International Journal of Automotive Engineering, Vol. 10, No. 1, (2020), 3140-3148

Iran University of Science and Technology

International Journal of Automotive Engineering

Journal Homepage: ijae.iust.ac.ir

ISSN: 2008-9899

Performance evaluation of PEM fuel cells; impact of relative humidity, pressure and temperature of inlet species on the current density of the PEMFCs

Hamed Davardoust[1], Golamreza Molaeimanesh[2]*, Sepehr Mousavi[3],

1Research Laboratory of Automotive Fluids and Structures Analysis, Automotive Engineering School, Iran University of science and technology, Tehran, Iran

2 Automotive Engineering School, Iran University of science and technology, Tehran, Iran

3 Applied Multi-Phase Fluid Dynamics lab, School of Mechanical Engineering, Iran University of science and technology, Tehran, Iran

ARTICLE INFO

Article history:

Received: 02 April 2019

Accepted: 02 May 2019

Published: 1 March 2020

Keywords:

robust control,

sliding mode control,

fractional order PI,

Chattering, vehicle suspension system,

PSO algorithm

A B S T R A C T

Due to the increasing level of air pollution and the reduction of fossil fuels, the need for new technologies and alternative fuels is felt more than ever. Proton exchange membrane fuel cells (PEMFCs) are one of these technologies, which have been of great interest to the researchers due to the benefits of non-contamination, high efficiency, fast start-up, and high power density. The proper functioning of the fuel cell requires thermal management and water management within the cells. To this end, in this work, the effect of different parameters on the performance of PEM fuel cell was investigated. The results demonstrated that the performance of the cell increases with increasing the pressure in the low current densities, while in the high current density, performance decreases with increasing the pressure of the cell. Also, the study of the effect of relative humidity shows that increasing the relative humidity of the cathode does not have much effect on the performance of the cell while increasing the relative humidity of the anode improves the performance of the cell.

1. . Introduction

proton exchange membrane fuel cells are considered as one of the most important clean energy sources in the coming years. Also, the attention paid to it has increased due to the possibility of producing hydrogen from renewable energy sources [1-2]. Hydrogen, as the most abundant element in the Earth, can be produced in various ways. The conversion of chemical energy from hydrogen to electrical energy is carried out by a device called a fuel cell. Fuel cells are new energy-generating technologies that generate high-efficiency electrical energy without causing environmental and acoustic pollution by combining direct fuel and oxidation. The direct production of electricity is the replacement of the Carnot cycle to convert the chemical energy from the fuel to the thermal and mechanical energy, and eventually the electricity, which minimizes energy dissipation and yields high efficiency [3].

The proton exchange membrane fuel cells are one of the best candidates to use in transportation applications and replacing internal combustion engines. High efficiency, zero emissions and the ability to generate heat and electricity simultaneously, are the advantages of this type of fuel cells, which makes these fuel cells a proper replacement of power generation systems. In general, the conversion efficiency of chemical energy to electrical energy in fuel cells is higher compared to other devices and energy conversion processes. As an example, in combination with natural gas plants, their efficiency reaches 70% to 80%. In addition to transportation applications, the use of these types of cells in portable devices, such as laptops, cell phones, and especially emergency

*Corresponding Author
Email Address: molaeimanesh@iust.ac.ir
https://doi.org/10.22068/ase.2020.536

[DOI: 10.22068/ase.2020.536]

power systems, is also rapidly increasing. For the commercialization of PEM fuel cells, their prices should be reduced and their performance optimized [4-6].

