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A Three-Dimensional Model of Single PEM Fuel Cell Having Triple-Serpentine Flow Channel Developed with CFD

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Abstract

In this investigation, a three dimensional, single-phase proton exchange membrane (PEM) fuel cells with triple-serpentine flow channel was studied numerically, evaluating reactant gas humidification, water management and cell performance. The model equations were solved using CFD software ANSYS Fluent® 16.2 with Gambit® (2.4.6) as a pre-processor. This 3-D model with 19x50 mm2 active layer used to investigate the performance of fuel cell by determining the current density, oxygen, hydrogen and water molar concentration distributions took into account the mass, momentum, energy, species, charge conservation equation as well as combines electrochemistry reaction inside the fuel cell. The simulation results were illustrated polarization curves including I–V and I–P curves. Various properties of the GDL such as permeability, porosity, tortuosity and the hydrophobic texture can affect the flooding at flow channels. In this study, the effect of GDL porosity on flooding was investigated with different operating conditions. From the results, for lower operating voltages, as the cathode and anode relative humidity increases, the cell performance is enhanced because the cell performance is mainly dependent on the cathode mass transport limitations due to the liquid water blockage effect. As decreases, the oxygen concentration in the reactants increases and the water concentration on the cathode side decreases, this reduces flooding and improves the cell performance. Also, analysing the polarization curve it can be said the performance of the PEM fuel cell was improved by increasing the reactant gases humidification

Keywords

Flooding, Gas Diffusion Layer, Humidification, PEM Fuel Cell, Performance

1. INTRODUCTION

Fuel cell is an electrochemical device that continuously changes the chemical energy of a fuel (hydrogen) and oxidant (oxygen or air) directly to electrical energy and heat, without combustion. The proton exchange membrane fuel cell (PEMFC) is considered to be a promising power source, especially for transportation and stationary cogeneration applications due to its high efficiency, low operating temperature, high power density, low emission and low noise. A PEMFC is composed of the catalyst layers, membrane, gas diffusion layers and bipolar plate. The GDL have two major functions. First, the reaction gases can successfully diffuse into the catalyst layer and uniformly spread thereon because of the porous structure of the GDLs. Second, the electrons generated by the anode catalysis are drained from the anode and enter the external circuit. Bipolar plates are designed to accomplish many functions, such as distribute reactants uniformly over the active areas, remove heat from the active areas, carry current from cell to cell and prevent leakage of reactants and coolant.

The performance of a PEMFC is affected by many factors such as temperature, pressure, relative humidity, mass flow rate of feed gases, channel geometries in current collector plate and the characteristics of the membrane, catalyst layer, and gas diffusion layer. In literature, several modelling and experimental work has been investigated in order to understand the

effect of channel geometries in bipolar plate including, serpentine flow channels, parallel flow channels, interdigitated flow field, flow field with pins and the influence of these parameters to the fuel cell performance. Because experimental work is costly, numerical modeling becomes an efficient and convenient approach to fuel cell analysis. For the last decade, much effort has been involved in the development of a numerical model. However few studies have been reported on the flow field designs and the bipolar plates in the literature [1–7].

Xing et al. [1] developed a fully coupled 2D, along-the-channel, two-phase flow, non-isothermal, CFD model. In their results thinner GDL could result in more non-uniform and more significant temperature rise at high current densities. Also a new channel design featured with multi-inlets and outlets is proposed to reduce water flooding improve the cell performance.

Sierra et al. [2] in their research a 3D numerical study on a PEM fuel cell model is focused on the performance evaluation of three flow fields with cylindrical geometry (serpentine, interdigitated and straight channels) in a fuel cell. The results showed that the tubular design with the straight channels presented the lowest pressure drop in the flow channels, the interdigitated tubular design had the highest water generation at the cathode, the serpentine design presented the most uniform distributions of hydrogen concentration, temperature and current density on the active area of the cell.

