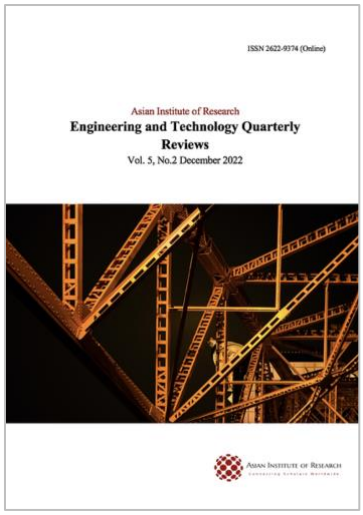

Engineering and Technology Quarterly Reviews

Kaplan, M. (2022), A Numerical Parametric Study on the Impacts of Mass Fractions of Gas Species on PEMFC Performance. In: *Engineering and Technology Quarterly Reviews*, Vol.5, No.2, 38-45.

ISSN 2622-9374

The online version of this article can be found at:
https://www.asianinstituteofresearch.org/

Published by:
The Asian Institute of Research

The Asian Institute of Research *Engineering and Technology Quarterly Reviews* is a peer-reviewed International Journal. The journal covers scholarly articles in the fields of Engineering and Technology, including (but not limited to) Civil Engineering, Informatics Engineering, Environmental Engineering, Mechanical Engineering, Industrial Engineering, Marine Engineering, Electrical Engineering, Architectural Engineering, Geological Engineering, Mining Engineering, Bioelectronics, Robotics and Automation, Software Engineering, and Technology. As the journal is Open Access, it ensures high visibility and the increase of citations for all research articles published. The *Engineering and Technology Quarterly Reviews* aims to facilitate scholarly work on recent theoretical and practical aspects of Education.

ASIAN INSTITUTE OF RESEARCH
Connecting Scholars Worldwide

The Asian Institute of Research
Engineering and Technology Quarterly Reviews
Vol.5, No.2, 2022: 38-45
ISSN 2622-9374

A Numerical Parametric Study on the Impacts of Mass Fractions of Gas Species on PEMFC Performance

Mahmut Kaplan[1]

[1] Department of Machine and Metal Technology, Naci Topcuoglu Vocational High School, Gaziantep University, Gaziantep, Turkey

Correspondence: Mahmut Kaplan, Department of Machine and Metal Technology, Naci Topcuoglu Vocational High School, Gaziantep University, Gaziantep 27600, Turkey. Tel: +90 536 231 92 81. E-mail: mahmutkaplan@gantep.edu.tr. ORCID: 0000-0003-2675-9229.

Abstract
Proton exchange membrane fuel cell (PEMFC) has attained increasing interest during the past decade owing to operating at low temperatures, generating higher efficiency power and having low pollutant emissions. Many parameters including operating temperatures, pressures and mass fraction of gas species affect PEMFC efficiency. In this work, a 3D Computational Fluid Dynamics approach is employed to study the influences of hydrogen mass fraction (0.1-0.6), oxygen mass fraction (0.1-0.2) and cathode water mass fraction (0.1-0.26) on the cell performance at 0.4-0.8 V. The numerical results using ANSYS Fluent reveal that decreasing hydrogen mass fraction and increasing water mass fraction augment the current density at 0.4 and 0.6 V. Besides, decreasing oxygen mass fraction from 0.2 to 0.16 also enhances the cell performance whereas the current density remains almost constant with further decreasing oxygen mass fraction. The highest current density of 2.30 A/cm^2 is achieved with mass fraction of oxygen of 1.6 and the current density increases by 82.5% compared to the base model at 0.4 V. However, the pressure drop of channels is not significantly affected by modifying mass fractions of gases. It is found that determining the optimum value of each species mass fraction at the anode and cathode plays a crucial role in the development of the cell efficiency.

