

CFD MODELLING OF PEMFC: ROLE OF H₂ RECIRCULATION (vs) SERPENTINE FLOW CHANNEL

Abstract

The proton-exchange membrane fuel cell (PEMFC) is an alternative power source for transport applications. In this study, the performance of PEMFC is numerically analyzed for a wide range of operating temperature and pressure through 3D CFD simulations. The predicted current and power density profiles are analyzed to find the optimum operating conditions for the fuel cell operation (343 K, 1 atm). The PEMFC performance is further quantified by calculating its fuel utilization efficiency. Different bends are introduced to improve the performance of PEMFC serpentine channels. The optimum number of bends that support fuel utilization efficiency is identified. The importance of H₂ recirculation (0% and 5%) in single-channel fuel systems is addressed. It is found that H₂ recirculation (5%) significantly enhances the performance of PEMFC without an increase in the pressure drop.

Keywords: PEMFC, CFD, Hydrogen recirculation, Serpentine channel, water saturation.

1. Introduction

PEMFC is an alternative technology in the field of clean energy for sustainable power generation. These devices are powered by electrochemical reactions that convert gas reactants (hydrogen and oxygen) into electricity and water without harmful emissions Awan et al. [1]. The components of PEMFCs are electrolytes, electrodes, gas diffusion layers, and catalysts, Chen et al. [2]. The membrane has high proton conductivity and very low to zero electron conductivity for efficient operation of PEMFC. The anode side of the cell receives the hydrogen gas, which is catalytically converted into protons and electrons. These protons diffuse from the anode current collector to the cathode current collector through a membrane with high zero electron conductivity. The electrons move from the anode side to the cathode side via an external circuit for current production as per Wilberforce et al. [3].

Over the past decade, computational and experimental investigations have been reported on hydrogen recirculation in PEMFC. Hydrogen utilization is an essential aspect of PEM fuel cell operation. Incomplete fuel utilization or fuel consumption in the fuel cell leads to poor performance.

Iranzo et al. [4] developed a 3D model for fuel cells for various channel designs. Their numerical predictions are comparable with experimental data. They found that operating pressure significantly influences fuel cell performance.

Lu et al. [5] investigated the multiphase flow behavior in a PEMFC. They observed that the semi-slugs or slugs dominate at low superficial air velocities due to significant pressure fluctuations and flow maldistribution. At higher superficial gas velocities, mist flow is observed with a small amount of water build-up.

Le and Zhou [20] used a 3D PEMFC model with parallel and serpentine flow channels. They predicted the liquid interfaces by solving the continuity, energy, momentum, species transport, and electrochemistry equations through the volume of fluid (VOF) model. They observed that liquid formation inside the flow channel increases pressure drop and affects performance.

Hsieh et al. [19] analyzed the performance of PEMFC by varying the cell temperatures and mass flow rates of gaseous reactant streams. They found that the extent of water accumulation has a strong relationship with cathode side pressure drop and its magnitude.

Du et al. [10] characterized gas-liquid flow behavior in PEMFC using CFD through the VOF approach and found that surface contact angle changes the flow pattern.

Zhu et al. [36] studied the effect of flow channel wall wettability on the droplet flow behavior using the VOF model. They found that significant water removal occurs at the hydrophobic side of the wall with high-pressure drop.

Lu et al. [24] investigated the importance of surface contact angle on gas-liquid flow behavior in PEMFC. The performance of a hydrophilically coated gas channel is superior to that of a hydrophobic channel.

Ding et al. [7] analyzed the effect of gas-liquid flow patterns in PEMFC flow channels through CFD simulations using the VOF model. They observed droplet flow at the corner, film flow at the wall, annular flow, and slug flow.

Hashemi et al. [10] compared serpentine performance with straight-type fuel cells by incorporating non-isothermal effects in their CFD model. Hydrogen and oxygen mass fraction distribution is superior in the serpentine flow PEMFC.

Ding et al. [9] analyzed the performance of PEMFC using the VOF model. They found that hydrophobic membrane electrode assembly improves performance. Ding et al. [10] further analyzed parallel PEMFC and found that increasing the stoichiometric ratio of gaseous reactants cannot reduce gas flow maldistribution.

Heidary et al. [11] studied the impact of flow blockage on the performance of PEMFC using a 3D CFD model. The blockage in the channels redirects the flow of the species towards the GDL. This leads to an increase in the mass flow rate of the species towards the catalyst layer and improves the performance of the fuel cell.

