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Numerical Simulation and Performance Evaluation of a Proton Exchange Membrane Fuel Cell

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Abstract

In the present study, a comprehensive numerical model of a Proton Exchange Membrane Fuel Cell (PEMFC) is developed and validated. The governing equations of mass diffusion, momentum transfer, species transport, heat transfer, and electric charge conservation are solved simultaneously. The simulations are performed using ANSYS FLUENT 15.0 at an operating temperature of 60 °C and atmospheric pressure. Model predictions are validated against experimental polarization data at the same operating conditions, showing good agreement. A mesh and iteration sensitivity analysis indicates that a mesh size of 224,280 cells and 500 iterations are sufficient to achieve a convergence criterion of 10^{-6}. Increasing the mesh density or iteration number beyond these values increases computational cost without improving accuracy. The numerical results include contours of molar concentrations of hydrogen, oxygen, and water, as well as temperature, enthalpy, and entropy distributions. The results provide detailed insight into transport phenomena and thermodynamic behavior inside the Proton Exchange Membrane (PEM) fuel cell.

Keywords: Proton exchange membrane fuel cell, Numerical simulation, ANSYS FLUENT, Transport phenomena, Thermodynamic analysis.

1 | Introduction

In recent years, many researches were promoted to find new efficient and green energy sources. Fuel cell is an attractive power generatuion device which is transformed chemical energy to electricity directly. This technique was established based on hydrogen energy. The energy shortage crisis in the world and production of green house gases reduces fossil fuel demand. The hydrogen can eliminate fossil fuel consumption and

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global warming. Since then, many researchers contributed in energy production of hydrogen in recent decade. In addition, various power systems were developed besde on energy of hydrogen rections [1], [2].

The initial fuel cell was introduced by Grove in 1843 [3]. The first work was developed on platinum electrodes and sulfuric acide that acts as electrolite. The electricity was obtained by reacting hydrogen and oxygen molecules in stochiometric rate. The water and vapor are two byproducts which may be produced and discharged through vent or drain. Since then, the solid and carbonate fuel cell were developed to promote the current density and efficiency of fuel cell. Low efficiency, safety problems and enviromental issues conducted the researches to new generation of fuel cells that was called Proton Exchange Membrane Fuel Cell (PEMFC). The temperature range 90ºC-180ºC was mentioned in various refrences. This technlogy is more viable for portable applications such as automoiles and space capsules.

In order to gain higher efficiency, differnt parameters were studied that help to commercialize the fuel cells.Temperature, electrolite, membrane charactristics and particularly catalyst layer, affect efficiency of fuel cell. The fuel cells are connected together in series configuration that builds a fuel cell stack. A stack obtains required voltage and current continously in the presence of H2 and O2.

Modeling of fuel cell systems plays a crucial role in improving the design, manufacturing, and operation of these systems. The use of numerical and analytical models leads to a reduction in experimental costs, enhancement of efficiency, and acceleration of fuel cell technology development. Reliable models must possess sufficient accuracy and robustness to predict fuel cell behavior under various operating conditions. An appropriate model should be capable of simulating fuel cell performance over a wide range of operating conditions, and even relatively simple models can exhibit significant predictive capability.

Models play a fundamental role in fuel cell development, as they provide deeper insight into the effects of key parameters on the performance of individual cell components as well as the overall system. Steady-state models describe fuel cell performance at a specific operating point, typically under constant temperature and reactant pressure, and are mainly used to predict experimental results. In contrast, dynamic models are employed to predict the transient behavior of fuel cells under time-varying operating conditions. These models are particularly useful for analyzing start-up and shutdown processes and for optimizing system response to load variations.

Siegel [4] presented a comprehensive review of published fuel cell models, addressing issues such as grid resolution, computational tools, and simulation time. In this study, one-dimensional, two-dimensional, and three-dimensional models were examined, and it was shown that one- and two-dimensional models are sufficient for many analyses. In addition, various modeling strategies, implementation approaches, as well as their advantages and limitations were discussed, and an overview of available fuel cell modeling software was provided.

In the context of developing new membrane materials for fuel cells, numerous studies have employed computational approaches. Cheddie and Munroe [5] developed a three-dimensional model to investigate the performance of a fuel cell employing a polybenzimidazole membrane, which is more advanced than one- and two-dimensional models. This type of membrane enables operation at higher temperatures, leading to increased reaction rates and reduced adverse effects of catalyst poisoning caused by carbon monoxide. The modeling results showed good agreement with experimental data.

One of the important applications of three-dimensional modeling in fuel cells is the optimization of flow channel design. Chen et al. [6] analyzed and simulated a wavy flow channel and validated their results using experimental data and the findings reported by Kaiser et al. [7]. The presence of obstacles in flow channels induces forced mixing regions and improves gas transport toward the Gas Diffusion Layer (GDL). The results demonstrated that wavy flow channels provide superior fuel cell performance compared to straight channels.

Modeling also enables the identification of faults and deficiencies during simulations. Such models can distinguish defective regions from the actual fuel cell behavior and prevent numerical errors from being

misinterpreted as real performance degradation. These approaches are particularly important for predicting fuel cell behavior under sudden failure conditions [8].