M.F.Torchio et al. [7] investigated The behavior of a PEM fuel cell using functional parameters such as temperature, pressure, and humidity. According to the results, increasing pressure can improve the performance of the cell. L Wang et al. [8] By examining the performance of a PEMFC, confirmed that increasing the temperature if the amount of required humidity enters the cell would improve the performance of the cell. Also, with increasing pressure, considerable improvement in the performance of the cell is achieved [9]. G.H.Guvelioglu and H.G.Stenger simulated fuel cell with MATLAB software and concluded that increasing the hydrogen rate and reducing the airflow with 100% humidity would result in better cell performance[10]. M.Zeroual et al. [11] studied the effect of pressure on cell performance. results demonstrate that Increasing pressure, on the one hand, leads to better water discharge and, on the other hand, increases the reaction rate [12].

In this work, in order to optimize the performance of the fuel cell, the effect of different parameters on the cell performance is investigated in detail.

2. theory and governing equations

In PEM fuel cells, hydrogen and oxygen interact with each other and their chemical energy converts to electrical energy, and as a result of this reaction, some heat is released and some liquid water is produced.

Inside a PEMFC, two half-reactions known as anodic and cathodic half-reactions take place in the anode and cathode side respectively. These half-reactions are:

$$2H_2 \rightarrow 4H^+ + 4e^- \quad (1)$$

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \quad (2)$$

In this simulation, a mathematical model based on continuity equations, thermal energy equation, species equation and electrochemical equations governing a PEMFC have been proposed and the phenomena of transmission and electrochemical phenomena in a PEMFC are examined. In addition, heat sources and heat sinks like water sorption/desorption at the GDL-membrane interfaces, water phase-change in the GDL, Half-reactions entropy, heat of Cathode electrochemical activation and convective heat transfer between gas flow channel and flow channels are also included.

2.1 Equations governing the transfer of species

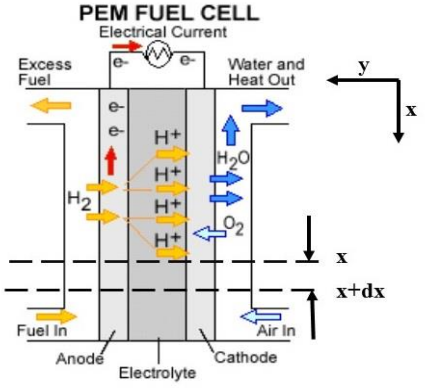
In a PEMFCs, hydrogen, and oxygen/air, enter as feeds into the anode and cathode flow channels, respectively. The molar rate of hydrogen and oxygen inputs in the anode and cathode flow channels can be obtained using relations (3) and (4).

$$\dot{N}_{H_2}^{cell} = \frac{S_a A_{cell} \bar{I}}{2F} \quad (3)$$

$$\dot{N}_{O_2}^{cell} = \frac{S_c A_{cell} \bar{I}}{4F} \quad (4)$$

which S_a is Anode stoichiometric coefficient, S_c is cathode stoichiometric coefficient, A_{cell} represents area of the cell, $\bar{I}$ is average current density and F stands for Faraday constant number(96485 C.mol^{-1}). Also $\dot{N}_{O_2}^{cell}$ and $\dot{N}_{H_2}^{cell}$ are input molar flow rates of oxygen and hydrogen.

The current density of a PEM fuel cell in a steady condition is determined using the transfer rate of the species participating in the reaction. In Figure 1, feeds to the anode and cathode channels in the direction of x and y are shown. In this modeling, it is assumed that the current flow and all the parameters change only in the x direction. This assumption is valid, since in order of magnitude, the magnitude of all the sizes of the cell is larger than its thickness.



[DOI: 10.22068/ase.2020.536]

Figure 1. View of a cell in a PEM fuel cell.

Consider a point like *x* in Fig. 1, in this point relation between the rate of production/consumption of the species participating in the reaction and the local current density is obtained by using equation (5):

$$\frac{dN_i}{dx} = \zeta_i \frac{wI(\mathrm{x})}{4F} \qquad (5)$$

That N_i is the molar flow rate of the species *i*, w is channel width, I(x) local current density and ζ_i stands for the stoichiometric parameter related to the species which in the channels of anode and cathode flow are :

Anode side:

$$\zeta_{H_2} = -2 \quad , \quad \zeta_{H_2O,a} = -4\alpha \qquad (6)$$

Cathode side:

$$\zeta_{O_2} = -1 \ , \ \zeta_{H_2O,\mathrm{c}} = 2 + 4\alpha \ , \ \zeta_{O_2} = 0$$

(7)

α is the net water drag coefficient and a and c stands for anode and cathode Respectively.