Macedo-Valencia et al. [12] analyzed single-phase flow characteristics in a PEMFC through a CFD model. The species concentration was high at the inlet, and its magnitude decreased along the flow channels.

Jourdan et al. [13] investigated the effect of different membrane thicknesses on PEMFC performance using Multiphysics flow modeling software (COSMOL). They found that the thickness of the PEMFC significantly improves cell performance.

Awan et al. [14] developed an isothermal and non-isothermal model to characterize single-channel PEMFC. They found that operating pressure has a significant effect on current density profiles.

Omeiri and Laouar [15] analyzed flow patterns in PEMFC for various channel geometries and operating conditions. They found that current density and velocity profiles are parabolic in flow channels' anode and cathode sections. The maximum velocity and current density are at the center of the flow channel.

Yu et al. [30] used a peristaltic pump to enhance the performance of PEMFC. This pump reduces flooding compared to the dead-end operational mode of the fuel cell.

In most of the published literature, fuel utilization efficiency has been improved through geometry modifications (baffles, indentation) and by active recirculation of hydrogen. In the present work, a serpentine flow channel is used to improve the fuel utilization efficiency of PEMFC. The manuscript is organized by discussing fuel cell geometry in section 3. Following this, the simulation methodology is discussed in section 4. Subsequently, simulation predictions are analyzed in the results and discussion section in section 5. Finally, the crucial findings are summarized in section 6.

3. Geometry of PEMFC

The schematic representation of the PEMFC is shown in Fig. 1(a-b). The corresponding orthogonal view of the fuel cell is depicted in Fig. 2. The dimensions of the anode and cathode flow channels are 1 mm in width and 1 mm in height, with an overall length of the channel is 50 mm. The GDL (Gas Diffusion Layer), CL (Catalyst Layer), and membrane have a thickness of 0.125 mm, 0.05 mm, and 0.05 mm, respectively. The overall height of the flow channel is 0.25 mm, and the width is 5 mm. The geometry of the PEMFC is developed using Design Modular (version 22.1). Ansys meshing is used to generate the mesh for the simulation. The system's geometry is created using a sweep technique with a minimum edge size of 0.1 mm. The orthogonal quality is maintained between 0.95-1. Grid independence studies ensure that CFD predictions are not dependent on grid elements.