Other studies have focused on cold-start conditions of fuel cells. At very low temperatures, fuel cell performance is severely affected, and phenomena such as ice formation and reduced membrane conductivity become significant. The results indicate a direct relationship between cathode gas humidity and ice formation, with the highest ice accumulation occurring in the cathode catalyst layer. Furthermore, increasing the gas flow rate can mitigate the adverse effects of cold-start operation.

Water formation and transport in flow channels and Gas Diffusion Layers (GDLs) represent key aspects of fuel cell performance. Numerous models have been developed to predict water formation and two-phase flow behavior. In some models, water droplets are represented as spherical particles suspended in the gas flow, which is a reasonable assumption at low current densities; however, at higher current densities, this assumption may lead to deviations from experimental observations [9].

Modeling of cooling channels is also of great importance, particularly in simulations of fuel cell stacks where significant heat generation occurs. Proper temperature control prevents component degradation and ensures long-term system performance. Some studies have utilized system-level models to design effective control strategies for coolant temperature regulation.

Moreover, innovative flow field designs such as interdigitated, serpentine, and radial channels have been investigated using Computational Fluid Dynamics (CFD) methods. The results of these studies indicate that modifying flow channel geometry can lead to a more uniform current density distribution, reduced pressure drop, and ultimately improved overall fuel cell performance.

Overall, the review of previous studies demonstrates that numerical modeling—particularly CFD-based approaches—is a powerful tool for the analysis, design, and optimization of fuel cells, providing deep insight into mass and heat transfer phenomena, electrochemical reactions, and transient system behavior [10].

2 | Modeling and Simulation

2.1 | Geometry

A PEMFC consists of different main parts, gas flow channels, anode and cathode, GDLs which are called GDLs, membrane and two catalyst layers in anode and cathode sides. Hydrogen diffuses through anode that a GDL plays as a barrier of hydrogen molecules. The GDL thickness is has an important effect on hydrogen diffusion and plays a key role in mass diffusion value. Each molecule of hydrogen oxidized to two protons and produces two electrons at anode catalyst layer. The electrons diffuse through GDL and anode side to current collector.Also, oxygen molecules diffuse in the opposite side through cathode layer. In the other word hydrogen acts as a fuel or energy source and oxygen as an oxidizer. *Fig. 1* shows the schematic of the Proton Exchange Membrane (PEM) fuel cell [11].

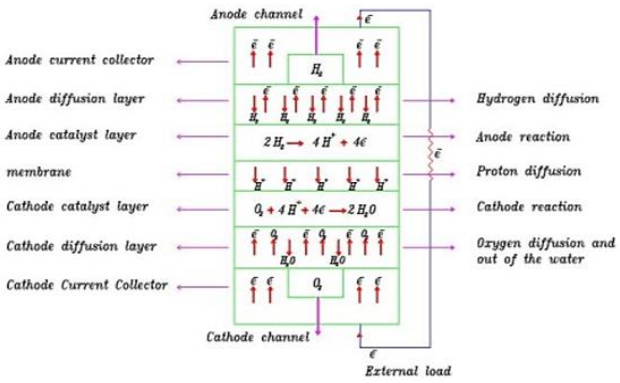


Fig. 1. Schematic of the PEM fuel cell.

During the reaction, energy released which can be validated by total enthalpy value of this reaction. The energy of H-O-H bond is lower than required energy for (O-O) and (H-H) bond breaking. Electricity is produced by moving the electrons in an external circuit and heat is released via fuel cell walls. The oxidation and reduction reactions must be balanced the electron production and consumption rate. This can be controlled by splitting the reaction sides. In the most cases nafion were applied as electrolyte that conducts H^+ ions, but acts as a barrier against electrons. Although rising temperature helps to promote reaction kinetic and fuel cell efficiency, but shows some shortcoming. Nafion is most cited electrolyte in PEMFC which is sensitive to temperature. This problem can be avoided by relative humidity control. As before mentioned, different parameters are effective in fuel cell operation and efficiency. In order to study and find the dependency of electricity production and operating and geometrical parameters, the fuel cell was modeled and simulated in this research. The geometric dimensions of the fuel cell model are given in *Table* 1.

Table 1. Geometric dimensions of studied PEMFC.

Parameter	Value	Units
Cell length	50	Mm
Gas channel width	1	Mm
Gas channel height	1	Mm
Current collector width	3	Mm
Current collector height	2	Mm
Gas diffusion layer thickness	0.3	Mm
Membrane thickness	0.125	Mm
Catalyst layer thickness	0.05	Mm

A single polymer exchange membrane fuel cell with abovementioned characteristics were modeled and studied in the following sections.

2.2 | Governing Equations

In this model, all areas inside the cell were supposed as a unit zone without internal boundaries between different regions. In this way to model the hydrodynamic behavior and electricity transfer in fuel cell, only one set of governing equations should be defined. As the heat loss is negligible, fuel cell was modeled at constant temperature.Therefore, conservation of mass, conservation of species, momentum and the electric potential equations (conservation of charge) are written as follows:

Conservation of mass

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

Conservation of momentum

$$\frac{\partial(\rho\varepsilon\vec{u})}{\partial t} + \nabla.(\rho\varepsilon\vec{u}\vec{u}) = -\varepsilon\nabla P + \nabla.\left(\varepsilon\mu^{eff}\nabla\vec{u}\right) + S_u. \quad (2)$$

Conservation of species

$$\frac{\partial(\varepsilon C_k)}{\partial t} + \nabla.(\varepsilon\vec{u}C_k) = \nabla.\left(D_k^{eff}\nabla C_k\right) + S_k. \quad (3)$$

Conservation of electrical charge

$$\nabla.\left(\sigma_{mem}^{eff}\nabla\phi_{mem}\right) + S_{mem} = 0. \quad (4)$$

$$\nabla.\left(\sigma_{sol}^{eff}\nabla\phi_{sol}\right) + S_{sol} = 0. \quad (5)$$

In the above equations u, P, C_k and ϕ are velocity vector, pressure, concentration of species k and electrical potential respectively. Also, S_u, S_k, S_{mem} and S_{sol} are the source terms of momentum, concervation of species,

electrolyte potential and solid phase potential respectively. The amount of these source terms are given in *Table* 2.

