

COMPUTATIONAL INVESTIGATION OF THE EFFECT OF THE INLET PRESSURE AND THE POROSITY OF GAS DIFFUSION LAYER ON THE PEM FUEL CELL PERFORMANCE

ÉTUDE NUMERIQUE DE L'EFFET DE LA PRESSION D'ENTREE ET DE LA POROSITE DE LA COUCHE DE DIFFUSION DE GAZ SUR LA PERFORMANCE DE LA PILE A COMBUSTIBLE PEM

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ABSTRACT

A proton exchange membrane fuel cell is an electrochemical device that can convert chemical energy directly into electric energy. The focus of this paper is to propose a three-dimensional computational fluid dynamics model of a straight single channel PEM fuel cell, including the effects of inlet pressure and diffusion layer porosity on the performance of fuel cell. The gas flow is supposed to be laminar, transient, non-isothermal and incompressible. The equations of conservation of mass, momentum and species are presented and the simulation is, carried out using the finite volume method tool of ANSYS FLUENT software based on a computational technique specific to fluid dynamics. The experimental results of the polarisation curves show how the performance of the PEM fuel cell varies under the effects of the considered operating parameters that are inlet pressure and gas diffusion layer porosity. Compared to the experimental and modelling results published in the literature, this work gives a good qualitative agreement.

KEYWORDS: PEM fuel cell, inlet pressure, porosity, Fuel cell performance, CFD, 3D model.

RESUME

La pile à combustible à une membrane échangeuse de protons est un dispositif électrochimique qui convertit l'énergie chimique directement en énergie électrique. L'objectif de cet article est de proposer un modèle numérique tridimensionnel de dynamique des fluides d'une pile à combustible à un seul canal direct. Dans ce travail, le flux de gaz est considéré laminaire, transitoire, non isotherme et incompressible. Les équations de conservation de masse, de mouvements et d'espèces sont présentées et la simulation est réalisée à l'aide de l'outil méthode des volumes finis du logiciel ANSYS FLUENT basé sur une technique de calcul spécifique à la dynamique des fluides. Les résultats expérimentaux des courbes de polarisation montrent comment la performance de la pile à combustible PEM varie sous l'effet des paramètres de fonctionnement considérés, à savoir la pression d'entrée et la porosité de la couche de diffusion gazeuse. Comparé aux résultats expérimentaux et de modélisation publiée dans la littérature, ce travail donne un bon accord qualitatif.

MOTS CLES : Pile à combustible PEM ; Pression d'entrée ; Porosité ; performance de la pile à combustible ; CFD ; modèle 3D

1 INTRODUCTION

A fuel cell is a converter of electrochemical energy that converts chemical energy of fuel, typically hydrogen, directly into electrical energy. Its operation is based on the electrochemical reactions coming simultaneously on the anode and the cathode. Over the last years, the proton exchange membrane fuel cell (PEMFC) has emerged as a favored technology for auto transportation and power generation [1] due to its high-energy efficiency, low operating temperature (100 Co), low emission, low

noise, fast start-up, and system robustness [2]. A PEM fuel cell is a multiple distinct parts device and a series of mass, energy, transport through gas channels, electric current transport through membrane electrode assembly and electrochemical reactions at the triple-phase boundaries [3].

Various models suggested many ways to predict the electrochemical behavior of PEMFC. The first two models were published in the early 1990s by Springer et al. [4]. Bernardi and Verbrugge. [5]. Chen-Yu Chenav et al. [6] studied the behavior of a Proton Exchange Membrane Fuel

Cell in Reformate of Gas. Jordan et al. [7] provided the diffusion layer parameter effects on fuel cell performances. M. Zerouala et al. [8] developed a numerical study of the effect of the inlet pressure and the height of the gas channel on the distribution and consumption of reagents in a fuel cell (PEMFC). Sridhar et al. [9] performed humidification studies on PEM fuel cell performances. Gurau V et al. [10] investigated Two-dimensional model for proton exchange membrane fuel cells.

The performance of PEM fuel cell is known as very sensitive to all the set of physical parameters mainly, Relative Humidity, Temperature, Porosity and Pressure. The recent publications focusing on the effect of the different physical parameter on the performance of a PEM fuel cell are developed as follows : Sukkee Um et al. [11] developed a transient, multidimensional model to simulate proton exchange membrane fuel cells. The model accounts simultaneously for electrochemical kinetics, current distribution, hydrodynamics, and multicomponent transport. Gurau et al. [12] discussed the variations of the concentrations and the partial pressures in the gas channels and developed a two-dimensional model for the entire sandwich of a PEMFC. Chen et al. [13] presented a two-phase transport in the cathode gas diffusion layer (GDL) of a proton exchange membrane fuel cell (PEMFC) with a porosity gradient in the GDL. Bernardi and Verbrugge [14] explained a one-dimensional model to examine the proton transport behaviors in the membrane. Zhang et al. [15] found a three-dimensional steady-state electrochemical mathematical model, where the mass, fluid, and thermal transport processes as well as the electrochemical reaction phenomena are considered the influences of the parameters of interest, which include on one hand porosity, permeability, and the thickness of the gas diffusion layer. Obayopo et al [16] explained a numerical investigation to analyze the flow field and reactant gas distribution in a PEM fuel cell channel with transversely inserted pin fins in the channel flow that aimed at improving the reactant gas distribution. The channel friction and pressure drop can be significantly reduced by increasing GDL porosity.

Yan et al [17] presented a two-dimensional model to investigate gas reactant transport at various conditions of flow channel width ratio and GDL porosity.

The PEMFC performance is target as a function of

operating conditions in almost of the examined studies where the computational modelling is the main tool in optimization of fuel cell performance [18, 19].

The handling of the FC modelling by using the computational fluid dynamics (CFD) method is of a wide interest due to its capability to consider more easily three-dimensional modelling [20-23] and two-phase transport phenomenon [24-26], what simplify the numerical calculations and makes the computational problem easier ; while straight gas flow channels in serpentine configuration are commonly the standard flow plate design of modelled fuel cells.