The electrolyte properties for Proton transfer are presented by Springer and his colleagues for Nafion membranes. Electro-osmotic drag coefficient for water inside membrane (n_d), has a direct relation with membrane water content(λm), and is defined as a function of the water activity as follows:

$$n_d = \frac{2.5\lambda_m}{22}$$

(8)

$$\lambda_m = \begin{cases} 0.043 + 17.81a_a - 39.85a_a^2 + 36.0a_a^3 \\ 14.0 + 1.4(\mathrm{a}_a - 1) \end{cases}$$

(9)

Diffusion of water, oxygen and hydrogen can be calculated according to the following relations:

$$D_{H_2O} = 1\times10^{-6}\exp[2416(\frac{1}{303}-\frac{1}{T})]\times(2.563-0.33\lambda+0.0264\lambda^2-0.000671\lambda^3) \qquad (10)$$

$$D_{O_2} = 2.88\times10^{-6}\exp[293314116(\frac{1}{303}-\frac{1}{T})] \qquad (11)$$

$$D_{H_2} = 4.1\times10^{-6}\exp[-2602(\frac{1}{T})] \qquad (12)$$

2.2. Continuity equation

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

$$\frac{\partial(\rho\varepsilon u)}{\partial x} + = S_m \qquad (13)$$

where u velocity in the x direction, ρ is density of reactant gases and S_m is mass sink term. This term is assumed to be zero because there is no reaction in the flow channels and gas diffusion layers. The sink term is not zero in the catalyst layer due to reaction of reactant species and can be calculated from the following equations [13]:

$$S_{H_2}(\mathrm{kg.s^{-1}.m^{-3}}) = -\frac{M_{H_2}}{2F}R_{an} \qquad (14)$$

[DOI: 10.22068/ase.2020.536]

$$S_{O_2}(\mathrm{kg.s^{-1}.m^{-3}}) = -\frac{M_{O_2}}{4F} R_{cat} \quad (15)$$

$$S_{H_2O}(\mathrm{kg.s^{-1}.m^{-3}}) = -\frac{M_{H_2O}}{2F} R_{cat} \quad (16)$$

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

2.4. Charge conservation equations

Electrochemical reactions within PEM fuel cell occur at the catalyst layers. The driving force of these reactions is surface activation overpotential. Activation overpotential is potential difference between solid phase and membrane. Therefore, two charge equations are needed. An equation for electron transfer through conductive solid phase and the other equation for proton transport through the membrane:

$$\nabla.(\sigma_{sol} \nabla \phi_{sol}) + R_{sol} = 0 \quad (17)$$

$$\nabla.(\sigma_{mem} \nabla \phi_{mem}) + R_{mem} = 0 \quad (18)$$

Volume sink terms are current density (A/m3). These terms are only defined in the catalyst layers:

For the solid phase:

$$R_{sol} = -R_{an} (< 0) \quad (19)$$

$$R_{sol} = +R_{cat} (> 0) \quad (20)$$

For membrane:

$$R_{mem} = +R_{an} (> 0) \quad (21)$$

$$R_{mem} = -R_{cat} (< 0) \quad (22)$$

The sink terms are calculated using the Butler–Volmer equation:

$$R_{an} = R_{an}^{ref} \left(\frac{C_{H_2}}{C_{H_2}^{ref}} \right)^{\gamma_{an}} \left(e^{(\alpha_{an} F/RT)\eta_{an}} - e^{-(\alpha_{cat} F/RT)\eta_{cat}} \right) \quad (23)$$

$$R_{cat} = R_{cat}^{ref} \left(\frac{C_{O_2}}{C_{O_2}^{ref}} \right)^{\gamma_{an}} \left(e^{-(\alpha_{cat} F/RT)\eta_{cat}} - e^{-(\alpha_{an} F/RT)\eta_{an}} \right) \quad (24)$$