Iranzo et al. [3] presented in this work a validation that was performed by comparing the local liquid water distributions obtained from the CFD model with experimental measurements developed CFD model for a 50 cm2 PEM fuel cell. Major conclusion of the study was that the CFD model used is not able to reproduce the liquid water accumulated in the channels, clearly observed in the neutron radiographs but not in the CFD results, given the treatment of the multiphase flow model.

Rahimi-Esbo et al. [4] in their paper seven flow fields were analyzed and their performances were investigated at the optimum channel to rib ratio. A novel serpentine flow field design aimed at effective water removal is introduced and examined. The results showed that 2-1-serpentine flow field has the highest performance especially at high current densities. It was founded that for operating voltages over 0.5 V, the geometry of the flow channels did not have a significant effect on performance.

Saco et al. [5] carried out a numerical analysis on scaled up model of PEM fuel cell (225 cm2) with four flow channel models. The study was mainly conducted to find the impact of flow field design on the performance of PEM fuel cell. From the results it was found that the current and power density of the straight zigzag flow channel was quite high compared to all other flow channels due to better consumption of hydrogen and oxygen molecules, better water removal rate in the flow channels.

Rostami et al. [6] studied a three-dimensional numerical model to understand the effect of bend sizes on a PEM (polymer electrolyte membrane) fuel cell in this work. The obtained results showed that as bend size increases from 1 mm to 1.2 mm, not only did the over potential reduce significantly but temperature gradient was also alleviated. Moreover, it was shown that the serpentine flow channels with 1.2 mm square bend size acted successfully in preventing secondary flows internal thereby decreasing pressure drop about 90.6% compared to serpentine flow channels with a bend size of 0.8 mm.

Vazifeshenas et al. [7] employed a novel compound flow field design concerned in PEM fuel cell to investigate the effectiveness developed with computational fluid dynamics (CFD). A typical serpentine and parallel flow field designs was verified through three dimensional simulations. From the results, the parallel design had the lowest current density and power in comparison with the other designs. Compound design could perform as well as the typical serpentine design, and also in some aspects could be a better choice than the serpentine one.

The goal of this study was to present the effects of various operating factors on the performance of a PEMFC with the most common bipolar plate design that is the triple serpentine flow field in fuel cells. In this design the gas flows through the channels circulating throughout the active area of the fuel cell. The polarization curves of the fuel cell were plotted under similar operating conditions with different GDL porosity.

2. ANALYSIS OF MODEL

In this study, the model presented is a three-dimensional, isothermal, single-phase, steady-state model that resolves coupled transport processes in membrane, catalyst layers, gas diffusion layers and reactant flow channels of a PEM fuel cell (Fig.1). Operating conditions and general geometrical properties of the PEM fuel cells components are given at Table 1 and Table 2.

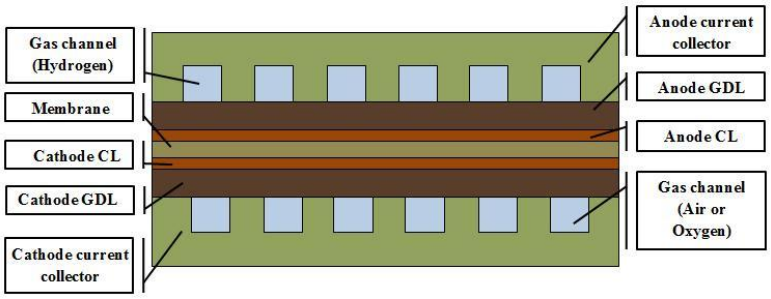

Figure 1. Schematic of the PEM fuel cell Geometry of Model

Table 1.Operating conditions of PEM fuel cell model

Parameters	Units	Value
Operation pressure	kPa	200
Cell temperature	K	343
Cathode stoichiometric ratio	-	2
Anode stoichiometric ratio	-	2
Cathode terminal	V	0.4-0.9
Anode terminal	V	0.0
Cathode mass flow rate	kg/s	calculated
Anode mass flow rate	kg/s	calculated
Cathode RH	-	10%,50%,100%
Anode RH	-	10%,50%,100%