The purpose of this study is to present a transient, single-phase, three-dimensional cell model of the PEMFC system, including the conservation of mass, momentum, species, charges and energy with electrochemical reactions that are valid for the flow channel and gas diffusion electrodes. These complete equations are solved using a finite-volume-based computational fluid dynamics (CFD) approach. The work is depending on the combination of two parameters : The effect of inlet pressure and porosity of GDL with straight geometry on the distribution of current density.

2 MODEL DESCRIPTIONS

In Figure.1 a single straight-channel of PEMFC assembled of four layers : the bipolar plate, gas diffusion layer (GDL), catalyst layer, and the membrane. Each layer offers different purposes and the design and composition of the various layers are all of important effects on the modelling of the fuel cell performances.

This work presents a comprehensive three-dimensional, non-isothermal model of a straight single channel PEM fuel cell. The model takes into account the transport phenomena of gaseous species, liquid water, protons, energy and water dissolved in the ion conducting polymer. This work reflects the influence of many parameters on the fuel cell performance, including geometry, materials operating and others. The present model is capable to improve the effects of inlet pressure and porosity of the gas diffusion layer (GDL) on the performance and modelling of PEM fuel cell

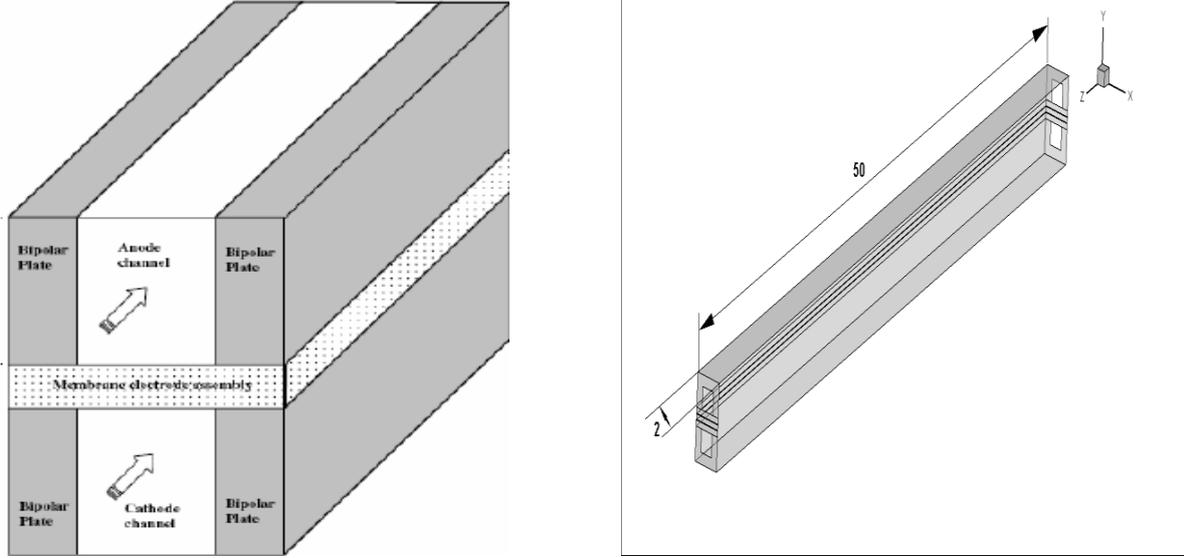


Figure 01 : Schematic of a single straight channel of PEMFC

2.1 Model Assumptions

For computing constraints, due to solving this three-dimensional model of a complete cell we considered the following reasonable simplifying assumptions:

- The system operates under a transient condition.
- The gas mixtures are considered as perfect gases.
- The incoming gas mixtures are considered as an incompressible fluid.
- The fluid flow in the channels is supposed to be laminar.
- Isotropic and homogeneous porous media, catalyst layer and membrane.
- In the cell, due to electrochemical reaction, the process is non-isothermal; but the walls of the cell and inlet gases have a constant temperature (isothermal).

3 GOVERNING EQUATIONS

The governing equations corresponding to the various regions of the fuel cell are given below.

The flow in the reactant gas channels is governed by the Navier–Stokes equation.

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial \rho \varepsilon \mathbf{u}}{\partial t} + \nabla \cdot (\varepsilon \rho \mathbf{u} \mathbf{u}) = -\varepsilon \nabla P + \nabla \cdot (\varepsilon \mu^{eff} \nabla \mathbf{u}) + S_u \sqrt{a^2 + b^2} \quad (2)$$

$$\frac{\partial (\varepsilon X_k)}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u} X_k) = \nabla \cdot (D_k^{eff} \nabla X_k) + S_k \quad (3)$$

$$\nabla \cdot (\sigma_e^{eff} \nabla \phi_e) + S_{\Phi_e} = 0 \quad (4)$$

$$\nabla \cdot (\sigma_s^{eff} \nabla \phi_s) + S_{\Phi_s} = 0 \quad (5)$$

$$\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\varepsilon \rho H \mathbf{u}) = \nabla \cdot (-K_{eff} \nabla T) + S_e \quad (6)$$

where u , ρ , ε , P , X_k , Φ_e , Φ_s , K_{eff} , μ and H represent respectively the intrinsic velocity vector, the fluid density, the porosity, the pressure, the molar fraction of specie k , the electrolyte potential in the

membrane, the solid phase potential, the effective thermal conductivity, the viscosity and the enthalpy.