Average current density is calculated from the equation below:

$$i_{ave} = \frac{1}{A} \int_{V_{an}} R_{an} dV = \frac{1}{A} \int_{V_{cat}} R_{cat} dV \quad (25)$$

2.5. Equations governing electrochemistry of the cell

The output voltage of a cell($Ecell$), in a PEM fuel cell can be obtained from the following equation:

$$E_{cell} = E_{oc} - \eta_{act} - \eta_{ohm} - \eta_{conc} \quad (26)$$

which E_{oc} is open circuit voltage. Also η_{act}, η_{ohm}, η_{conc} represent activation overpotential, ohmic overpotential and concentration overpotential respectively. The value of the open circuit voltage can be obtained by using equation 27:

$$E_{oc} = 1.229 - 0.85 \times 10^{-3}(\mathrm{T} - 298.15) + 4.31 \times 10^{-5} T (\ln P_{H_2} + 0.5 \ln P_{O_2}) \quad (27)$$

Activation overpotential of the cathode can be obtained from equation (13):

$$\eta_{act}(\mathrm{x}) = \frac{RT}{0.5F} \ln\left(\frac{I(\mathrm{x})}{I_{\circ} P_{O_2}^{cat}(\mathrm{x})}\right) \quad (28)$$

Which $I_{\circ}$ is exchanged current density at a reference pressure and $P_{O_2}^{cat}(\mathrm{x})$ is partial

[DOI: 10.22068/ase.2020.536]

pressure of oxygen in the catalyst layer and can be calculated using equation 29.

$$P_{O_2}^{cat}(\mathrm{x}) = C_{O_2}^{bulk}(\mathrm{x}) - \frac{I(\mathrm{x})}{4F}\left(\frac{1}{h_{O_2}} + \frac{t_{GDL}}{D_{O_2-g}^{eff}}\right)RT \quad (29)$$

$C_{O_2}^{bulk}(\mathrm{x})$ is concentration of oxygen in the flow channel and $D_{O_2-g}^{eff}$ represents Effective diffusion coefficient of oxygen in the gas mixture and can be calculated with Bruggeman equation as follows:

$$D_{O_2-g}^{eff} = D_{O_2-g}[(1-s)\phi]^{3/2} \quad (30)$$

Where ϕ is the porosity of GDL layer and D_{O_2-g} is diffusion coefficient of oxygen in the cathode channel.

2.6. Equations governing thermal energy

The general equation governing energy in a flow channel in a PEM fuel cell is according to equation (31):

$$\rho_{mix} C_{p,mix} v_x \frac{\partial T}{\partial x} = k_{mix} \frac{\partial^2 T}{\partial x^2} + Q_{total}^{source} \quad (31)$$

3. Results and discussion

3.1. validation

In Fig. 2, simulation results are compared with experimental results in the polarization curve. Not considering the contact resistance and internal leakage, as well as using the estimation of the Nurst equation in the reference article, cause differences in the results.

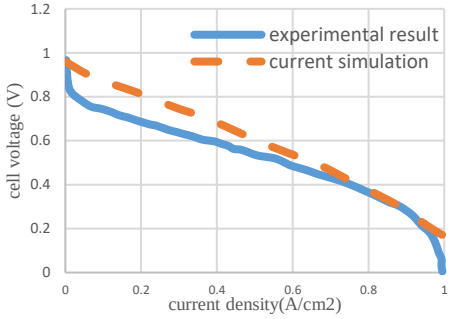


Fig.2. Validation of current simulation with experimental model results [14]