The geometric model is created in Gambit 2.4.6. ANSYS-Fluent 16.2 PEMFC module is used in this research to compile the appropriate user-defined functions for a PEMFC. In this model, the numerical domain is a single-cell geometry domain. Pure hydrogen and air are used as reactant gases in the model. The inlet flow velocity was controlled by stoichiometry numbers of 2 at the anode and 2 at the cathode. The operating pressure was 200 kPa absolute at the exit of the cell. The active surface area is 19x50 mm², with triple-serpentine flow field configuration. The channels are 1 mm in width and 1 mm in depth. The width of the rib is 1 mm. Also the flow channels are shown in Figure 2.

Figure 2.The bipolar plate flow channel pattern

Table 2. General geometrical property of the PEM fuel cells components

Parameters	Units	Value
Channel width	mm	1
Channel length	mm	50
Gas diffusion layer thickness	mm	0.27
Catalyst layer thickness	mm	0.02
Membrane thickness	mm	0.127
Active area	m^2	0.00095

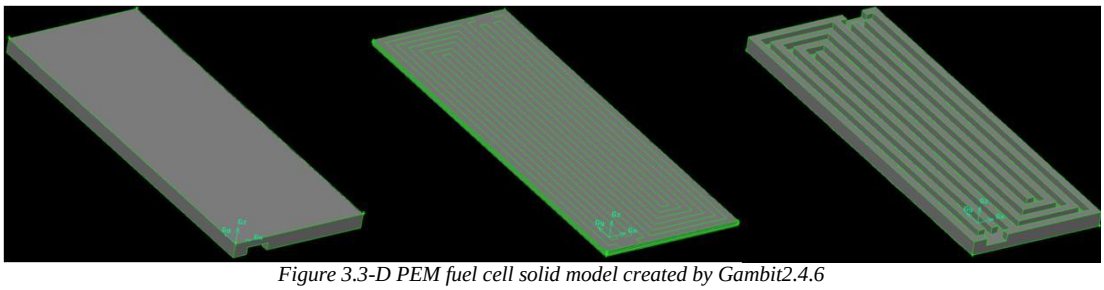

Figure 3.3-D PEM fuel cell solid model created by Gambit2.4.6

2.1. Theoretical Formulation

Basic equations used during fuel cell operation are as follows:

Conservation of mass equation:

$$\nabla.(\rho\vec{u}) = S_m \tag{1}$$

So the source terms are;

$$S_m = S_{H_2} + S_{wv_p} + S_{wl_p} + S_{awv_e} \tag{2}$$

$$S_m = S_{O_2} + S_{wv_p} + S_{wl_p} + S_{cwv_e} \tag{3}$$

$$S_{H_2} = -\frac{M_{H_2} A_{cv} I}{2F} \tag{4}$$

$$S_{O_2} = -\frac{M_{O_2} A_{cv} I}{4F} \tag{5}$$

Momentum transport equation:

$$\nabla.(\rho\vec{u}\vec{u}) = -\nabla P + \nabla.(\mu\nabla\vec{u}) + S_{p,i} \tag{6}$$

Here $\beta$is the permeability. $S_{p,i}$is the sink source term for porous media in x, y and z-directions;

$$S_{p,i} = -\left(\sum_{j=1}^{3} \frac{1}{\beta_j} \mu u_j\right) \tag{7}$$

Species transport equation:

$$\nabla.(\rho m_n \vec{u}) = \nabla.(J_n) + S_s \tag{8}$$

Here *n* denotes for H_2-O_2water vapor and liquid water. The source terms are the same as those of the conservation of mass equation. The diffusion mass flux (*J*) of species *n* in n-direction is:

$$J_{\xi,n} = -\rho D_{\varepsilon,n} \frac{\partial m_{K,n}}{\partial \xi} \tag{9}$$