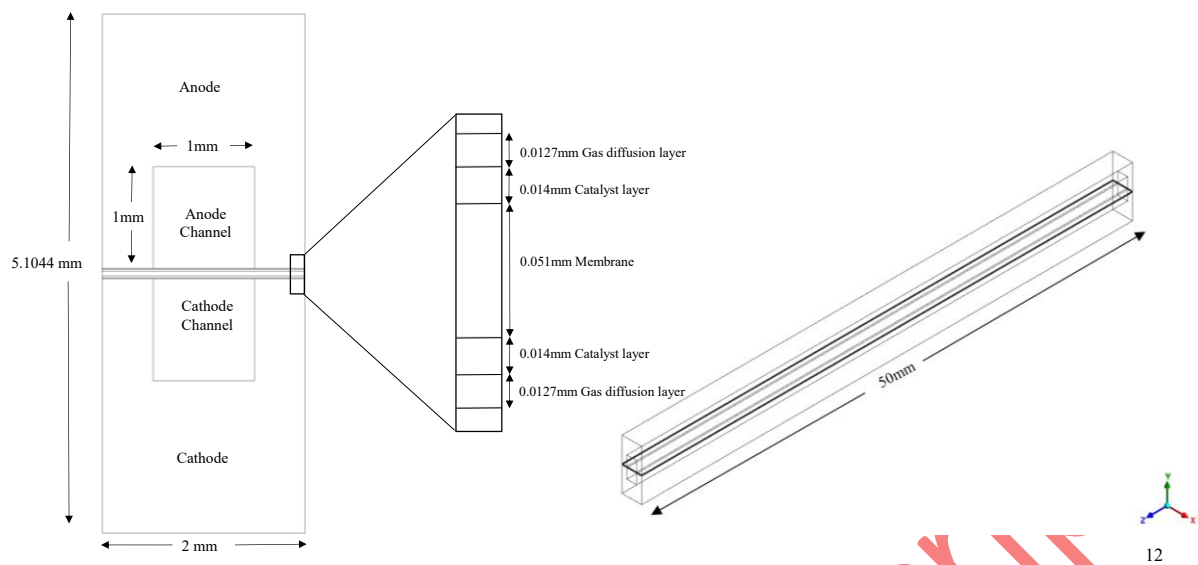


Fig 1. a) Schematic of PEM fuel cell

b) 3-D view of PEM fuel cell

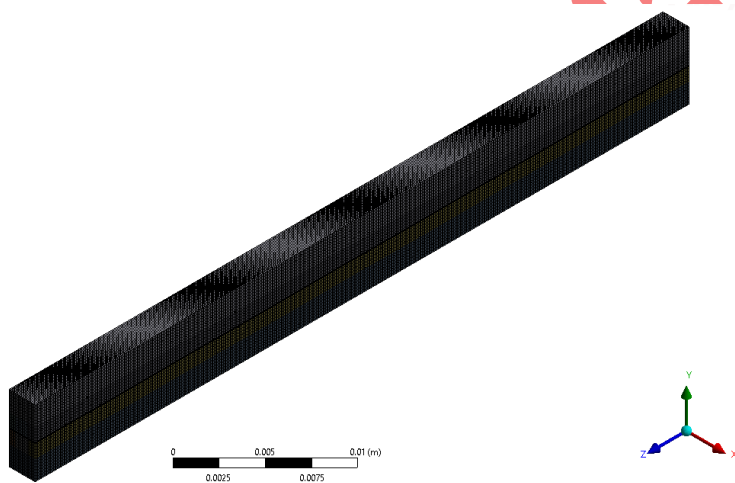


Fig 2. Adopted computational grid for PEM fuel cell

3. Methodology

3.1 CFD Modelling

The flow field in a PEMFC is analyzed by solving continuity, momentum, energy, and species transport equations. These equations are computed simultaneously with charge transport, such as the Joule heating reaction and Butler–Volmer and Nernst equations. The transport equations are ,

Continuity equation:

$$\nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

Momentum equation:

$$\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\mu^{eff} \nabla \vec{v}) + S_p \quad (2)$$

The porous media characteristics are incorporated through the source term (S_p),

$$S_p = -\left(\frac{\mu}{k}\right) \vec{v} \quad (3)$$

Species transport equation :

$$\nabla \cdot (\rho \vec{v} y_i) = -\nabla \cdot \vec{J}_i + S_i \quad (4)$$

The diffusive flux for the species i ($\vec{J}_i$) is obtained using,

$$\vec{J}_i = -\rho D_i \nabla y_i \quad (5)$$

Energy balance equation:

$$\nabla \cdot [\vec{v}(\rho E + p)] = \nabla \cdot (K_{eff} \nabla T - \sum_i h_i \vec{J}_i) \quad (6)$$

The transport equations and other details are obtained from the literature (ANSYS, FLUENT Theory Guide 2011). The performance of PEMFC is analyzed by calculating fuel utilization efficiency using (C. H. Woo and J. B. Benziger, 2007)

$$\beta_H = \frac{Q_{bulk,A}^{in} \cdot P_{H,A}^{in} - Q_{bulk,A}^{out} \cdot P_{H,A}^{out}}{Q_{bulk,A}^{in} \cdot P_{H,A}^{in}} \quad (V)$$

where, Q_A , is volumetric flow rate, m³/s, $Q_A = U_{bulk,A} A_A$, P_H is hydrogen partial pressure, $P_H = P_{abs} \chi_H$, P_{abs} , is absolute pressure Pa, U_{bulk} bulk velocity m/s, χ_H , mole fraction of hydrogen

3.2 Simulation Methodology

To characterize the performance of PEMFC, *3D steady state CFD simulations are performed using commercial software (Ansys CFD 2022V1) for a wide range of operating conditions.*

The reaction heating, Joule heating, Butler-Volmer rate, water transport of the membrane, and porous electrodes were considered in the CFD model. The velocity inlet boundary conditions (BC) are specified at the anode and cathode inlets for the gaseous reactants. The pressure outlet BC is imposed at the anode and cathode outlets. No slip BC is specified at the anode and cathode channel walls. The operating condition of PEMFC is reported in Table 1. The velocity is kept constant (0.2 m/s) at both anode and cathode inlets with the operating temperature (313-353 K), operating pressure (1 to 5 atm), and operating voltage (0.1 V to 0.9 V).

Table 1. Operating conditions for numerical simulation.