Table 2. Definition of the source terms.

	Gas Flow Channels	GDLs	Catalyst Layers	Membrane
Momentum	$S_u = 0$	$S_u = \frac{-\mu}{k}\varepsilon^2\vec{u}$	$\vec{u} = 0$	$\vec{u} = 0$
Conservation of species	$S_k = 0$	$S_k = 0$	$S_k = -\nabla.\left(\frac{n_d}{F}I_e\right) - \frac{s_k j}{nF}$	$S_k = -\nabla.\left(\frac{n_d}{F}I_e\right)$
Potential	$S_\phi = 0$	$S_\phi = 0$	$S_\phi = j$	$S_\phi = 0$

Also, the physical and geometrical properties of case study fuel cell should be defined which are presented in *Table 3*.

Table 3. Model parameters.

Current Collector		Electrode Parameters	
Thermal conductivity	20 W.(m.K)$^{-1}$	H_2 diffusivity	8×10^{-5} m^2.s^{-1}
Electrical conductivity	22000 (ohm.m)$^{-1}$	O_2 diffusivity	2×10^{-5} m^2.s^{-1}
Gas diffusion layer		H_2O diffusivity	5×10^{-5} m^2.s^{-1}
Porosity	75%	Pore blockage saturation exponent	2
Thermal conductivity	2 W.(m.K)$^{-1}$	Anode reference concentration	1 kmol.m^{-3}
Electrical conductivity	2500 (ohm.m)$^{-1}$	Cathode reference concentration	1 kmol.m^{-3}
Contact angle	165 °	Anode concentration exponent	0.5
Catalyst layer		Cathode concentration exponent	1
Porosity	50%	Anode exchange coefficient	1
Thermal conductivity	2 W.(m.K)$^{-1}$	Cathode exchange coefficient	1
Electrical conductivity	2500 (ohm.m)$^{-1}$	Anode reference current density	10000 A.m^{-2}
Anode CL surface/Volume ratio	7.6×10^6 m^{-1}	Cathode reference current density	20 A.m^{-2}
Cathode CL surface/Volume ratio	1.0×10^7 m^{-1}	Open-circuit voltage	0.98 V
Membrane			
Thermal conductivity	0.36 W.(m.K)$^{-1}$		
Ionic conductivity	(ohm.m)$^{-1}$		

2.3 | Boundary Conditions

In order to investigate the performance of a PEMFC, the governing equations should be solved numericall simultaneously. In this work, simulation was carried out using software ANSYS FLUENT 15.0. Then all parameters including boundary conditions of equations must be defined exactly. The mass flow rates at anode and cathode inlet are specified. In the other hand the flow rates of H_2 and O_2 should be determined at the inlet of gas flow channel. The mass flow rate of fuel and air at the inlet of gas flow channels are calculated based on stoichiometry, current density, temperature, relative humidity and Faraday constant [12].

Also, pressure at the outlet of anode and cathode side can be supposed constant. As a result the pressure gradient goes to zero at these sides. Therefore, the pressure outlet boundary condition is selected at the outlet of anode and cathode gas flow channels. The pressure and the other flow charactristics can be extrapolated with regard to interior values. The walls confined the fluid region, and then the no-slip condition is enforced

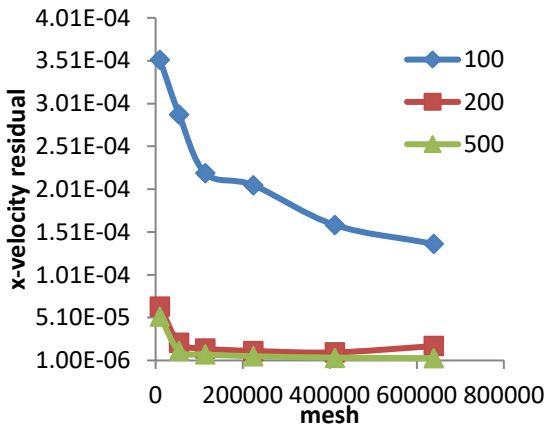
at the walls of fuel cell. The shear stress, velocity vector and heat transfer via the walls are calculated based on the aforementioned assuption. The appropriate boundary condition at upper and lower walls and the sides of the fuel cell is considered as wall boundary condition that was selected. The boundary conditions are given in *Table* 4.

Table 4. Boundary conditions.