S_{Φ_s} and S_e are presented in Table 1. [19]

The expressions of sources terms S_u , S_k , S_{Φ_e} ,

Table 01 : Governing source terms in various regions

	Source and sink terms			
	Flow Channel	Gas diffusion layer	Catalyst Layer	Membrane
Momentum	0	$\frac{\mu}{k_p} \varepsilon^2 \mathbf{r}$	$-\frac{\mu}{k_p} \varepsilon_m \varepsilon_{mc} \mathbf{r} + \frac{k_{\emptyset}}{k_p} Z_f C_f F \nabla \emptyset_e - \frac{\mu}{k_p} \varepsilon_m \mathbf{r} + \frac{k_{\emptyset}}{k_p} Z_f C_f F \nabla \emptyset_e$	
Species	0	0	$\frac{j_a}{2FC_{total}} \text{ for } H_2$ $\frac{j_c}{4FC_{total}} \text{ for } O_2$ $\frac{-j_c}{2FC_{total}} \text{ for } H_2O$	
Solid potential	0	0	$-\frac{J_a}{J_c}$	0
Membrane potential	0	0	$\frac{J_a}{-J_c}$	0
Heat	0	0	$J_a \eta_a \text{ in the Anode Catalyst Layer}$ $J_c \eta_c \text{ in the cathode Catalyst Layer}$	$\frac{i^2}{\sigma_m}$

Using the Bruggman correlation [11], the effective diffusion coefficient of specie (k) and the ionic conductivity in the membrane can be expressed by the following formulas :

$$D_m^{eff} = \varepsilon_m^{1.5} D_k \quad (7)$$

$$\sigma_k^{eff} = \varepsilon_m^{1.5} \sigma_k \quad (8)$$

With : ε_m is the membrane phase porosity. The effective thermal conductivity and isotropic multiphase composition were determined by Hashin and Shtikman [16]. It was expressed as follows :

$$K_{eff} = \frac{1}{\frac{1-\varepsilon}{3k_s} + \frac{\varepsilon}{2k_s + k_f}} - 2k_s \quad (9)$$

With : k_f is the thermal conductivity in the fluid phase and k_s is the thermal conductivity in the solid phase.

For some particular situations of the porosity, we can write [27] :

$$\varepsilon = 0 \text{ and } \varepsilon = 1$$

$$k_{eff}(\varepsilon = 1) = k_f \quad k_{eff}(\varepsilon = 0) = k_s$$

The diffusion coefficient depends on temperature and pressure :

$$D(T) = D_0 \left(\frac{T}{T_0}\right)^{\frac{3}{2}} \left(\frac{P_0}{P}\right) \quad (10)$$

The proton conductivity in the membrane phase (S/cm) is related with the water content of the membrane, λ which is in turn a function of the water activity, a :

$$\sigma(T) = \sigma_m(T) = (0.5139\lambda - 0.326) \exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right] \quad (11)$$

The membrane water content is given by the following empirical formula (Springer and Gottesfeld, 1997) [28]

$$\lambda = \begin{cases} 0.043 + 17.18a - 39.85a^2 + 36a^3 & \text{for } 0 < a \leq 1 \\ 14 + 1.4(a-1) & \text{for } 1 \leq a \leq 3 \end{cases} \quad (12)$$

The water activity is expressed as follows [4]

$$a = \frac{\omega_w RT}{P^{sat}} \quad (13)$$

Where : ω_w is the molar fraction of water vapor.

Once the membrane phase potential, ϕ_m and the proton conductivity on the membrane, σ_m are obtained, local current density, I , can be calculated by

$$I = -\sigma_m \nabla \phi_m \quad (14)$$

The diffusion coefficient of H2O in the membrane (m²/s)

$$D_w^m = \begin{cases} 3.1 \times 10^{-7} \times \lambda \left(e^{0.28\lambda} - 1 \right) e^{\left(\frac{-2346}{T} \right)} & \text{for } 0 < \lambda < 3 \\ 4.17 \times 10^{-8} \times \lambda \left(161e^\lambda + 1 \right) e^{\left(\frac{-2346}{T} \right)} & \text{outside} \end{cases} \quad (15)$$

The diffusivity of H2 in the gas (m²/s)

$$D_{H_2} = 1.1 \times 10^{-4} \left(\frac{T}{353} \right)^{\frac{3}{2}} \left(\frac{1}{P} \right) \quad (16)$$

The diffusivity of O₂ in the gas (m²/s)

$$D_{O_2} = 3.2 \times 10^{-5} \left(\frac{T}{353} \right)^{\frac{3}{2}} \left(\frac{1}{P} \right) \quad (17)$$

The diffusivity of H2O in the gas (m²/s)

$$D_{H_2O} = 7.35 \times 10^{-5} \left(\frac{T}{353} \right)^{\frac{3}{2}} \left(\frac{1}{P} \right) \quad (18)$$

The enthalpy H (J/kg)

$$H = C_p \Delta T \quad (19)$$

The local current density along the axial direction can be calculated as the following :

$$I(y) = -\sigma_e^{\text{eff}} \frac{\partial \Phi_e}{\partial x} \Big|_x = IF \quad (20)$$

IF : is the interface between the membrane and cathode catalyst layer. The average current density is calculated as :

$$I_{\text{avg}} = \frac{1}{L} \int I(y) dy \quad (21)$$

I : is the current density (A/cm²).

The transfer current densities in these equations are expressed by linear and Tafel approximations of Butler-Volmer equation respectively in the anode and cathode.

They are expressed as the following (Um et al., 2000) [11] :

$$i_a = a j_{0,a}^{\text{ref}} \left(\frac{X_{H_2}}{X_{H_2,\text{ref}}} \right)^{\frac{1}{2}} \left(\frac{\alpha_a + \alpha_c}{RT} \cdot F \cdot \eta \right) \quad (22)$$

$$i_c = -a j_{0,c}^{\text{ref}} \left(\frac{X_{O_2}}{X_{O_2,\text{ref}}} \right)^{\frac{1}{2}} \cdot \exp \left(\frac{-\alpha_c}{RT} \cdot F \cdot \eta \right) \quad (23)$$

The overpotential is described as

$$\eta(x, y) = \Phi_s - \Phi_e - V_{oc} \quad (24)$$

With j , a , η , Φ and VOC represent respectively the current transfer (A/cm³), transfer coefficient, over potential (V), potential (V) and potential of open-circuit (V).

For the solid phase potential, the potential at the interface between the anode current collector and the diffusion layer is zero, and for the membrane phase potential, the potential at the interface between the anode catalyst layer and the membrane is set to be zero also.