3.2. effect of pressure

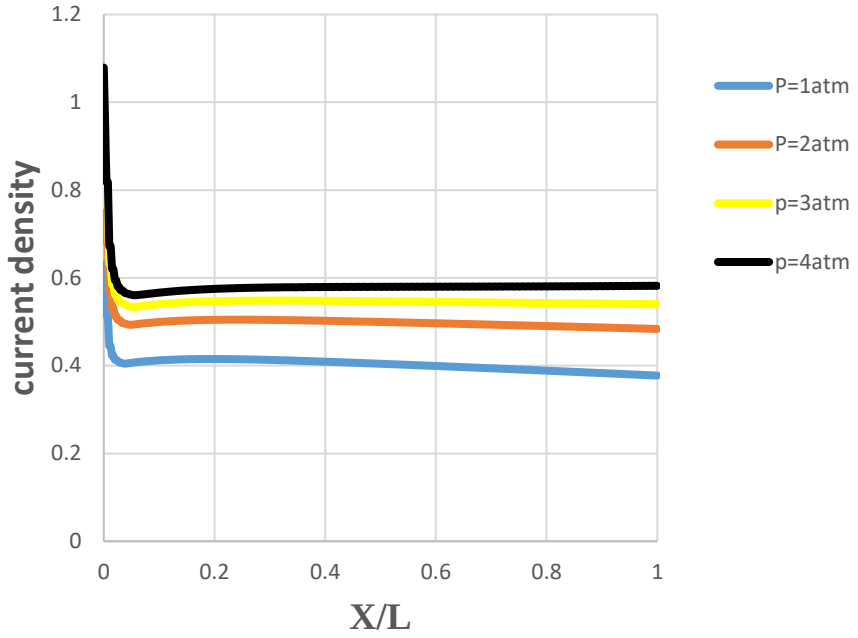
The following figures present effect of pressure of the anode and cathode side of a PEM fuel cell on the performance of the cell. Fig 3 (a) and 3(b) show the current density of the PEM fuel cell in different pressures. It can be understood from the figures that increasing the pressure in the cathode side causes enhancing the current density but in the anode side, increasing the pressure causes decreasing the current density. Looking accurately to the figure 3(b), one can consider that as the ratio X/L (computational domain is divided into L segments) increases from zero to unity, the current density rate becomes greater for P=2atm in comparison with the case of P=1atm. In other words, if the goal is to sustain the current density, it is suggested that the system operate under the pressure of 1atm at the anode side as P=2atm experiences significant current density change which is believed to be a vital drawback for PEM fuel cells.

3.3. effect of relative humidity

relative humidity in the anode and cathode side was studied as seen in the figures 4(a) and 4(b). In the cathode side (Fig 4(a)) with increasing the relative humidity from 0.3 to 1, current density is also increasing along the cell. The increment in the current density is more at higher relative humidity. In the Fig 4(b) that represents the current density changes in different relative humidities of anode side, no significant changes take place in the current density and it is almost constant along the cell in the anode side.

[DOI: 10.22068/ase.2020.536]

(a)



(b)