Keywords: PEMFC, CFD Model, Species Mass fractions, Cell Performance, Pressure drop, Optimization

1. Introduction

Proton exchange membrane fuel cell (PEMFC) is regarded to be an encouraging technology for producing clean and efficient energy at low operating temperatures (333-353 K). PEMFC transforms the chemical energy of the fuel into electricity by oxidizing hydrogen as a fuel. There are three major application areas for PEMFC systems such as transportation (aviation, marine, rail and road), stationary (backup systems) and portable power (Wang et

al., 2020). Membrane, catalyst layer (CL), gas diffusion layer (GDL) and bipolar plate are main parts of PEMFC. The flow channel machined into bipolar plate surfaces supplies reactant gases (hydrogen and oxygen) and takes away water and heat from the cell (Xing et al., 2019). The electrochemical reactions that occur at the surfaces of CL are as follows:

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

$$½O_2 + 2e^- + 2H^+ \rightarrow H_2O \ (Cathode) \quad (2)$$

Recently, transport and electrochemical phenomena associated with the components of PEM fuel cell have gained significant attention in academia for augmenting the cell efficiency (Song and Meng, 2013; Salva et al. 2016; Wu, 2016; Subin & Jithesh, 2018; Ahmadi & Rostami, 2019; Ogungbemi et al. 2021; Yang et al., 2022). Salva et al. (2016) developed a 1D analytical model to determine the current densities under different operating conditions including pressure, temperature, relative humidity and stoichiometry in the cathode. They reported that the suggested PEMFC model had a potential to optimize operating parameters to obtain maximum possible power output. It was also found that for higher current density, it was required to elevate the cathode stoichiometry and decrease the relative humidity gradually. Subin & Jithesh (2018) conducted an experiment to study the impact of operating parameters including temperature and air flow rate on the performance of the self-humidified PEMFC having dry feed condition at the cathode. It was found that the high operating temperature leaded to performance losses related to membrane dehydration. They also concluded that optimization of the air flow rate was necessary for achieving high efficiency. Ahmadi & Rostami (2019) experimentally and numerically examined the influence of inlet velocity of gases on PEMFC efficiency. The results showed that higher inlet velocity (> 0.2 m/s) affected the penetration of gases from the channels adversely whereas lower inlet velocity (< 0.05 m/s) resulted in the loss of species concentration which affected the long-term performance. Yang et al. (2022) experimentally studied the influencing of air velocity and operating temperature on cell performance of open-cathode PEMFC. They revealed that increasing temperature and velocity augmented the cell efficiency due to taking out excessive water in pores of GL and CL.

Literature studies show that it is common practise to assess the influences of operating parameters on PEMFC performance. However, the combined influence of mass fractions of anode and cathode gases on the enhancement of PEMFC efficiency is not readily available in the literature. The goal of this work is to analyse the influence mass fraction of gases involved in PEMFC electrochemical reactions on the PEMFC performance using a single-phase computational model developed in the previous study (Kaplan, 2021). The organization of the paper is as follows. In the second part, the PEMFC model is described in detail. In the third part, the numerical results and their discussion are introduced. In the fourth part, the conclusions obtained from the present numerical study are presented.

2. CFD Model Details

In the present work, 3D geometry is generated using SOLIDWORKS. Then computational mesh is produced and divided into 9 parts containing a membrane and CL, GDL, flow channel and current collector in the anode and cathode sides using ANSYS Meshing as seen in Figure 1. These parts are required to specify anode and cathode characteristics in the FLUENT Fuel Cell module (ANSYS, 2011).