Parameters	Value	Unit
Anode Velocity	0.2	m/s
Cathode Velocity	0.2	m/s
H ₂ mass fraction at anode inlet	0.1-1	-
H ₂ O mass fraction at anode inlet	0.0, 9	-
O ₂ mass fraction at cathode inlet	0.18	-
H ₂ O mass fraction at cathode inlet	0.2	-
Anode/Cathode inlets temperature	313-353	K
Open circuit voltage	1.0	V

Operating Pressure	1 - 3	atm
Operating Voltage	0.1 - 0.9	V

The QUICK algorithm discretizes spatial and temporal derivative terms in the transport equations. The velocity and pressure are coupled through the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm. The convergence criteria (10^{-5}) are specified for all the dependent variables. The hydrogen recirculation is carried out by recirculating the outlet mass flow to the inlet of the PEMFC.

ξ. Results and Discussion

The flow characteristics in a PEMFC are numerically investigated using 3D CFD simulations. At first, the predicted contours of current density distribution at the interface between GDL and catalyst layer are analyzed for various operating pressures (1-3 atm). This is shown in Fig 3. Its magnitude is observed to increase with an increase in pressure. This is quantitatively analyzed through polarization curves. This is depicted in Fig 4. Three distinct regions characterize the polarization curve. The voltage drop is significant at low and high current density regions. Its value is moderate at moderate current density regions. As the operating voltage increases, the predicted current density increases, and its magnitude is found to be high (3.4 A/cm^2) when the operating voltage is 3 atm. At this condition, fuel utilization efficiency is calculated [48% (3 atm) and 33% (1 atm)], and it is found to be high at 3 atm. This is attributed to the increase in gaseous reactants' diffusion rate into the catalyst layer and cell performance. This is further analyzed by computing the power density for various operating pressures. This is depicted in Fig 5. The predicted power density is high at 0.9 V and 3 atm. Hence, this condition is considered an optimum for the operation of PEMFC.

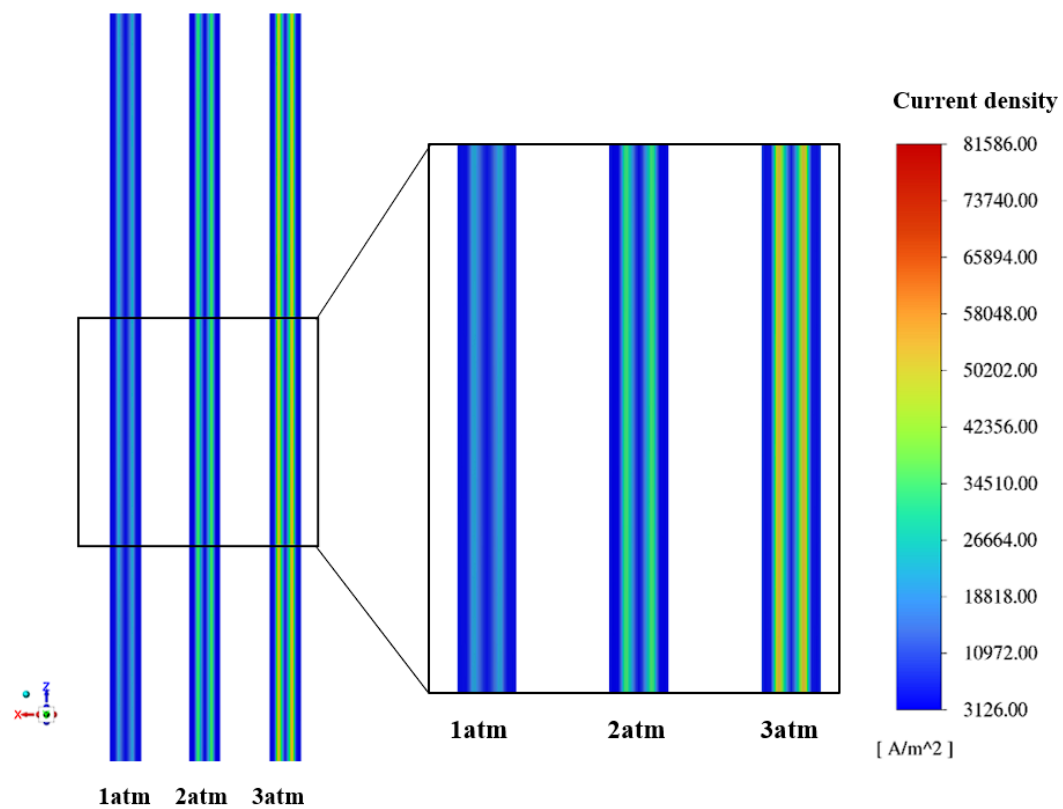


Fig 3. Effect of operating pressure on current density distribution at GDL/Catalyst interface