Parameter		Value	
Fuel cell temperature		60 °C	-
Fuel cell operating pressure		1 atm	-
Relative humidity		100%	-
Anode stoichiometry		1.5	-
Cathode stoichiometry		3.5	-
Anode flow rate		9.675×10^{-8} kg.s^{-1}	Calculated
Cathode flow rate		8.636×10^{-6} kg.s^{-1}	Calculated
Inlet mass fraction anode	H_2	30.77%	Calculated
	H_2O	69.23%	Calculated
Inlet mass fraction cathode	O_2	20.16%	Calculated
	H_2O	13.49%	Calculated
	N_2	63.35%	Calculated

3 | Results and Discussion

This PEM fuel cell model was solved using ANSYS FLUENT 15.0 software. The hexahederal mesh was selected in order to descritize the fuel cell geometry. Sensitivity analysis was carried out to test the accuracy of the proposed model. The model was solved for different mesh number and iteration. Velocity vector residual, energy residual, mass concentration residual, electrical potential residual and voltage residual were measured, compared and depicted in various graphs in *Fig. 2*. The results show that the best convergency was obtained at 500 iteration and 224280 mesh number. Although the precision for iteration number =200 is acceptable (single precision order) but due to the low run time, the results are reported at iteration number 500.



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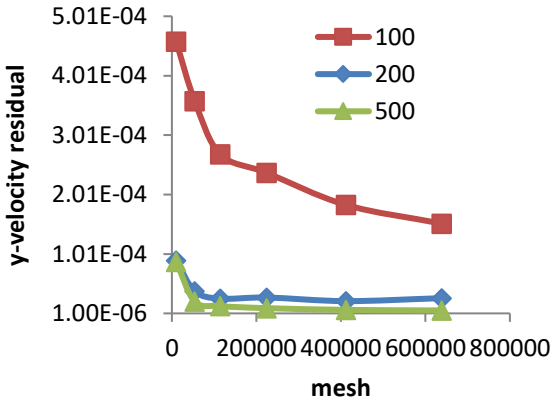

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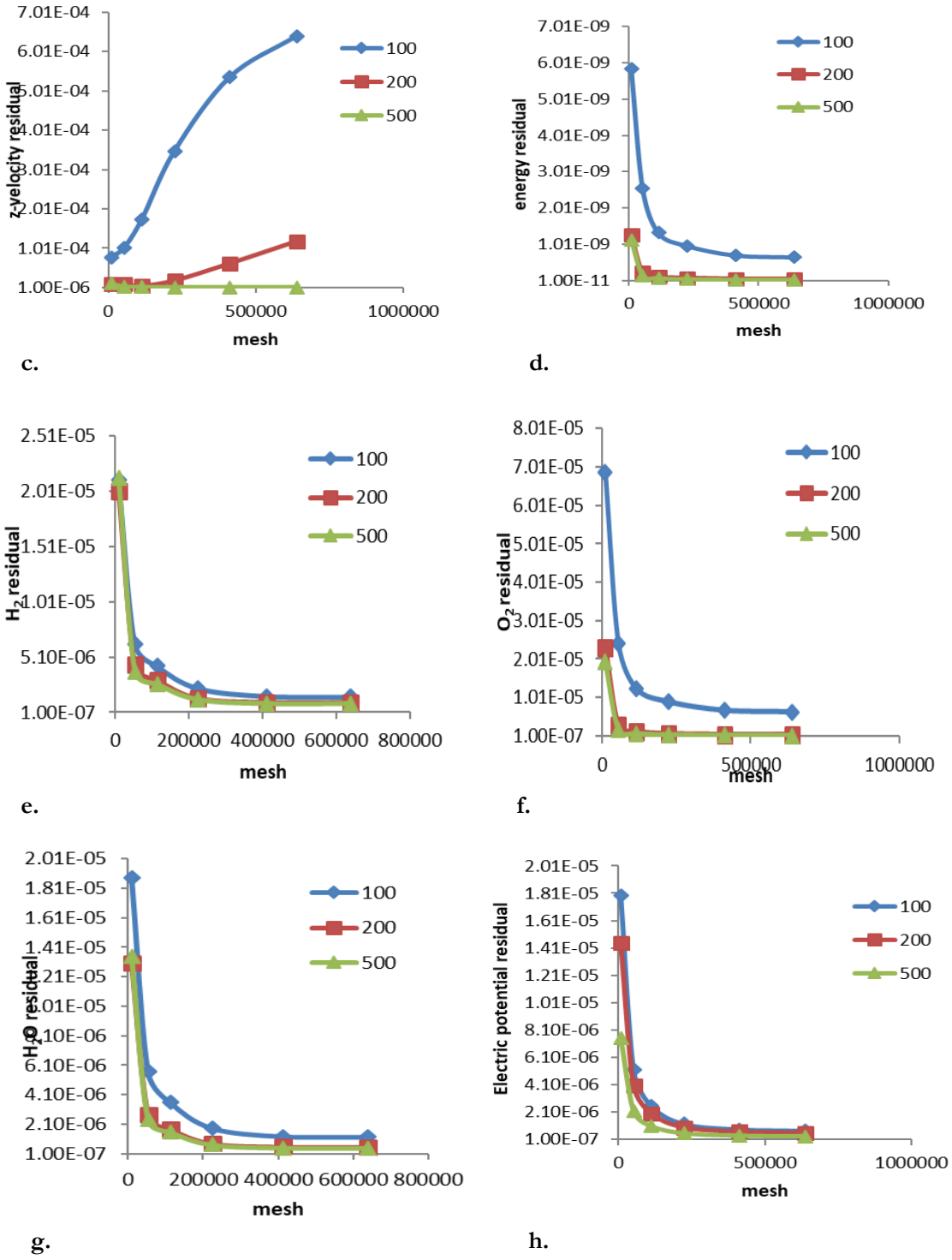


Fig. 2. The residual values at different mesh number and iterations.