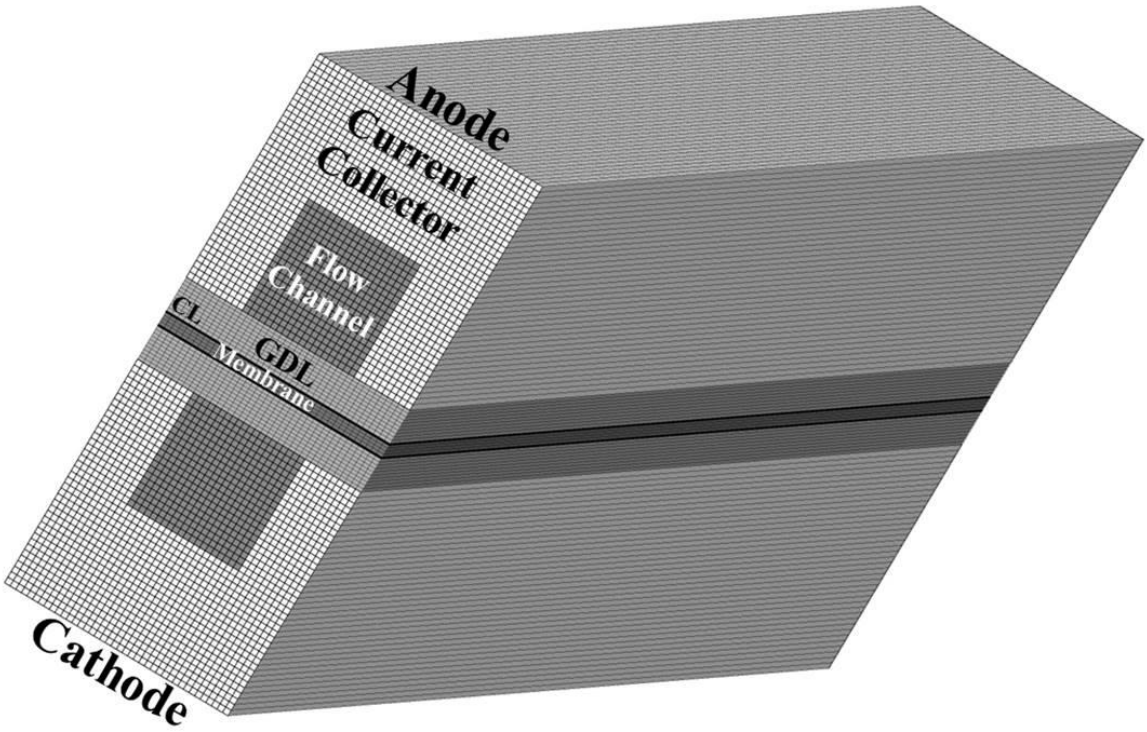

Figure 1: Grid structure of PEMFC model

The dimensions of PEMFC geometry are obtained from the experiment performed by Wang et al. (2003). The cell width and length are 2 and 70 mm, respectively. The membrane, GDL and CL thicknesses are 0.108, 0.3 and 0.0129 mm, respectively. The flow channel is 1 mm in width and height. The operational parameters employed for the model are summarized in Table 1.

The following assumptions have been made when constructing the computational model:

- The flow is steady state, laminar, single phase and incompressible.
- Assume the species behave as ideal gases and exist only in gas phase in the flow channel.
- A homogeneous isotropic porous medium is considered for the GDL, CL and membrane.

Table 1: Electrochemical properties of PEMFC

Parameter	Value
Anode mass fraction of H_2 and H_2O at the inlet	0.2 and 0.8
Cathode mass fraction of O_2 and H_2O at the inlet	0.2 and 0.1
Reference exchange current density (anode)	4000 A/m^2
Reference exchange current density (cathode9	0.1 A/m^2
Reference H_2 and H_2O diffusion	7.33 x 10^{-5} m^2/s (Mazumder & Cole, 2003)
Reference O_2 diffusion	2.13 x 10^{-5} (Mazumder & Cole, 2003)
Reference other species diffusion	4.9 x $10^{-5}m^2/s$ (Mazumder & Cole, 2003)
Operating temperature and pressure	343 K and 101.325 kPa (Wang et al., 2003)
GDL and CL porosity and viscous resistance	0.5 and 1 x 10^{12} $1/m^2$ (Kahveci & Taymaz, 2018)
CL surface/volume ratio	200000 1/m
Open-circuit voltage	0.94 V

Mass, momentum, species, energy and charge equations are used to simulate physical phenomena taking place in the PEMFC as shown in Table 2 (Kaplan, 2021; Spiegel, 2008; Barbir, 2013).

Table 2: Governing equations

	Equations
Mass	$\nabla(\rho\vec{u}) = 0$
Momentum	$\frac{1}{\left(\varepsilon^{eff}\right)^2}\nabla(\rho\vec{u}\vec{u}) = -\nabla P + \nabla(\mu\nabla\vec{u}) + S_m$
Species	$\nabla(\vec{u}C_k) = \nabla(D_k^{eff}\nabla C_k) + S_k$
Energy	$\nabla(\rho\vec{u}T) = \nabla(k^{eff}\nabla T) + S_h$
Charge	$\nabla(\sigma_{mem}\nabla\phi_{mem}) + R_{mem} = 0$ $\nabla(\sigma_{sol}\nabla\phi_{sol}) + R_{sol} = 0$ $\eta_{an} = \phi_{sol} - \phi_{mem}$ $\eta_{cat} = \phi_{sol} - \phi_{mem} - V_{oc}$