The operating potential of the cell is then calculated by

$$V_{cell} = V_{oc} - \eta_{a,tot} - \eta_{c,tot} - \eta_{m,pro} \quad (25)$$

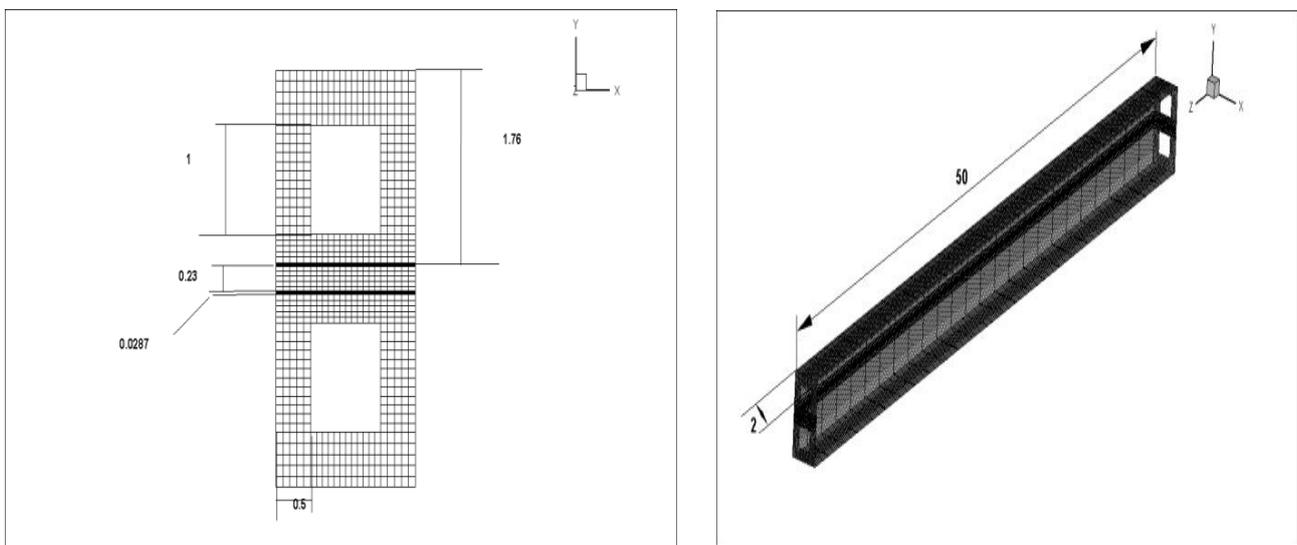
Where $\eta_{m,pro}$ is the Ohmic overpotential in the membrane, and V_{oc} is the open circuit potential, which is calculated by [14]:

$$V_{oc} = 1.23 - 0.9 \times 10^{-3} (T - 298) + 2.3 \frac{RT}{4F} \log(p_H^2 p_0) \quad (26)$$

4 RESULT AND DISCUSSION

4.1 Computational methodology

Modelling plays an important role in the development of the fuel cell as it allows the understanding of the influence of the various parameters on the performance of the cell via a numerical simulation that permits a systematic design and optimization of fuel cell systems. In the present work, a three dimensional numerical simulation is performed on the PEMFC. The adopted simulation platform is the software “ANSYS 14.5”, FLUENT”-module PEMFC.



(a) (b)
Figure 02: view of the computational mesh of domain: (a) X-y, (b) X-Y-Z

To implement the model in fluent software we operate in two major steps. The first is to generate the schema and the mesh of the cell, where we used the appropriated software of CFD code namely GAMBIT Version 2.4.6. It specifies the different areas of the cell respectively, giving them the appropriate physical characteristics. The second step is to export the schema of the cell towards Fluent with the defined boundary conditions (see the Cell Operating Condition in next paragraph) of the flow in order to proceed with the simulation.

4.2 Solver validation

A series of simulation were carried out on the model from low to high operating current densities. In order to evaluate the validity of the model, numerical simulation results compared with the experimental data presented by Cheng et al. [29], as shown in Figure. 3. Compared to the

experimental polarization curve, the polarization curve of cell potential appears in good agreement in case of low and intermediate load regions. However, the activation overpotential is predominant at low current densities. At a relatively high current density, the curve is linear owing to ohmic membrane resistance. The limiting current density is around 0.2 A/cm² when the mass transport of oxygen controls the rate of the electrochemical reaction. When we examine the behaviour in high load condition, one can note that accordingly to the results of Figure.3, the predicted values are higher than the experimental values as expected. In addition, as the polarization curve is the only experimental data available in the literature, polarization curves are typical, and commonly used to validate the agreement between model and experiments.

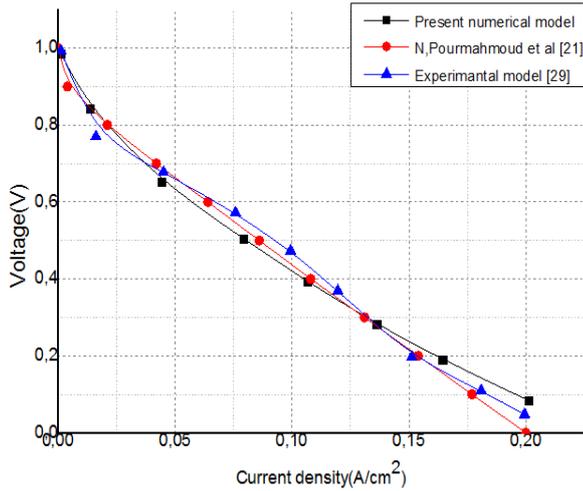


Figure 03 : Comparison of predicted performance curves with the model of Nader Pourmahmoud [21] and the experimental data of B. cheng [29]

Figure.4 as shows the response of the polarization curve current-tension. It's the easiest way to evaluate the performance of fuel cell. It is obtained by registering the voltage of the fuel cell by varying the current density, or conversely to measure the current produced at different voltages. This polarization curve shows three parts where a phenomenon of loss predominates over the others ; the first zone is the area of activation predominates at low current density $I=0$ (A/cm²). It depends on the activity of the species involved in the electrochemical reactions, and

mainly partial pressures of the reactants and products, the activity of the catalyst and surface developed by this one. The second zone is ohmic polarization ; the losses in this area are mainly due to the cathodic overvoltage because the reduction of oxygen is reaction kinetics is limited compared to the oxidation of hydrogen. The third part is the region of concentration where the current density is high $I=0.177$ (A/cm²) in the base case, the maximum flow of reagent is reached at one of the two electrodes and the concentration of the reactants at the level of the electro-active surface becomes very low.

