode water concentrations at different membrane thickness A, B, C, D

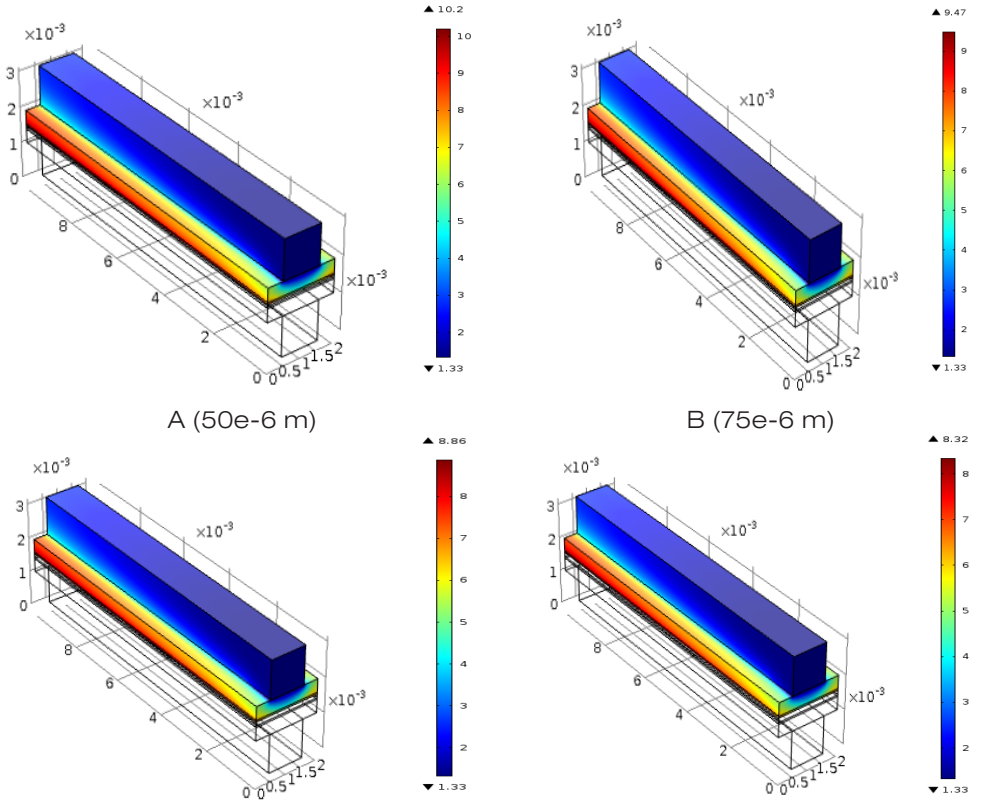


Figure 8. Cathode water concentrations at different membrane thickness A, B, C, D

## CONCLUSION

A 3D PEMFC model has been used to analyze the membrane thickness effect on the performance in a single fuel cell. According to the four thicknesses (100e-6 m, 75e-6m, 50 e-6m and 125e-6 m studied, 50 e-6m is found to be the best operating thickness for the PEMFC under the specified inlet operating conditions. At 333K, the fuel cell has the optimal relative humidity in the membrane and cathode diffusion layer, which allows both oxygen and hydrogen proton diffuse to the cathode catalyst layer. The detailed numerical results provide an understanding of the electrochemistry and transport phenomena in a PEM fuel cell. This model can be used as an effective CFD tool for fuel cell development to reduce cost in fuel cell design and optimization.

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