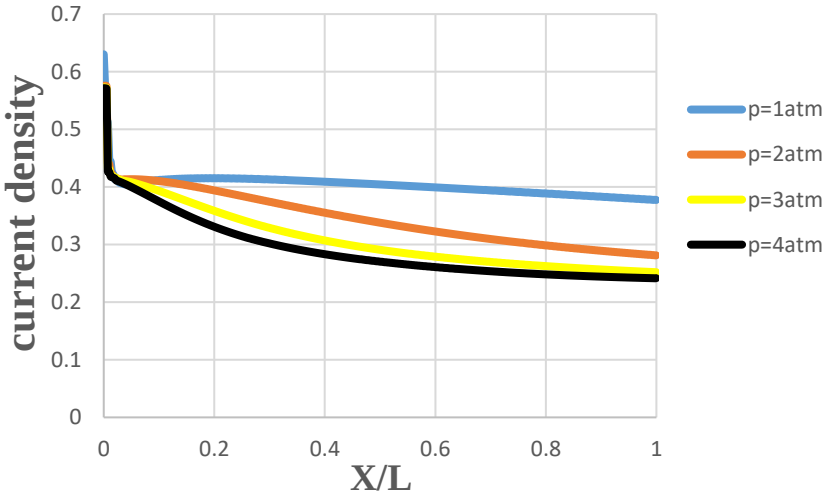


Fig3. Current density of PEM fuel cell in different pressures. (a)cathode side (b)anode side

[DOI: 10.22068/ase.2020.536]