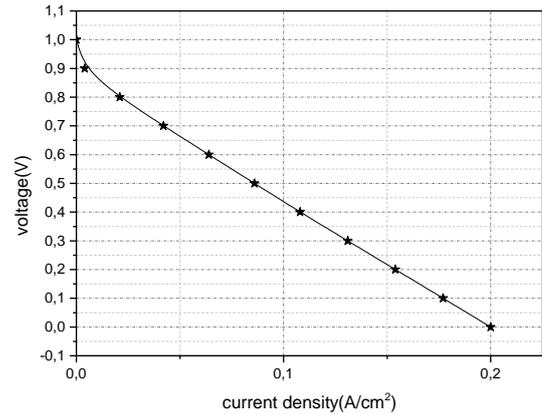


Figure 04: Polarization curve of PEMFC on the base case

All the Fuel cell operating conditions and geometrical parameters are illustrated in Table 2 and Table 3.

Table 02: Cell operating condition

Parameters	Symbol	Value
Anode Reference Exchange Current Density (A/cm ²)	$A_{s1a,ref}$	25000
cathode Reference Exchange Current Density (A/cm ²)	$A_{s1c,ref}$	0.5
Anode Reference Concentration (kmol/m ³)	$C_{h,ref}$	1
cathode Reference Concentration (kmol/m ³)	$C_{o,ref}$	1
Anode concentration exponent	$C_{h,exp}$	0.5
cathode concentration exponent	$C_{o,exp}$	1
Anode Exchange Coefficient	α_a	0.5
cathode Exchange Coefficient	α_c	1
Hydrogen Reference Diffusivity (m ² /s)	$D_{h,ref}$	0.00011
Oxygen Reference Diffusivity (m ² /s)	$D_{o,ref}$	3.23×10^{-5}
Vapor Reference Diffusivity (m ² /s)	$D_{h2o,ref}$	7.35×10^{-5}
Another Species Reference Diffusivity (m ² /s)		3×10^{-5}
Open circuit voltage(V)	V_{oc}	1.115775
Specific leakage current (A/m ³)		0
Porosity of GDL	ϵ_d	0.4
Viscous Resistance of GDL (1/m ²)		$1 \times 10^{+12}$
Porosity of CL	ϵ_{ct}	0.4
Surface/Volume Ratio of Catalyst Layer (1/m)		200000
Porosity of Membrane	ϵ_m	0.4
Membrane Equivalent Weight (kg/kmol)		1100

Membrane Protonic Conduction Coefficient		1
Membrane Protonic Conduction Exponent		1
Faraday constant (C mol ⁻¹)	F	96,487

Table 03: Geometrical and operational parameters for base case

<i>conditions</i>		
Operating parameters	Symbol	Value
Relative humidity of inlet fuel and air (%)	RH _a , RH _c	100
Humidified Temperature (K)	T	353.15
Operating Temperature (K)	T	353.15
Outlet Temperature (K)	T _{out}	353.15
<hr/>		
fuel inlet	Flow Rate (kg/s)	FR _{H₂} 6.632 × 10 ⁻⁸
	Temperature (K)	T _{in} 353.15
	Hydrogen mass fraction	X _{H₂} 0.378
	Water mass fraction	X _{a, H₂O} 0.621
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Air inlet	Flow Rate (kg/s)	FR _{O₂} 9.752 × 10 ⁻⁷
	Temperature (K)	T _{in} 353.15
	Oxygen mass fraction	X _{O₂} 0.208
	Water mass fraction	X _{c, H₂O} 0.103
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Channel length (mm)	L	50
Channel width (mm)	W	1
Channel height (mm)	H _{ch}	1
Gas diffusion layer thickness(mm)	Th _d	0.26
Wet membrane thickness (Nafion_ 117) (mm)	Th _m	0.23
Catalyst layer thickness (mm)	Th _c	0.0287
Fuel stoichiometric ratio ξ _{H₂}	ξ _{H₂}	2
Air stoichiometric ratio ξ _{O₂}	ξ _{O₂}	2
Gauge pressure (Pa)	p	303975
Outlet Temperature (K)	T _{out}	353.15

4.3 Effect of inlet pressure

As the inlet pressure is an important operating parameter because its large effects on fuel cell performance, the change of the pressure will cause change of gas composition, exchange current density and electrode potential parameters as they are parameters of the input pressure.

In this parametric study, the cell operating temperature is kept at 353.15 K, while the inlet pressure is varied from 1 atm to 6 atm. The Polarization curves are presented in Figure. 5. The values of inlet pressures of anode and cathode sides were presented as a loop to determine side has the most effect on the performance of the cell. In each case (a), (b), (c), (d) we fixed the inlet pressure from 1,3,5,6 atm at the anode and increases in the cathode. The results show that the performance of the fuel cell improves with the increase of inlet pressure. In addition to this the current density increase more and more when the value of anode inlet pressure is bigger than the cathode one, as it is shown in the Table.4. The higher open circuit voltage at the higher inlet pressures is explained by the Nernst equation and the overall polarization curves shift positively as the inlet pressure increases. Another reason of the performance improvement is the partial pressure increase of the reactant gases with increasing operating pressure.