Voltage values at various current densities were plotted in the range 0 mA/cm². The accuracy of results was compared with experimental data which were reported. Polarization curve was performed at 60°C and atmospheric pressure as shown in *Fig. 3*. The results show good agreement between model and experimental data.

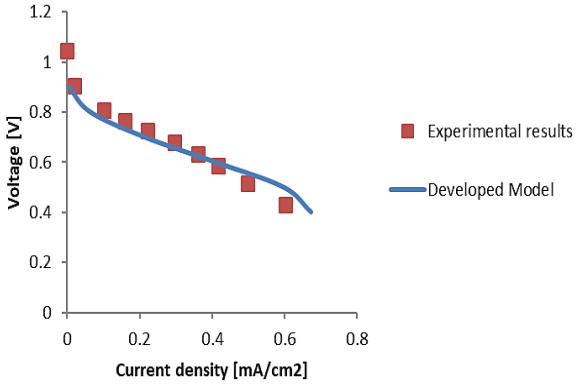


Fig. 3. Comparision between polarization curve and experimental data.

Temperature contours at 0.4 V were depicted in *Fig. 4*. Temperature at current collector and inlet plated were defined as boundary or initial condition as can be seen in *Fig 4*. Each molecule of oxygen reacts with four protons and 4 electros at cathod catalyst layer. This reaction is exothermic that causes coniderable temperature rise in fuel cell [13]. The generated water was dispsed through a drain and heat released via the fuel cells and outlet materials. Maximum temperature was observed at mid-plane of PEMFC. Temperature of this layer reaches to 346 K.

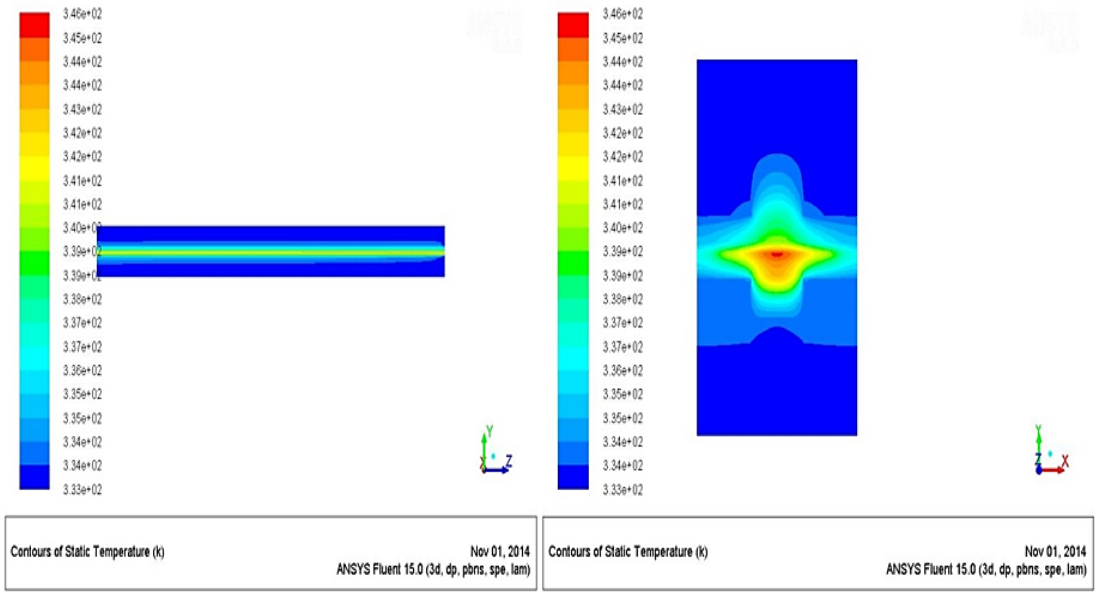


Fig. 4. Countoures of temperature at 0.4 V at mid plane of PEM fuel cell of yz and xy.

As mentioned before water and heat are the main products of PEM fuel cell which are obtained from (H-H) and (O-O) bonds breaking. The contours of molar concentration of water for at 0.4 V were depicted in *Fig. 5*. The results show that molar concentration of water increases along the flow channel. Water plays the key role in performance analysis of PEM fuel cell. It shows essential impact on ionic conductivity. Also an increase in water content causes water flooding and decreases performance of the PEM fuel cell.