Energy equation:

$$\nabla.(\rho\vec{u}h) = \nabla.(k\nabla T) + S_h \tag{10}$$

The source term S_n can be obtained by energy losses and heat source by phase change. The heat source from the electrochemical reaction:

$$S_{he} = h_{rxn}\left[\frac{IA_{cv}}{2F}\right] - IV_{cell}A_{cv} \tag{11}$$

The local current density of the cell is calculated from the open circuit voltage (V_{oc}) and the losses;

$$I = \frac{\sigma_m}{t}\{V_{oc} - V_{cell} - \eta\} \tag{12}$$

Where *t* is the membrane thickness and $\sigma_m$is the membrane conductivity and defined as;

$$\sigma_m = \left(0.514\frac{M_{m,dry}}{\rho_{m,dry}} C_{wa} - 0.326\right).exp\left(1268\left(\frac{1}{T_0} - \frac{1}{T}\right)\right) \tag{13}$$

2.2. Numerical Solutions

The procedure to model PEM fuel cell is;

1) Creating and defining the geometry of the fuel cell with Gambit 2.4.6
2) Creating an appropriate mesh for geometry with Gambit 2.4.6.
3) Assigning zone names and types that is required in the FLUENT PEM fuel cell add-on module.
4) Importing the mesh file into FLUENT.
5) Defining fuel cell parameters, setting up of the case and then running calculations.
6) Postprocessing the results.

The model equations were solved using the commercial computational fluid dynamics (CFD) software ANSYS Fluent®16.2 with Gambit® (2.4.6) as a pre-processor. The CFD code has an add-on module for fuel cells, which has therequirement of the source terms for species transport equations, heat sources, and liquid water formation (ANSYS 2015). Afinite volume method was used for solving the problem. The conservation of mass, momentum and energy equations weresolved until the iterative process meets the convergence criteria.(Fig.4) The number of iterations was determined as 200. AHP-PC-Intel®Xeon® CPU E5-2650v2@2.6 GHz, 2.6 GHz, 64 GB was used to solve the set of equations.