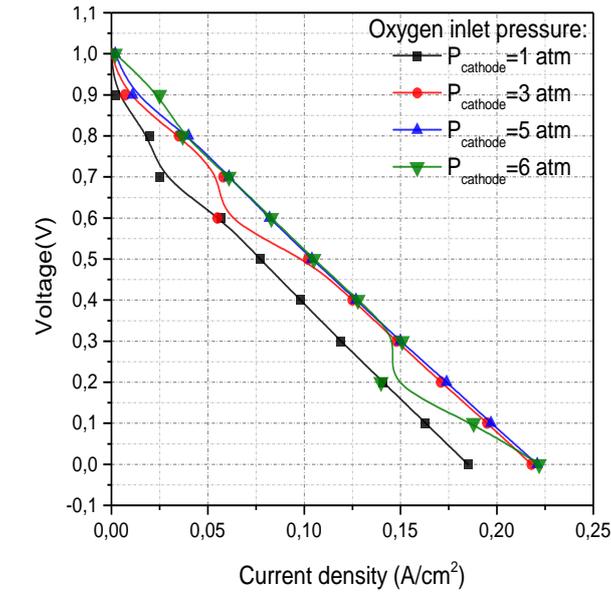
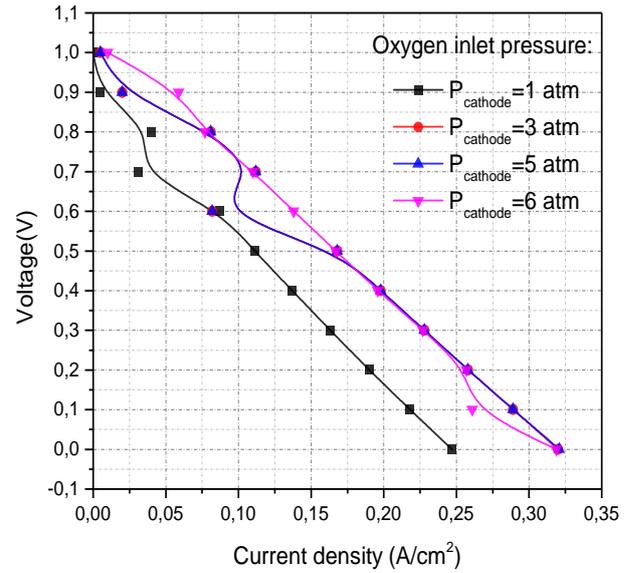
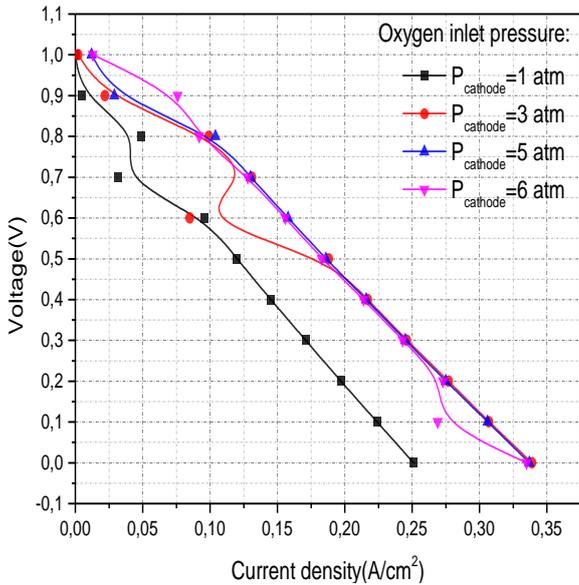
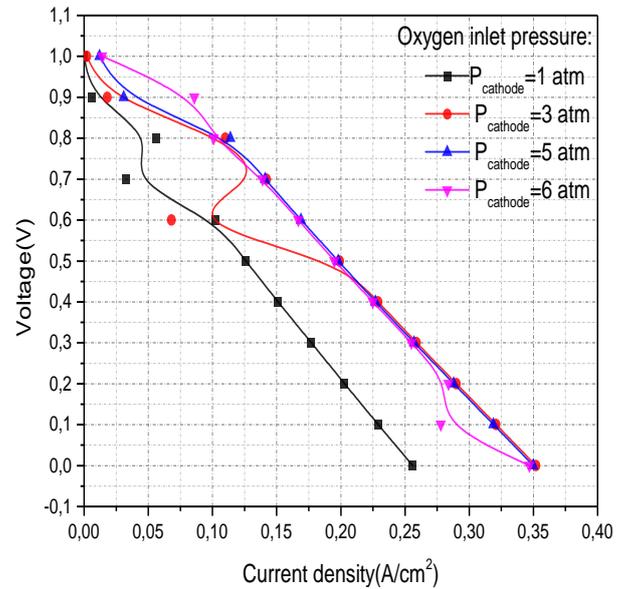

 (a) P_{anode} fixed to 1 atm, increases in $P_{cathode}$

 (b) P_{anode} fixed to 3 atm, increases in $P_{cathode}$

 (c) P_{anode} fixed to 5 atm, increases in $P_{cathode}$

 (d) P_{anode} fixed to 6 atm, increases in $P_{cathode}$

Figure 05: Polarization curves for different cases of inlet pressure

Table 04: The effect of inlet pressure on the current density

Case	The best value of P_{anode} and $P_{cathode}$	The best value of current density in $V=0.1V$
(a)	$P_{anode} = 1, P_{cathode} = 6$	$I = 0.188 \text{ (A/cm}^2\text{)}$
(b)	$P_{anode} = 3, P_{cathode} = 3$	$I = 0.298 \text{ (A/cm}^2\text{)}$
(c)	$P_{anode} = 5, P_{cathode} = 3$	$I = 0.307 \text{ (A/cm}^2\text{)}$
(d)	$P_{anode} = 6, P_{cathode} = 3$	$I = 0.321 \text{ (A/cm}^2\text{)}$

4.4 Effect of diffusion layer porosity

The electrode porosity affects the mass transport of reactant gases from the channel towards the catalyst layers because higher volume porosity provides less resistance to mass transport, what affects the gas diffusion coefficients through

the Bruggemann correction

A second effect of the diffusion layer porosity variation is that higher volume porosity increases resistance to electron transport in the gas diffusion layers, what is a negative effect of the electrode porosity on electron conduction.