The constant mass flow boundary condition is applied at the flow channel inlet with mass flow rate of 5.398 x 10^{-6} and 3.294 x 10^{-5} kg/s at the anode and cathode, respectively (Biyikoglu & Alpat, 2011). Pressure at the outlet of flow channels is fixed and atmospheric. The upper and lower current collector faces are specified as the wall. The electrical potential at the anode and cathode terminals is fixed as zero and the operating voltage, respectively. The same boundary conditions are employed for the model and the cases including different mass fractions of gases.

3. Results and Discussions

3.1 Model Validation

In the current study, the model is verified by comparing the computational results with measured data from Wang et al. (2003) in Figure 2.

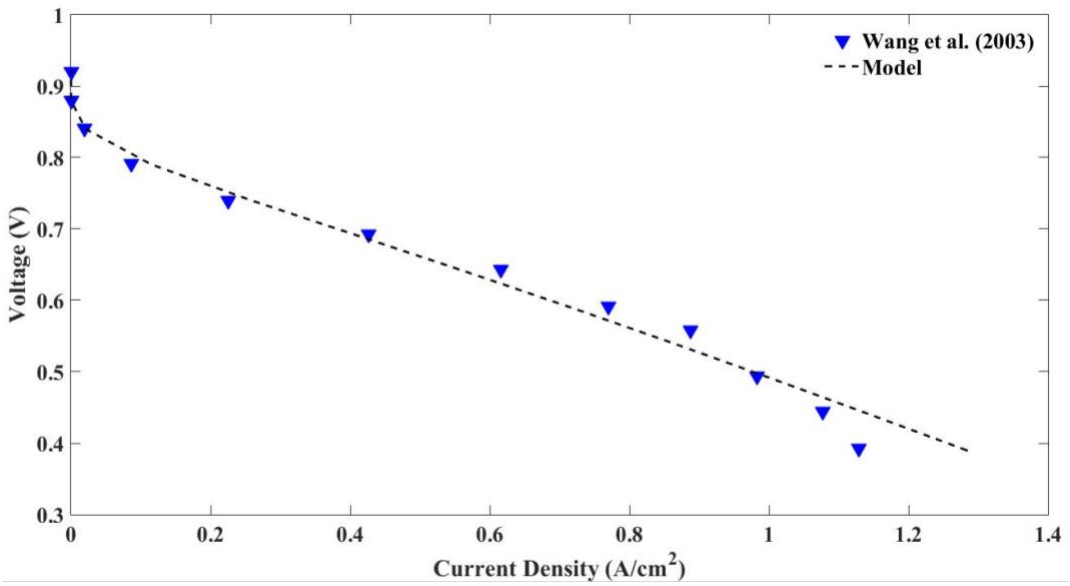

Figure 2: Comparison mathematical model with experimental data (Wang et al., 2003)

The predicted results agree well with the measured data, especially at lower current densities. But the present model overestimates the experimental data at higher current densities. It may be owing to the model ignoring the liquid water in the GDL and CL resulting in decreasing the GDL and CL porosity and increasing the resistance to mass transfer in gas phase.

3.2 Influence of Mass Fraction of Gas Species on Current Density

In this section, the effect of mass fraction of hydrogen, and oxygen and water (cathode) on PEMFC performance is presented. Figure 3 displays the calculated current densities for various mass fractions of hydrogen (0.1-0.6) at three voltages of 0.4, 0.6, and 0.8 V.