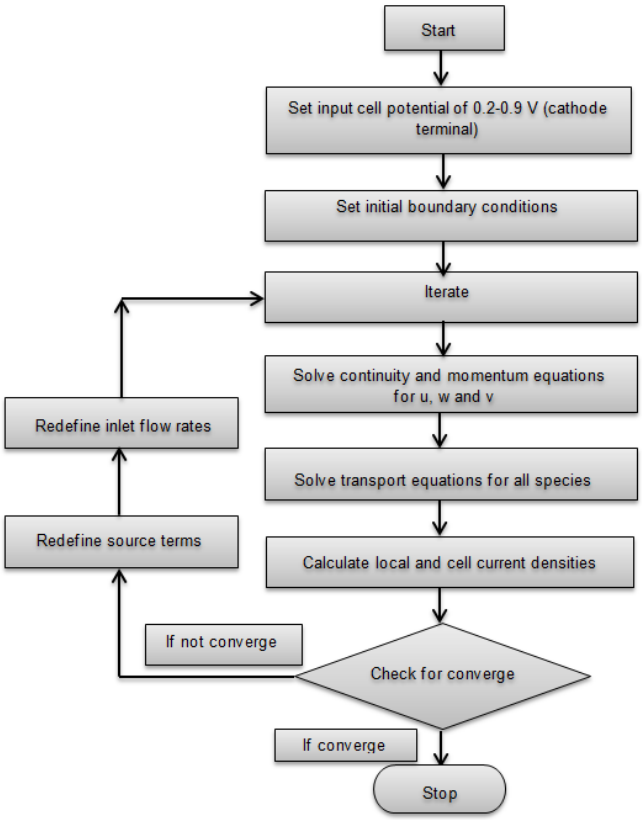

Figure 4.Solution Algorithm

3. RESULTS AND DISCUSSION

3.1. Relative Humidity Effect at Anode Side

In order to reach good cell performance, there must be water balance between anode and cathode. When hydrogen at the anode inlet is fully humidified, the humidity of the membrane can be well maintained. However if hydrogen is insufficiently humidified, membrane dehydration could occur on the anode side. The problem of water deficiency on the anode side of the membrane can be solved by humidification of hydrogen flow at anode side. For each of the gas humidification configurations for the double-serpentine PEMFC model, it was investigated the water accumulation in the membrane operated with constant operating conditions. In Fig. 5 it is shown that I–V and I–P curves anode RH =10%, 50%, 100% respectively. According to the simulated results in figure, as anode relative humidity increase, the overall water uptake in the system increases. This increase enhances the cell performance. Maximum power density was reached at 0.7 V, 1.136 A/cm^2 with the value of 0.4754W/cm^2.

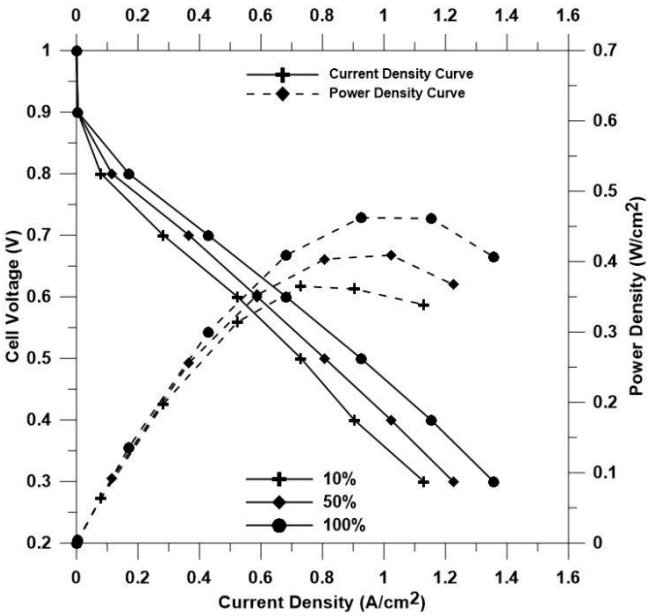

Figure 5.I–V and I–P curves cathode RH= 100% and anode RH =10%, 50%, 100% respectively

As mentioned above, the reason for this decrease is that diffusing the oxygen from channel through the GDL in order tooccur the electrochemical reaction. As shown in the Fig. 6, it is also noted that the optimal oxygen consumption of thechannels was achieved at 100% relative humidity obtained the maximum current and power density to improve the performance of fuel cell.

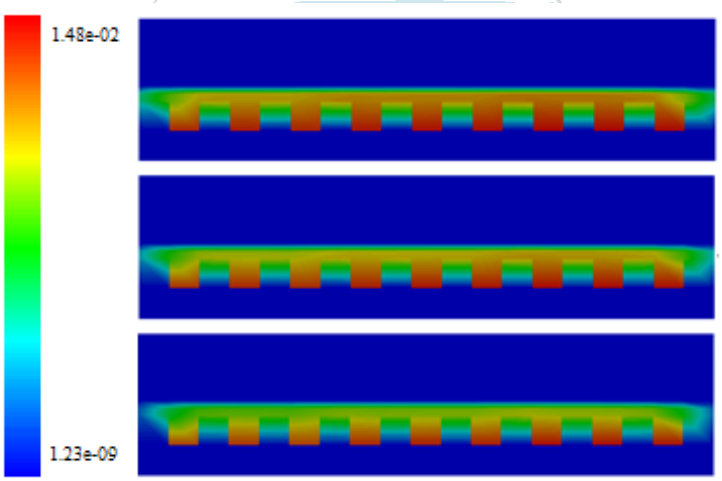

Figure 6. Contours of oxygen molar concentration distribution (kmol/m3) in the middle of model with different relativehumidity at x-z plane, 0.6V, (a) 10%, (b) 50 %, (c) 100%.