These are the main two effects of diffusion layer porosity on fuel cell performance.

In this work, we present the effect of the porosity of the gas diffusion layer on the distribution of current density. In the first part, the simulation is done by choosing the best case where the values of inlet pressure of channels ($P_{anode} = 6 \text{ atm}$ and $P_{cathode} = 3 \text{ atm}$) that are given the best performance $I = 0.352 \text{ (A/cm}^2\text{)}$, While in the second part we

choose multiple values of porosity $\epsilon_d = 0.2, 0.3, 0.4, 0.5, 0.7, 0.8$ to apply it to find the variation of polarization curve for the chosen model.

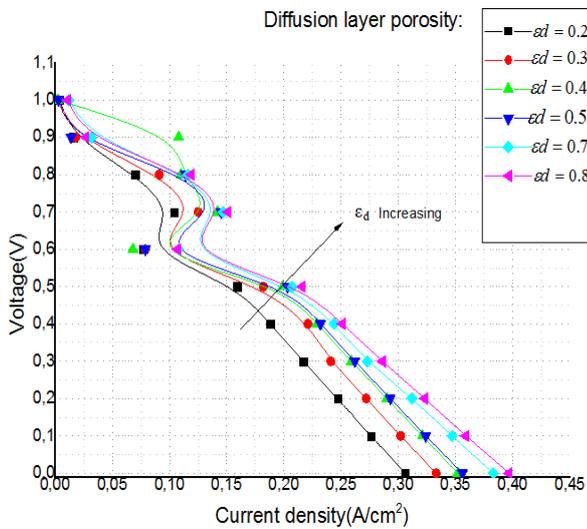


Figure 06: Effects of diffusion layer porosity for $P_{anode}=6 \text{ atm}$ and $P_{cathode}=3 \text{ atm}$

Figure.6 shows the effects of the diffusion layer porosity on the performance of the PEMFC and the simulation results show that the effect of the diffusion layer porosity on the PEMFC performance is significant when the porosity is in the low value region ranging from 0.2 to 0.3. With the increase of the diffusion layer porosity, its effect becomes lower and lower. When the diffusion layer porosity increases from 0.5 to 0.8, its effects augment this leads to increase the current density. Another point to bring up is when $\epsilon_d=0.8$, the higher value of current density is produced and fixed in $I=0.397(\text{A}/\text{cm}^2)$ whatever is the value of diffusion layer porosity. These results indicate that the limiting current density of the cell increases significantly with the increasing of the diffusion layer porosity. In result, the increase of porosity means that the onset of mass transport limitations occurs at higher current densities and the molar oxygen fraction at the catalyst layer increases with more distribution by increasing the porosity.

5 CONCLUSION

In this work, a three-dimensional, non-isothermal computational fluid dynamics model of a Proton Exchange Membrane Fuel Cell (PEMFC) with straight flow channels was proceeded to investigate the influence of common standard parameters on the performances of fuel cell. For this purpose, the effects of the porosity of gas diffusion layer and inlet pressure of the anode and cathode side on the current density was numerically calculated.

This result shows that the increase of the inlet pressure in channel gases imply the increasing on current density and higher inlet pressure in the anode channel than the cathode channel leads to increase the performance. In the other side the various values of diffusion layer porosity, $\epsilon_d=0.2, 0.3,$

$0.5, 0.7, 0.8$ were used to simulate the behavior of fuel cell. Numerical results reveal that cell performance (voltage and current density) can be increased by growing of ϵ_d , because reagents broadcast much more on the area of reaction as more as the gas diffusion layer is porous. When the diffusion layer porosity goes up to the superior value ($\epsilon_d=0.8$) we attain the high current density region and the fuel cell attains its maximum amount of performance. The polarization curve shows that there is a critical point at $V=0.4 \text{ v}$ and $I=0.251(\text{A}/\text{cm}^2)$ which represents the optimal functioning point for the Fuel Cell. These results shows that the model presented in this work allows to understand the complex electrochemistry occurring during the operation of fuel cell and is a useful tool for simulating the real operating conditions of a PEM fuel cell.

NOMENCLATURE

- a water activity
- A area (m^2)
- As specific area of catalyst layer (m^{-1})
- D diffusion coefficient (m^2s^{-1})
- F Faraday's constant (C mol^{-1})
- iref reference exchange current density (A m^{-2})
- I current density (A m^{-2})
- k thermal conductivity ($\text{W m}^{-1}\text{K}^{-1}$)
- K electrode absolute permeability (m^2)
- M molar mass (kg mol^{-1})
- R universal gas constant ($8.314 \text{ J mol}^{-1}\text{K}^{-1}$)
- S source term of governing equations
- u velocity vector (m s^{-1})
- V potential (V)
- W width (m)

GREEK SYMBOLS

- α transfer coefficient
- ζ stoichiometric flow ratio
- η overpotential (V)
- κ electrical conductivity (S m^{-1})
- λ membrane water content
- μ Viscosity ($\text{kg m}^{-1}\text{s}^{-1}$)
- ν kinetic viscosity (m^2s^{-1})
- ρ density (kg m^{-3})
- σ surface tension (N m^{-1})
- ω species molar fraction

SUBSCRIPTS AND SUPERSSCRIPTS

av	average value
eff	effective
in	inlet
oc	open circuit
ref	reference values
sat	saturation
Panode	Anode inlet pressure
Pcathode	Cathode inlet pressure
ϵ_d	diffusion layer porosity