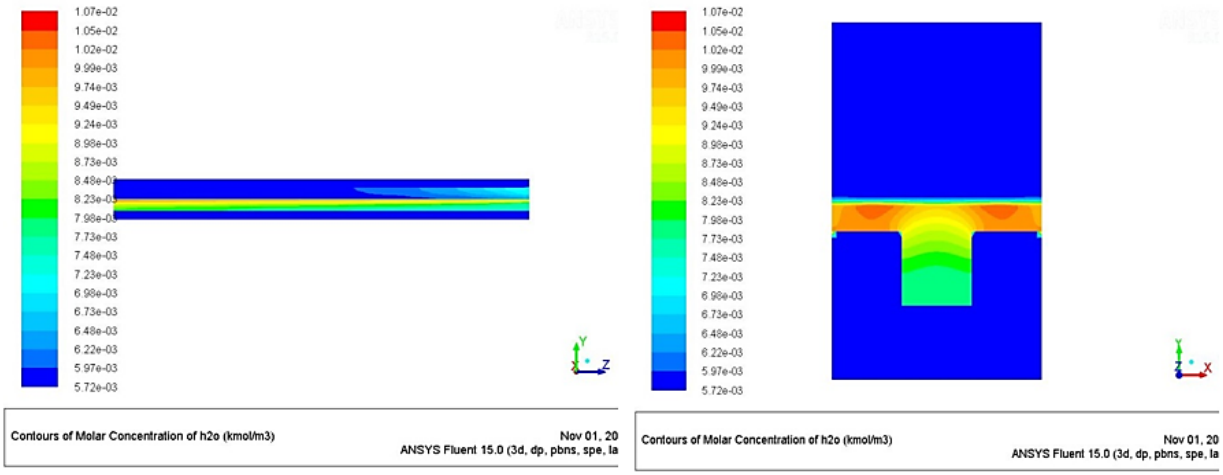


Fig. 5. Contour of molar concentration of water at 0.4 V at mide plane of PEM fuel cell of yz and xy.

The produced water content is a function of reaction kinetic. The water molar concentration should be defined based on hydrogen and oxygen molar flow rate and reaction efficiency. In the other hand the initial value of H_2 and O_2 and obtained water content must be confirmed each other. *Fig. 6* shows the contours of molar concentration of oxygen at 0.4 V. Oxygen enters to the fuel cell via cathode flow channel and diffuses through the GDL. At cathode catalyst layer, oxygen reacts with protons and electrons which were produce heat. Therefore due to O_2 concentration difference (mass gradient) between cathode inlet flow and catalyst layer, oxygen tend to diffuses through porous GDL. Then O_2 molar flow rate decreases at gas catalyst layer that can be seen in *Fig. 6* [14].

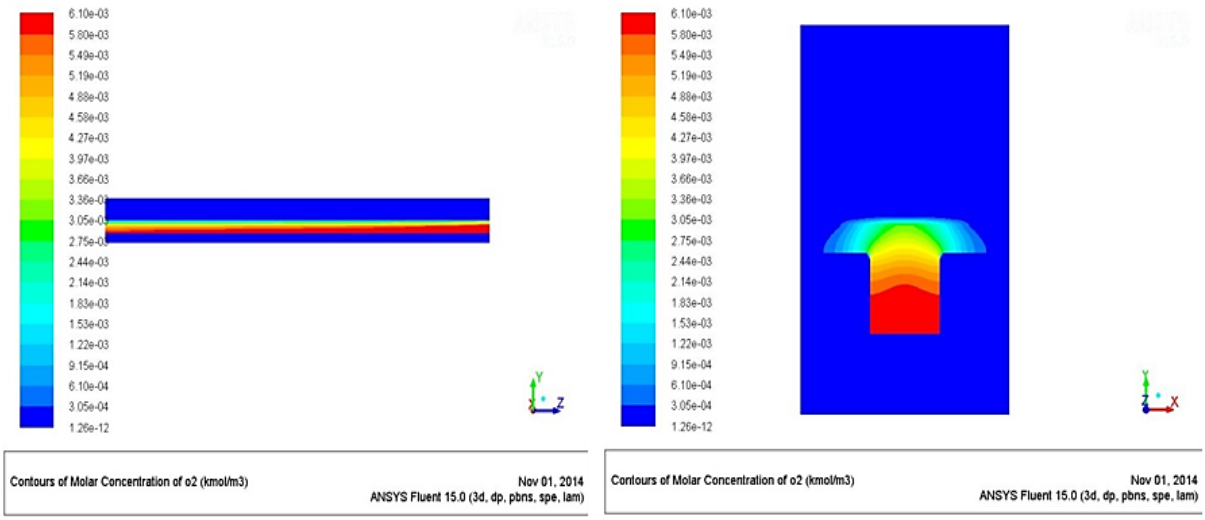


Fig. 6. Countor of molar concentration of oxygen at 0.4 V at mide plane of PEM fuel cell of yz and xy.

Fig. 7 shows the contours of H_2 molar concentration at 0.4 V. Hydrogen enters the fuel cell from the anode side and diffuses through the GDL due to H_2 concentration gradient. At anode catalyst layer, each hydrogen molecule lost two electrons and oxidized. The reaction between O_2 and protons are carried out at cathode catalyst layer, and then hydrogen concentration decreases.