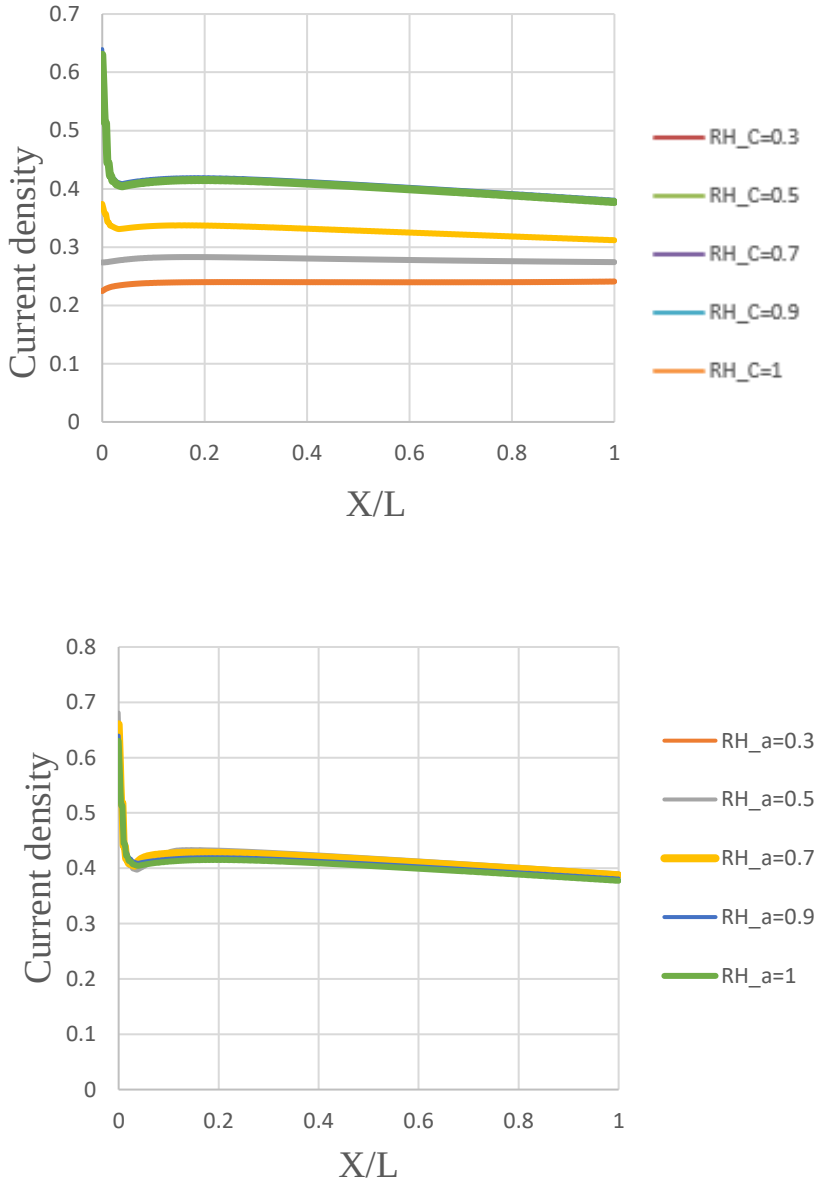


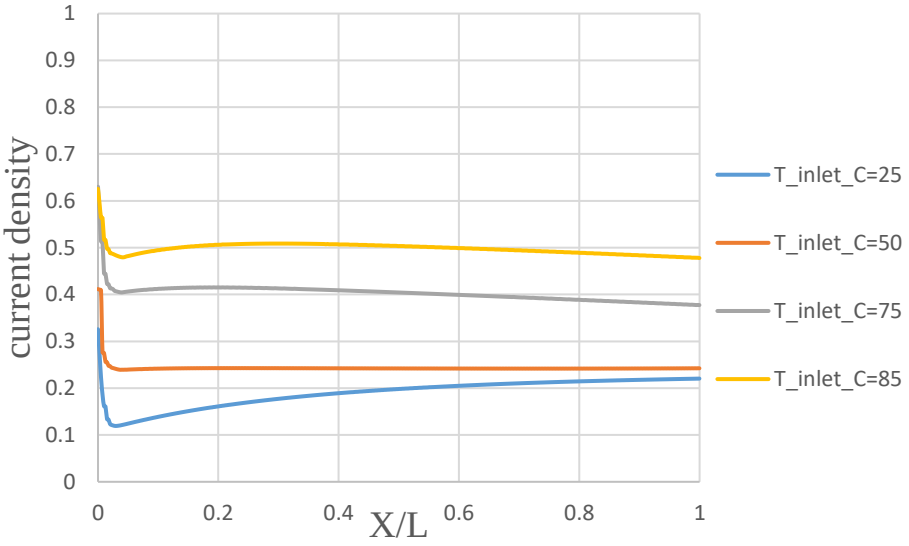
Fig.4. Current density of PEM fuel cell in different relative humidity. (a)Cathode side of PEMFC (b)Anode side of PEMFC

3.4. effect of temperature of inlets

In the fig.5(a) and 5(b) impact of temperature changes in the inlet of the PEMFC (temperature of hydrogen and oxygen) on the performance of the cell is shown. It can be derived from figure 5(a) that while the temperature of the inlet in the cathode side increases, better performance of the PEMFC takes place and current density indicates 30 percent of growth in the case with inlet temperature of 85 ^{0}C in comparison with the case that has an inlet temperature of 25 ^{0}C. but in Fig 5(b) that represents current density in the anode side, there is not much difference in cell performance i.e. temperature of inlets in the anode side doesn't have a significant effect on the current density of the PEM fuel cells.

[DOI: 10.22068/ase.2020.536]

(a)



(b)

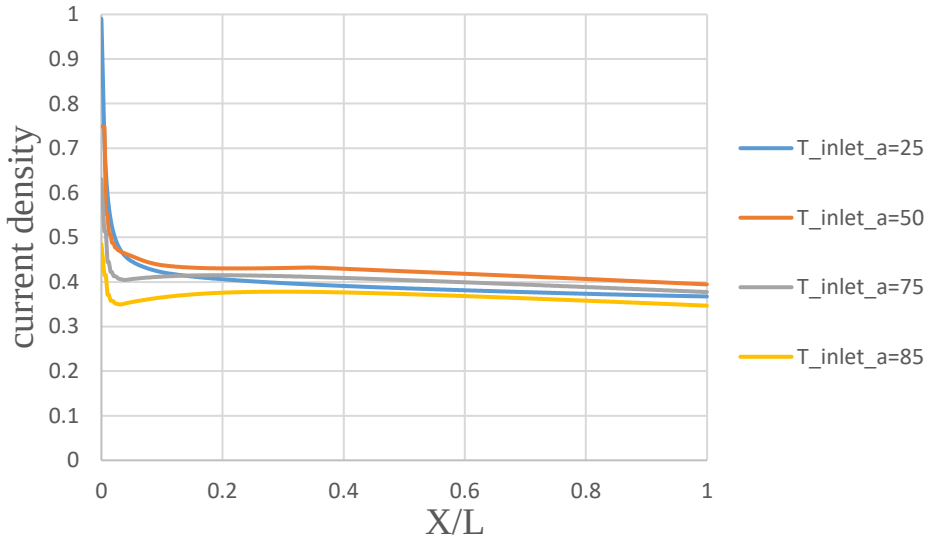


Fig.5. Current density of PEM fuel cell in different inlet temperatures. (a)Cathode side of PEMFC (b) Anode side of PEMFC