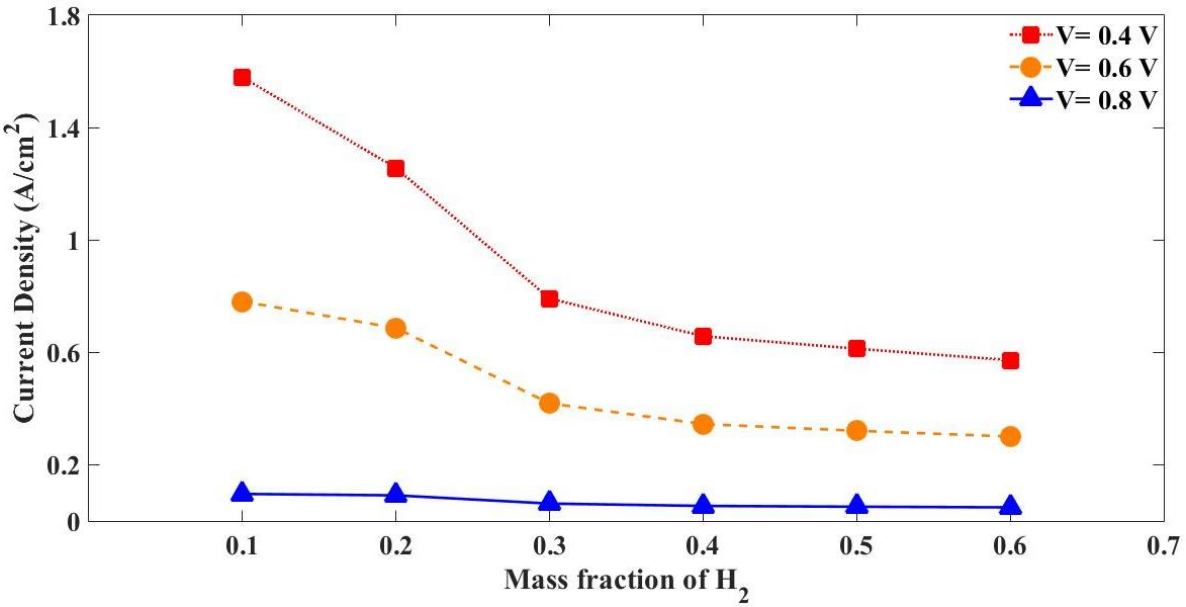

Figure 3: Change of current density for different mass fractions of hydrogen at various cell voltages of 0.4-0.8 V

As seen in Figure 3, the influence of hydrogen mass fraction on the current density is almost negligible at 0.8 V whereas the current densities increase linearly with a decrease in hydrogen mass fraction from 0.6 to 0.4 at 0.4 and 0.6 V. After this, the hydrogen mass fraction has a more obvious impact on the current density. Then a sudden increase of the current density is detected when the value of hydrogen mass fraction reaching 0.3 at 0.4 and 0.6 V. The results in Figure 3 indicate that increasing water mass fraction with decreasing hydrogen mass fraction plays a dominant role for augmenting the cell efficiency at 0.4 and 0.6. The peak value of 1.58 A/cm^2 is achieved with hydrogen mass fraction value of 0.1 at 0.4 V. Figure 4 illustrates the computed current densities for various mass fractions of oxygen (0.1-0.2) at three different voltages of 0.4, 0.6, and 0.8 V.