Fig. 7 displays the distribution of the H_2O molar concentration through the membrane domain with different relative humidity. The simulated results showed that water distribution and membrane conductivity in the fuel cell depended onanode humidification and the related water management. The increase of concentration of water at membrane is significant when the relative humidity is increased from 10% to 100%.

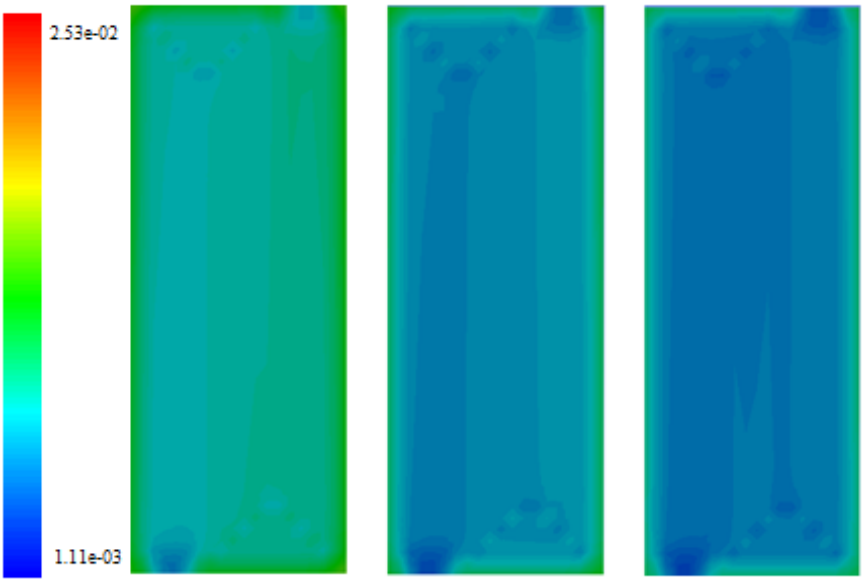

Figure 7.Contours ofmolar concentration distribution of H_2O (kmol/m^3) in membrane with different relative humidity at x-x-y plane, 0.6 V (a) 100%, (b) 50 %, (c) 10%

3.2. Relative Humidity Effect at Cathode Side

The water generated at the cathode must be transported away from the catalyst layer by evaporation, water–vapor diffusion and capillary transport of liquid water through the GDL into the flow channels of the flow field. If this does not occur, excess water exists at the cathode side and condenses. This causes blocking the pores of the GDL and reducing the active sites of the cathode catalyst layer. This phenomenon is known as "flooding", and is an important limiting factor of PEM fuel cell performance. The extent of flooding and the effects of flooding depend on the operating conditions and the properties of PEM materials like bipolar plates, MEA. In Fig. 8 it is shown that I–V and I–P curves anode RH= 100% andcathode RH =10%, 50%, 100% respectively. However, it is clearly seen from the figure that the current density is increased by the increasing cathode relative humidity.