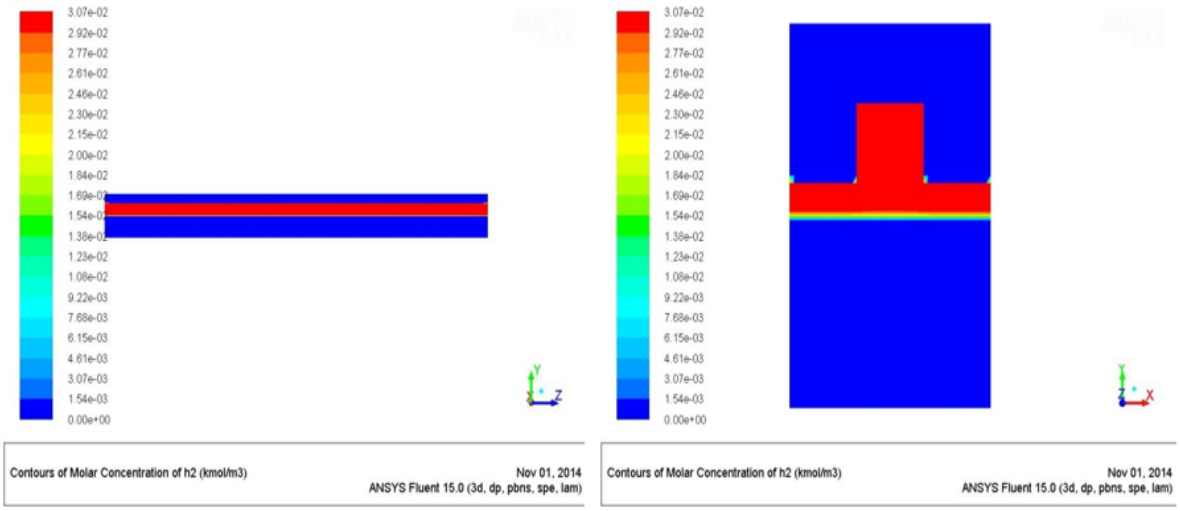
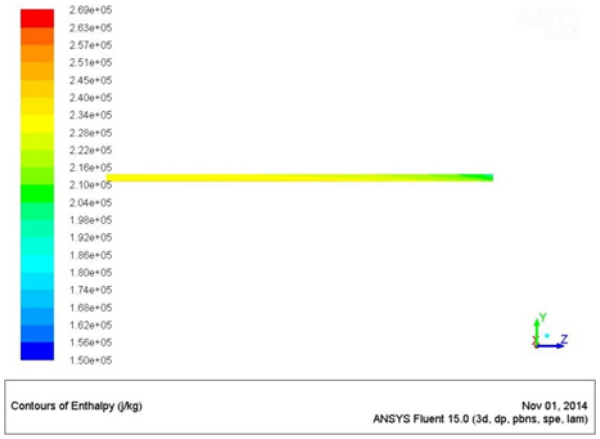


Fig. 7. Countor of molar concentration of hydrogen at 0.4 V at mide plane of PEM fuel cell of yz and xy.

Enthalpy changes of the anode and cathode flow is demonstrated in *Fig. 8*. According to the figure can be seen that the enthalpy increases along the cell length. As the chemical reaction releases heat to the fuel cell and this increase in temperature will cause an increase in enthalpy.



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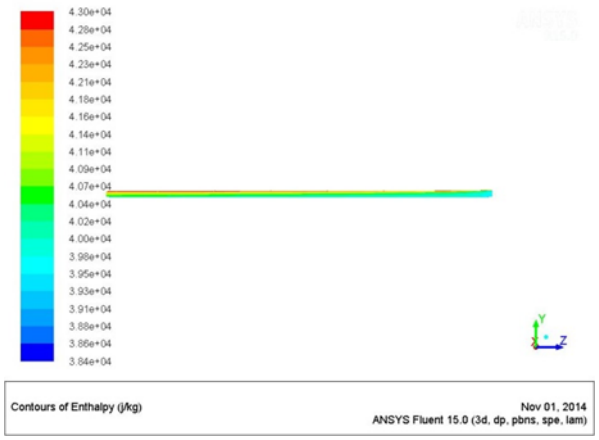

b.

Fig. 8. Enthalpy changes; a. anode flow, and b. cathode flow.

Fig. 9 shows the entropy changes of anode and cathode flow. In energy conversion to different typesor use of energy for work production, the amount of energy is destroyed as heat generated by friction or other factors. So the entropy increases along the cell length.

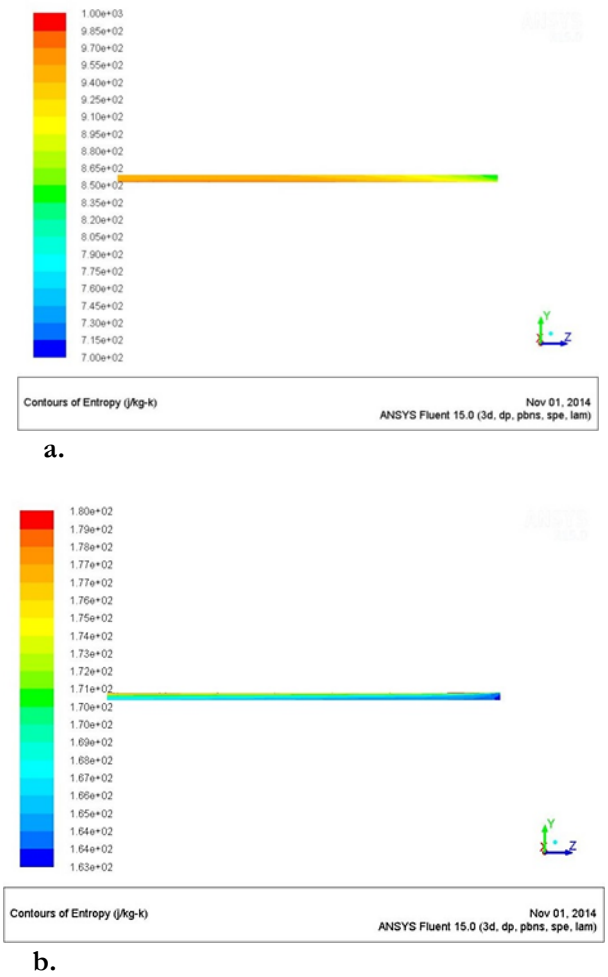

Fig. 9. Entropy changes; a. anode flow and b. cathode flow.