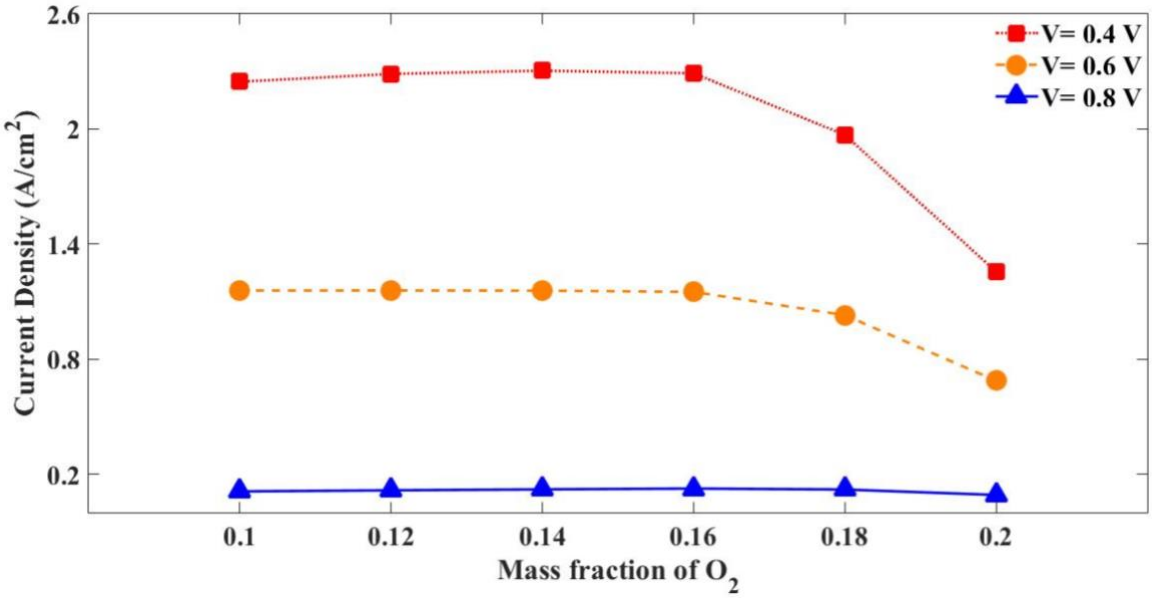

Figure 4: Change of current density for different mass fractions of oxygen at various cell voltages of 0.4-0.8 V

As seen in Figure 4, decreasing oxygen mass fraction from 0.2 to 0.16 significantly improves the cell performance at 0.4 and 0.6 V whereas the current density is almost independent of oxygen mass fraction for its values between 0.1 and 0.16 at all cell voltages. Due to the sum of all mass fractions of cathode gases being equal to unity, an increase in oxygen mass fraction results in decreasing water mass fraction. Like the previous results obtained with variation of hydrogen mass fraction, higher cathode water mass fraction results in elevating the cell current density at 0.4 and 0.6 V. The maximum value of 2.30 A/cm^2 is observed with oxygen mass fraction value of 0.14 at 0.4 V. Figure 5 illustrates the current densities for different water mass fractions (0.1-0.26) for three different voltages of 0.4, 0.6, and 0.8 V at the cathode.

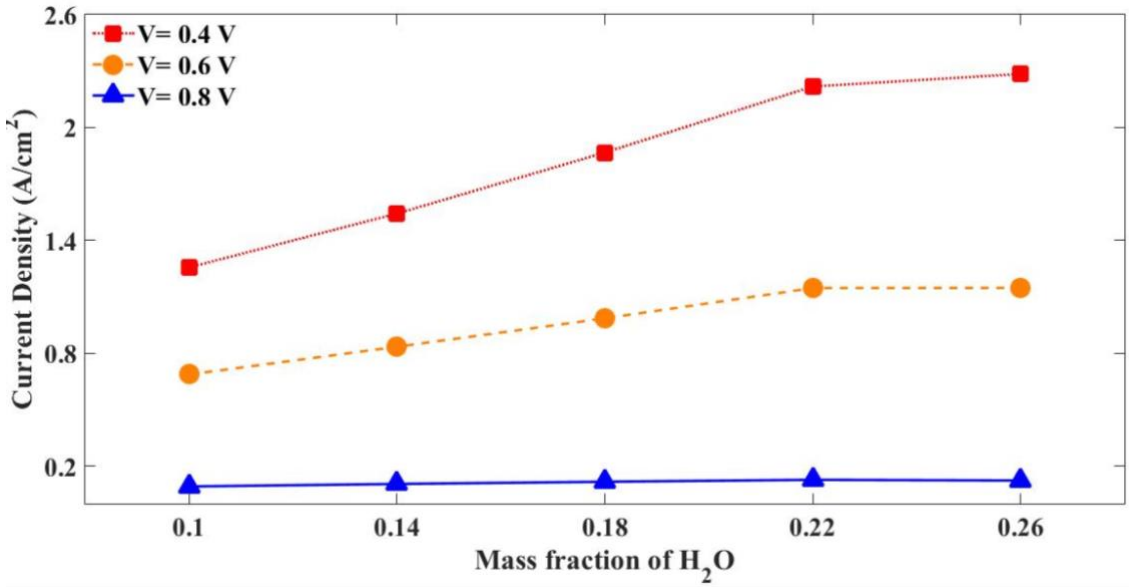

Figure 5: Change of current density for different mass fractions of water (cathode) at various cell voltages of 0.4-0.8 V

As illustrated in Figure 5, increasing water mass fraction until reaching a value of 0.22 enhances the current density remarkably at 0.4 and 0.6 V. However, the current density remains almost constant with further increase in hydrogen mass fraction at 0.6 V. The highest value of 2.28 A/cm^2 is obtained with water mass fraction value of 0.26 at 0.4 V. The results in Figures 3, 4 and 5 reveal that finding the optimal values for the mass fractions of anode and cathode gases is a key factor to improve PEMFC efficiency.