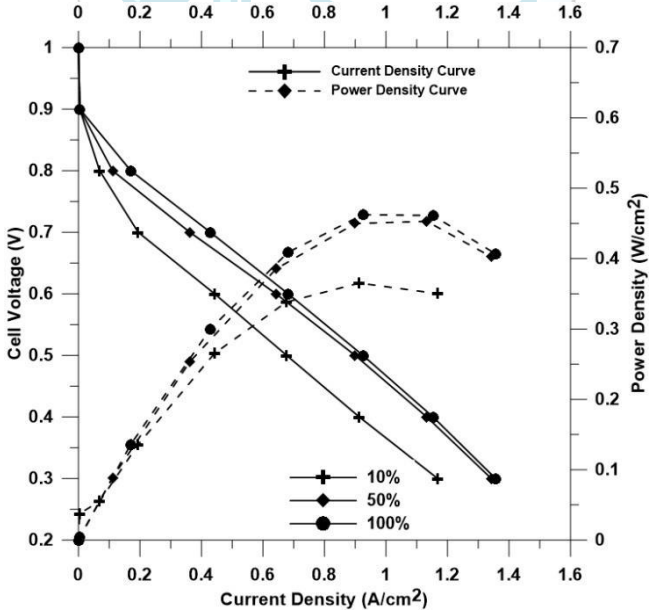

Figure 8.I–V and I–P curves anode RH= 100% and cathode RH =10%, 50%, 100% respectively

3.3. Effect of Cell Voltage on Water Content

The effects of cell voltage on the fuel cell performance have been shown that include the membrane and cathode channel water content of the in Fig.9 and Fig.10 at different cell voltages. It can be seen in both figures the water content increases with increasing the voltage value. After the voltage rises to a certain value, the increase of cathode humidification adverselyaffect the cell performance due to a decrease in current density. As mentioned above, the reason for this decrease is thatmuch water, because of water production in the electrochemical reaction at the cathode and excessive humidification

of thecathode side, will stay in the porous cathode GDL, preventing the oxygen from diffusing through the GDL to catalyst layer. And this causes flooding at porous sides of fuel cell. Consequently the best performance occurs at 0.6 V

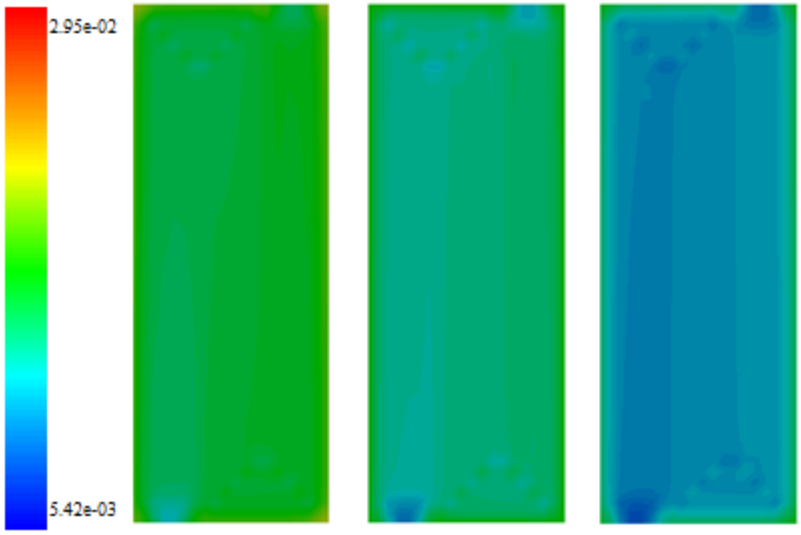

Figure 9.Contours ofmolar concentration distribution of water (kmol/m^3) in membrane with different cell voltage at x-y plane (a) 0.3V, (b) 0.6V, (c) 0.9V

As the cell voltage decreases, the cell performance is enhanced because the cell performance is mainly dependent on thecathode mass transport limitations due to the liquid water blockage effect. The water concentration in the reactants decreases. This reduces means that the cathode flooding is prevented and it improves the cell performance.