REFERENCES

- [1] Maher A.R. Sadiq Al-Baghdadil, modelling of proton exchange membrane fuel cell performance based on semi-empirical equations, *Renewable Energy*, 30, (2005), 1587-1599.
- [2] W.Q. Tao, C.H. Min, X.L. Liu, Y.L. He, B.H. Yin, W. Jiang, Parameter sensitivity examination and discussion of PEM fuel cell simulation model validation Part I. Current status of modeling research and model development, *Journal of Power Sources*, (2006).
- [3] A. Boucetta, H. Ghodbane, M. Y. Ayad, M. Bahri. A review on the performance and modelling of proton exchange membrane fuel cells. AIP conference proceedings. (2016)
- [4] [4] T.E. Springer, T.A. Zawodzinski, S. Gottesfeld, *J. Electrochem. Soc.* 138 (8) (1991) 2334–2342.
- [5] D.M. Bernardi, M.W. Verbrugge, *AIChE J.* 37 (8) (1991) 1151–1162.
- [6] Chen-Yu Chena, Chun-Chi Chena, Sui-Wei Hsuc, Ming-Pin Laia, Wei-Hsiang Laia, Wei-Mon Yangd “Behavior of a Proton Exchange Membrane Fuel Cell in Reformate Gas”, *Energy Procedia* 29 (2012) 64– 71
- [7] Jordan LR, Shukla AK, Behrsing T, Avery NR, Muddle BC, Forsyth M. Diffusion layer parameters influencing optimal fuel cell performance. *J Power Sources* 2000; 86:250–4.
- [8] M. Zerouala, S. Belkacem Bouzidab, H. Benmoussac, H. Bouguettaiad “Numerical study of the effect of the inlet pressure and the height of gas channel on the distribution and consumption of reagents in a fuel cell (PEMFC)”, *Energy Procedia* 18 (2012) 205 – 214
- [9] Sridhar P, Perumal R, Rajalakshmi N, Raja M, Dhathathreyan KS. Humidification studies on polymer electrolyte membrane fuel cell. *J Power Sources* 2001; 101:72–8.
- [10] Gurau V, Liu H, KakacS. Two-dimensional model for proton exchange membrane fuel cells. *AIChE J* 1998; 44:2410–22.
- [11] Sukkee Um, Wang CY, Chen KS. Computational Fluid Dynamics Modeling of Proton Exchange Membrane Fuel Cells. *Journal of the Electrochemical Society* 2000; 147:4485–4493.
- [12] Gurau V, Barbir F, Liu H. An analytical solution of a half-cell model for PEM fuel cells. *J. Electrochem Soc* 2000; 147:2468–2477.
- [13] Chen Falin, Chang Min-Hsing, Hsieh Ping-Tso. Two-phase transport in the cathode gas diffusion layer of PEM fuel cell with a gradient in porosity. *International Journal of Hydrogen Energy* 2008; 33:2525- 9.
- [14] Bernardi DM, Vebrunge MW. A mathematical model of the solid polymer electrolyte fuel cell. *Journal of Electrochemical Society* 1992; 139(9):2477e91.
- [15] Zhang Zhuqian, Jia Li, He Haiting, Wang Xia, Yang Lixin. Modelling dynamic behaviors of a single cell proton exchange membrane fuel cell under different operating conditions. *Journal of the Taiwan Institute of Chemical Engineers* 2010; 41:689- 98.
- [16] Obayopo SO, Bello-Ochende T, Meyer JP. Modelling and optimization of reactant gas transport in a PEM fuel cell with a transverse pin fin insert in channel flow. *International Journal of Hydrogen Energy* 2012; 37:10286- 98.
- [17] Yan WM, Soong CY, Chen F, Chu HS. Effects of flow distributor geometry and diffusion layer porosity on reactant gas transport and performance of proton exchange membrane fuel cells. *Journal of Power Sources* 2004; 125:27–39.
- [18] K. Z. Yao, K. Karan, K. B. McAuley, P. Oosthuizen, B. Peppley and T. Xie, A review of mathematical models for hydrogen and direct methanol polymer electrolyte membrane fuel cells, *Fuel Cells*, 4 (1/2) (2004) 3-29.
- [19] Badreddine Larbi, Wael Alimi, Ridha Chouikh, Amenallah Guizani. Effect of porosity and pressure on the PEM fuel cell performance. *international journal of hydrogen energy* 38 (2013) 8542-8549.
- [20] T. Berning, D.M. Lu, N. Djilali, *J. Power Sources* 106 (2002) 284–294.
- [21] Nader Pourmahmoud, Sajad Rezazadeh, Iraj Mirzaee, Sonita Motaleb Faed. A computational study of a three-dimensional proton exchange membrane fuel cell (PEMFC) with conventional and deflected membrane electrode assembly, *Journal of Mechanical Science and Technology* 26 (9) (2012) 2959-2968.
- [22] Maher A.R. Sadiq Al-Baghdadi. Three-dimensional computational fluid dynamics model of a tubular shaped PEM fuel cell, *Renewable Energy* 33 (2008) 1334–1345.
- [23] Phong Thanh Nguyen, Torsten Berning, Ned Djilali. Computational model of a PEM fuel cell with serpentine gas flow channels, *Journal of Power Sources* 130 (2004) 149–157.
- [24] Z.H. Wang, C.Y. Wang, K.S. Chen. Two-phase flow and transport in the air cathode of proton exchange membrane fuel cells, *J. Power Sources* 94 (1) (2001) 40-50.
- [25] D. Natarajan, T.V. Nguyen. A Two-Dimensional, Two-Phase, Multicomponent, Transient Model for the Cathode of a Proton Exchange Membrane Fuel Cell Using Conventional Gas Distributors, *J. Electrochem.*

- Soc. 148 (12) (2001) 1324–1335.
- [26] T. Berning, N. Djilali, 3D, Multiphase, Multicomponent Model of the Cathode and Anode of a PEM Fuel Cell, *J. Electrochem. Soc.* 150 (12) (2003) A1598–A1607.
- [27] Dunn Martin L, Taya Minoru. The effective thermal conductivity of composites with coated reinforcement and the application to imperfect interfaces. *Journal of Applied Physics* 1993; 73:1711e22.
- [28] Springer T, T.Zawodzinski, Gottesfeld S. Electrode materials and process for energy conversion and storage. *Journal of Electrochemical Society* 1997; 13:1e14.
- [29] B. Cheng, O. Minggao and Y. Baolian, Analysis of water management in proton exchange membrane fuel cells, *Tsing. Sci. Technol.*, 11 (1) (2006) 54-64