3.2 Optimization of Mass fractions of Gas Species

The calculated values of current densities and pressures for the cases with different mass fractions of gases at 4 V are given in Table 3. It is obvious from Table 3 that changing mass fractions of anode and cathode gases significantly affects the cell performance. Modifying oxygen and water mass fractions has nearly no significant impact on the pressure drop in the anode and cathode. However, increasing hydrogen mass fraction results in elevating pressure drop in the anode channel. The maximum pressure drop of 1.35 kPa is gained with hydrogen mass fraction value of 0.6 at 4 V. The results suggest that the influence of mass fractions of gas species on the current density is more dominant than that on the pressure drop.

Table 3: The calculated results for different mass fractions of gases at 4 V

Mass fraction of anode gases		**Mass fraction of cathode gases**		**Current density (A/cm^2)**	**Pressure drop (kPa)**	
H_2	**H_2O**	**O_2**	**H_2O**		**Anode**	**Cathode**
0.10	0.90	0.20	0.10	1.58	0.45	2.48
0.20*	0.80*	0.20*	0.10*	1.26	0.66	2.23
0.30	0.70	0.20	0.10	0.79	0.89	2.34
0.40	0.60	0.20	0.10	0.66	1.05	2.31
0.50	0.5	0.20	0.10	0.61	1.20	2.31
0.60	0.40	0.20	0.10	0.57	1.35	2.30
0.20	0.80	**0.10**	0.53	2.25	0.63	2.42
0.20	0.80	**0.12**	0.44	2.29	0.66	2.53
0.20	0.80	**0.14**	0.36	2.30	0.69	2.62
0.20	0.80	**0.16**	0.27	2.29	0.69	2.55
0.20	0.80	**0.18**	0.19	1.97	0.65	2.26
0.20	0.80	0.19	**0.14**	1.54	0.67	2.33
0.20	0.80	0.18	**0.18**	1.87	0.66	2.29
0.20	0.80	0.17	**0.22**	2.22	0.70	2.48
0.20	0.80	0.15	**0.26**	2.28	0.69	2.53

*Mass fractions of gases for the model

3. Conclusion

In this work, a three-dimensional single phase PEMFC model is developed to scrutinize the impact of varying mass fraction of hydrogen, oxygen and water (cathode side) on the cell performance. The findings are summarized as follows:

- Altering mass fractions of gases at the anode and cathode sides has a considerable impact on the cell power output.
- Decreasing hydrogen mass fraction and increasing water mass fraction lead to augmenting the current density at 0.4 and 0.6 V.
- The current density remains nearly unchanged with increasing oxygen mass fraction from 0.1 to 0.16 whereas further increasing oxygen mass fraction leads to reducing the cell efficiency at 0.4 and 0.6 V.
- There is not a significant impact of mass fractions of gas species on performance of PEMFC at 0.8 V.
- An increase in hydrogen mass fraction results in pressure drop in the anode whereas the pressure drop in the cathode remains nearly fixed for varying mass fractions of gases compared the model.
- The highest current density of 2.30 A/cm^2 is gained with 0.16 oxygen mass fraction and the current density increases by 82.5% compared to the model at 0.4 V.
- Optimizing mass fraction of anode and cathode gases is necessary to achieve better cell performance.

References

Ahmadi N., & Rostami S. (2019). Enhancing the performance of polymer electrolyte membrane fuel cell by optimizing the operating parameter. *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, 41, 220. https://doi.org/10.1007/s40430-019-1720-0

ANSYS FLUENT Fuel Cell Modules Manual, Release 14.0, ANSYS Inc., November 2011.

Barbir F. (2013). *PEM fuel cells: theory and practice*. Elsevier/Academic Press.

Spiegel C. (2008). *PEM fuel cell modeling and simulation using MATLAB.* Elsevier/Academic Press.