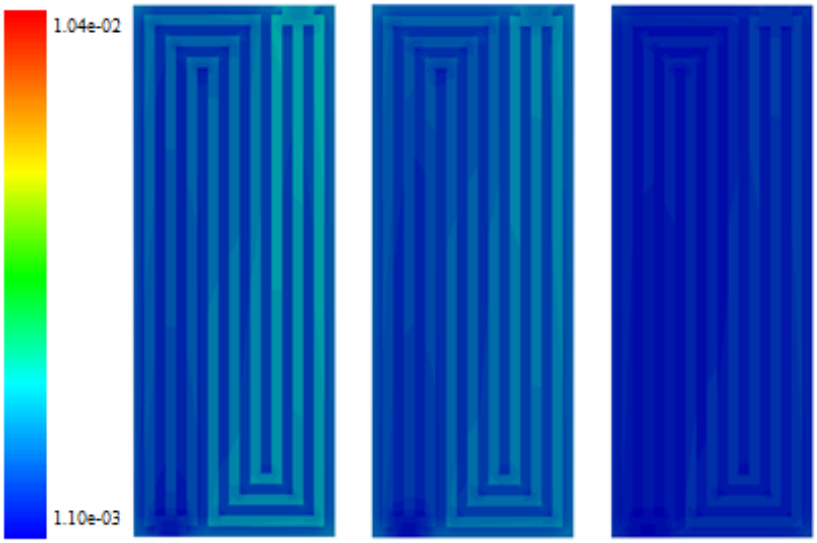

Figure 10.Contours ofmolar concentration distribution of water(kmol/m^3)in cathode channel with different cell voltageat x-y plane (a) 0.3V, (b) 0.6V, (c) 0.9V

3.4. Effect of GDL Porosity on Current and Power Density

In Figure 11 the I–V curves demonstrate that a better performance can be obtained by using a gas diffusion layer of higher porosity. A gas-diffusion layer of higher porosity has an ability of stronger diffusion transport, which is beneficial in that it supplements the reactant gas to the catalyst layer. Increasing operation temperature is helpful to enhance electrochemical reaction rate and ionic transport in PEMFC, and the cell performance.

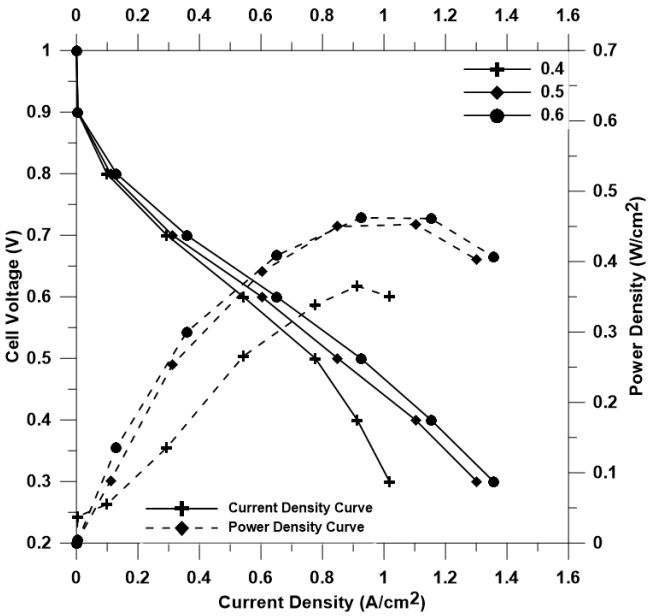

Figure 11.I–V and I–P curves of the effect of GDL porosity on current and power density with ε=0.4, 0.5, 0.6 respectively

4. CONTENT

A three-dimensional computational fluid dynamics model of a PEM fuel cell with triple-serpentine flow channels was developed to investigate the effects of cell voltage, gas diffusion layer porosity and reactant gases humidification on performance. Using a single-phase, steady-state, three-dimensional model of PEM fuel cell, the following conclusion was obtained; the humidity in the reactant gases is an important factor to consider for improving the cell performance. As the relative humidity of anode side increases, both the chemical reaction and mass transfer of hydrogen are enhanced due to the increase of water content in the membrane, which leads to a better cell performance. The maximum power density for thehighest performing was 0.4754 W/cm^2 and occurred at maximum anode /cathode humidification with 0.6 GDL porosity at 0.6 cell voltage.

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