4. conclusion

in this research, the numerical simulation was accomplished to analyze the effect of different operation parameters of the PEM fuel cell on its performance and the following results were obtained:

With increasing pressure in the cathode side, due to the improvement of the mass transfer in the cell and the improvement of the value of the open circuit voltage, the efficiency of the cell increases

Increasing the temperature if the required humidity provided, will significantly improve the performance of the cell.

Reducing the humidity can be a factor in lowering the performance of the cell in low currents.

5. References

[1] O'hayre, R., Cha, S.W., Prinz, F.B. and Colella, W., 2016. Fuel cell fundamentals. John Wiley & Sons.

[DOI: 10.22068/ase.2020.536]

[2] Natarajan, D. and Van Nguyen, T., 2001. A two-dimensional, two-phase, multicomponent, transient model for the cathode of a proton exchange membrane fuel cell using conventional gas distributors. Journal of the Electrochemical Society, 148(12), pp. A1324-A1335

[3] J. Larminie, A. Dicks, Fuel Cell Systems Explained, second ed., John Wiley & Sons, Chichester, 2003.

[4] Zong, Y., Zhou, B., Sobiesiak, A., "Water and thermal management in a single PEM fuel cell with non-uniform stack temperature", J. of Power Sources, 161: 143-159, 2006.

[5] Y.M. Ferng & A. Su, "A three-dimensional full cell CFD model used to investigate the effects of different flow channel designs on PEM performance", Hydrogen energy, vol. 32, 4466-4476(2007).

[6] K. Sadeghzadeh, M.B. Salehi, Mathematical analysis of fuel cell strategic technologies development solutions in the automotive industry by the TOPSIS multi-criteria decision-making method, International Journal of Hydrogen Energy 36 (2011) 13272–13280.

[7] M.G. Santartelli, M.F. Torchio, " Experimental analysis of the effect of the operating variables on the performance of a single PEMFC", Energy conversion and management, vol. 48,40-51(2007).

[8] L. Wang, A. Husar, T. Zhou, H. Liu, "A parametric study of PEM fuel cell performances", hydrogen energy, vol. 28, 1263-1272(2003).

[9] G.H. Guvelioglu & H.G. Stenger, "Flow rate and humidification effects on a PEM fuel cell performance and operation", Power source, vol. 163, 882-891(2007).

[10] B. Kim, Y. Lee, A. Woo, Y. Kim, "Effect of cathode channel size and operating conditions on the performance air blowing PEMFCs", Applied energy, vol. 111, 441-448(2013).

[11] M. Zeruoal, B.S. Bouzida, H. Benmoussa, H. Bouguettaia, "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, vol. 18, 205-214(2012).

[12] Larbi, W. Alimi, R. Chouikh, A. Guizani, "Effect of porosity and pressure on the PEM fuel cell performance", hydrogen energy, vol. 38, 8542-8549(2013).

[13] N.P. Siegel, M.W. Ellis, D.J. Nelson, M.R. von Spakovsky, A two-dimensional computational model of a PEMFC with liquid water transport, Journal of Power Sources 128 (2004) 173–184.

[14] Ramousse, J., Lottin, O., Didierjean, S., Maillet, D., "Heat sources in proton exchange membrane (PEM) fuel cells", J. of Power Sources, 192: 435-441, 2009

[DOI: 10.22068/ase.2020.536]