4 | Conclusion

The molar concentration of hydrogen from the anode flow channel to the anode catalyst layer decreases.Molar concentration of oxygen from the cathode flow channel to the catalyst layer decreases.Also, due to the consumption of oxygen, its concentration along the fuel celldecreases.Note that the overall reaction in fuel cells is associated with the production of the water and heat, the molar concentration of water and temperature raise in the cathode catalyst layer is high and the temperature achieve to 346 K. The amount of entropy and enthalpy of both the anode and cathode side also increases.

Authors' Contributions

All aspects of the research and manuscript preparation were carried out by the author. The author has read and approved the final version of the manuscript.

Consent for Publication

The author has given consent for the publication of this manuscript.

Ethics Approval and Consent to Participate

This study does not involve any research conducted on human participants or animals.

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Data Availability

All data are included in the text.

Conflicts of Interest

The authors declare no conflict of interest.

References

[1] Liu, W., Sun, L., Li, Z., Fujii, M., Geng, Y., Dong, L., & Fujita, T. (2020). Trends and future challenges in hydrogen production and storage research. *Environmental science and pollution research*, *27*(25), 31092–31104. https://doi.org/10.1007/s11356-020-09470-0%0A%0A

[2] Zou, C., Li, J., Zhang, X., Jin, X., Xiong, B., Yu, H. (2022). Industrial status, technological progress, challenges, and prospects of hydrogen energy. *Natural gas industry b*, *9*(5), 427–447. https://doi.org/10.1016/j.ngib.2022.04.006

[3] Grove, W. R. (1843). On the gas voltaic battery experiments made with a view of ascertaining the rationale of its action and its application to eudiometry. *Philosophical transactions of the royal society of london*, (133), 91–112. https://doi.org/10.1098/rstl.1843.0009

[4] Siegel, C. (2008). Review of computational heat and mass transfer modeling in polymer-electrolyte-membrane (PEM) fuel cells. *Energy*, *33*(9), 1331–1352. https://doi.org/10.1016/j.energy.2008.04.015

[5] Cheddie, D. F., & Munroe, N. D. H. (2006). Three dimensional modeling of high temperature PEM fuel cells. *Journal of power sources*, *160*(1), 215–223. https://doi.org/10.1016/j.jpowsour.2006.01.035

[6] Chen, X., Yu, Z., Yang, C., Chen, Y., Jin, C., Ding, Y., Wan, Z. (2021). Performance investigation on a novel 3D wave flow channel design for PEMFC. *International journal of hydrogen energy*, *46*(19), 11127–11139. https://doi.org/10.1016/j.ijhydene.2020.06.057

[7] Kaiser, R., Ahn, C. Y., Kim, Y. H., & Park, J. C. (2024). Performance and mass transfer evaluation of PEM fuel cells with straight and wavy parallel flow channels of various wavelengths using CFD simulation. *International journal of hydrogen energy*, *51*, 1326–1344. https://doi.org/10.1016/j.ijhydene.2023.05.025

[8] Wang, Y., Diaz, D. F. R., Chen, K. S., Wang, Z., & Adroher, X. C. (2020). Materials, technological status, and fundamentals of PEM fuel cells--a review. *Materials today*, *32*, 178–203. https://doi.org/10.1016/j.mattod.2019.06.005

[9] Pasaogullari, U., & Wang, C. Y. (2010). *Modeling and diagnostics of polymer electrolyte fuel cells*. Springer Science & Business Media. https://doi.org/10.1007/978-0-387-98068-3

[10] Wang, Y., Chen, K. S., Mishler, J., Cho, S. C., & Adroher, X. C. (2011). A review of polymer electrolyte membrane fuel cells: Technology, applications, and needs on fundamental research. *Applied energy*, *88*(4), 981–1007. https://doi.org/10.1016/j.apenergy.2010.09.030

[11] Larminie, J., Dicks, A., & McDonald, M. S. (2003). *Fuel cell systems explained* (Vol. 2). J. Wiley Chichester, UK. https://doi.org/10.1002/9781118878330?urlappend=%3Futm_source%3Dresearchgate.net%26utm_medium%3Darticle

[12] Demuren, A., & Edwards, R. L. (2020). Modeling proton exchange membrane fuel cells—a review. *50 years of cfd in engineering sciences: A commemorative volume in memory of d. brian spalding*, 513–547. https://doi.org/10.1007/978-981-15-2670-1_15%0A%0A

[13] Mukherjee, P. P., & Wang, C. Y. (2011). Polymer electrolyte fuel cell modeling--a pore-scale perspective. In *Green energy: Basic concepts and fundamentals* (pp. 181–221). Springer. https://doi.org/10.1007/978-1-84882-647-2_5%0A%0A

[14] Springer, T. E., Zawodzinski, T. A., & Gottesfeld, S. (1991). Polymer electrolyte fuel cell model. *Journal of the electrochemical society*, *138*(8), 2334. https://doi.org/10.1149/1.2085971%0A%0A