Biyikoglu A., & Alpat C. O. (2011). Parametric study of a single cell proton exchange membrane fuel cell for a bundle of straight gas channels. *Gazi University Journal of Science*, 24(4), 883–899.

Kahveci E. E., & Taymaz I. (2018). Assessment of single-serpentine PEM fuel cell model developed by computational fluid dynamics. *Fuel*, 217, 51-58. https://doi.org/10.1016/j.fuel.2017.12.073

Kaplan M. (2021). Numerical investigation of influence of cross-sectional dimensions of flow channels on PEM fuel cell performance. *Journal of Energy Systems*, 5(2), 137–148. https://doi.org/10.30521/jes. 871018

Mazumder S., & Cole J. V. 2003. Rigorous 3-D mathematical modeling of PEM fuel cells II. Model predictions with liquid water transport. *Journal of The Electrochemical Society*, 150(11), A1510-A1517. https://doi.org/10.1149/1.1615609

Ogungbemi E., Wilberforce T., Oluwatosin I., Thompson J., & Olabi A. G. (2021). Review of operating condition, design parameters and material properties for proton exchange membrane fuel cells. *International Journal of Energy Research*, 45(2), 1227-1245. https://doi.org/10.1002/er.5810

Salva J. A., Iranzo A, Rosa F., Tapia E., Lopez E, & Isorna F. (2016). Optimization of a PEM fuel cell operating conditions: Obtaining the maximum performance polarization curve. *International Journal of Hydrogen Energy*, 41(43), 19713-19723. https://doi.org/10.1016/j.ijhydene.2016.03.136

Subin K., & Jithesh P. (2018). Experimental study on self-humidified operation in PEM fuel cells. *Sustainable Energy Technologies and Assessments* 27, 17-22. https://doi.org/10.1016/j.seta.2018.03. 004

Song G. H., & Meng S. (2013). Numerical modeling and simulation of PEM fuel cells: Progress and perspective. *Acta Mechanica Sinica*, 29(3), 318–334. https://doi.org/10.1007/s10409-013-0037-y

Xing L., Shi W., Su H., Xu Q., Das P. K., Mao B., & Scott K. (2019). Membrane electrode assemblies for PEM fuel cells: A review of functional graded design and optimization. *Energy*, 177, 445-464. https:// doi .org/10.1016/j.energy.2019.04.084

Wang L., Husar A., Zhou T., & Liu H. (2003). A parametric study of PEM fuel cell performances. *International Journal of Hydrogen Energy*, 28(11), 1263–1272. https://doi.org/10.1016/S0360-3199 (02)00284-7

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*, 3, 178-203. https://doi.org/10.1016/j. mattod.2019.06.005

Wu H. W. (2016). A review of recent development: Transport and performance modeling of PEM fuel cells. *Applied Energy*,165, 81-106. https://doi.org/10.1016/j.apenergy.2015.12.075

Yang Y. Jia H., Liu Z. Bai N., Zhang X., Cao T., Zhang J., Zhao P., & He X. (2022). Overall and local effects of operating parameters on water management and performance of open-cathode PEM fuel cells. *Applied Energy*, 315, 118978. https://doi.org/10.1016/j.apenergy.2022.118978

Nomenclature

C	Molar concentration (mol/m^3)	σ	Electrical conductivity (1/Ωm)
D	Diffusion coefficient (m^2/s)	ϕ	Electric potential (V)
k	Thermal conductivity (W/mK)	*Subscript*	
P	Pressure (Pa)	*an*	Anode
R	Volumetric transfer current, A/m^3	*cat*	Cathode
S_h	Energy source term	*k*	Chemical species
S_k	Species source term	*mem*	Membrane
S_m	Momentum source term	*sol*	Solid
T	Temperature (K)	*Superscript*	
$\vec{u}$	Velocity vector (m/s)	*eff*	Effective
V_{oc}	Open-circuit voltage (V)	*Abbreviations*	
Greek letter		*CL*	Catalyst layer
ε	Porosity	*CFD*	Computational fluid dynamics
η	Overpotential (V)	*GDL*	Gas diffusion layer
μ	Viscosity (kg/ms)	*PEM*	Proton exchange membrane
ρ	Density (kg/m^3)		