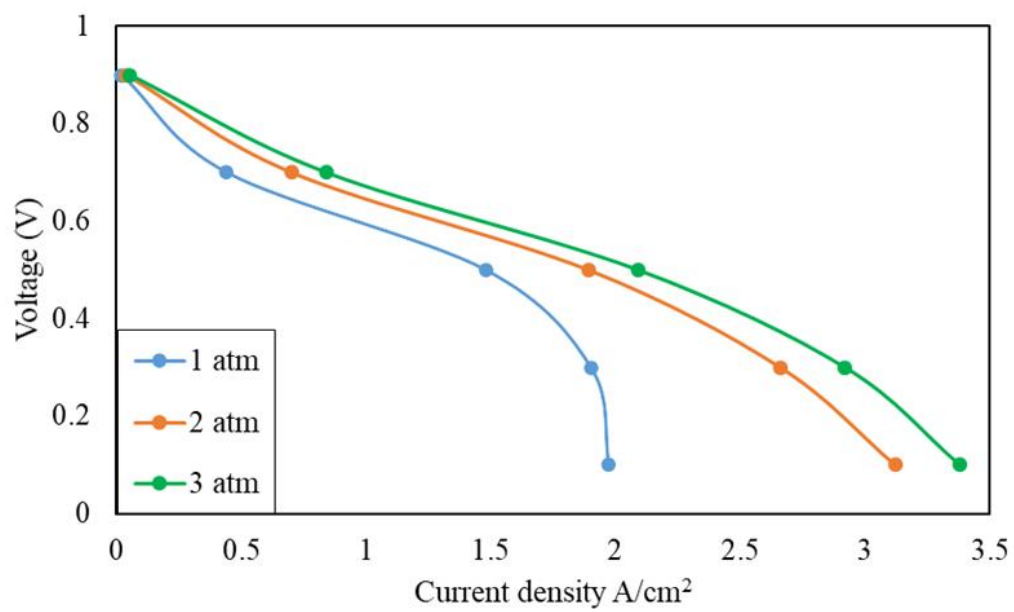


Fig 4. Effect of operating pressure on Polarization curve

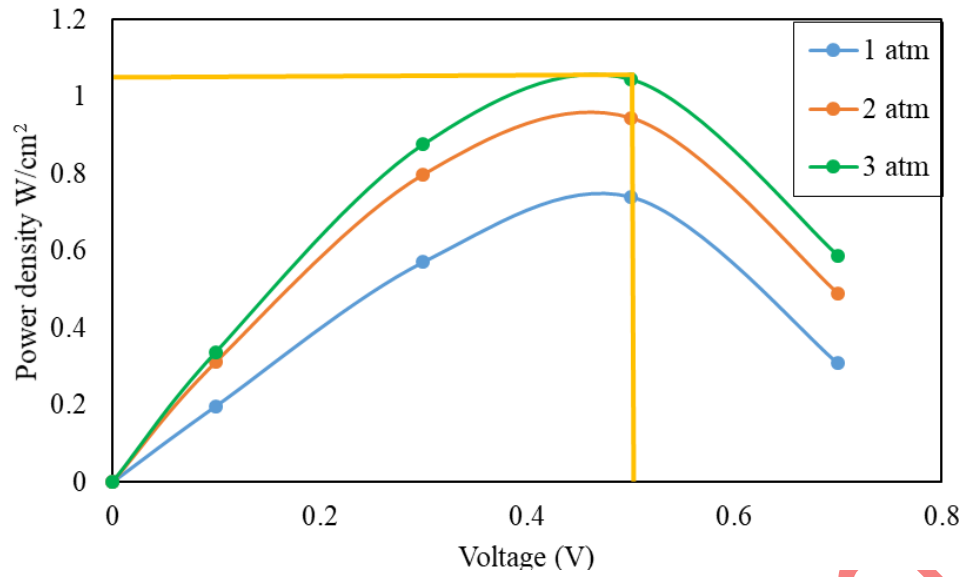


Fig 9. Effect of operating pressure on power density curve

Further, the influence of operating temperature on cell performance is investigated. The operating temperature has been varied from 313 K to 333 K while maintaining a constant pressure of 3 atm and keeping other parameters unchanged. The predicted polarization and Power density curves are shown in Fig 6 and Fig 7. The current and power density magnitude is observed to be high at 333 K (optimum). At this temperature (333 K), the reaction kinetics are significantly improved, and hence, the power output of PEMFC is high (48 %) at 0.5 V (operating voltage).

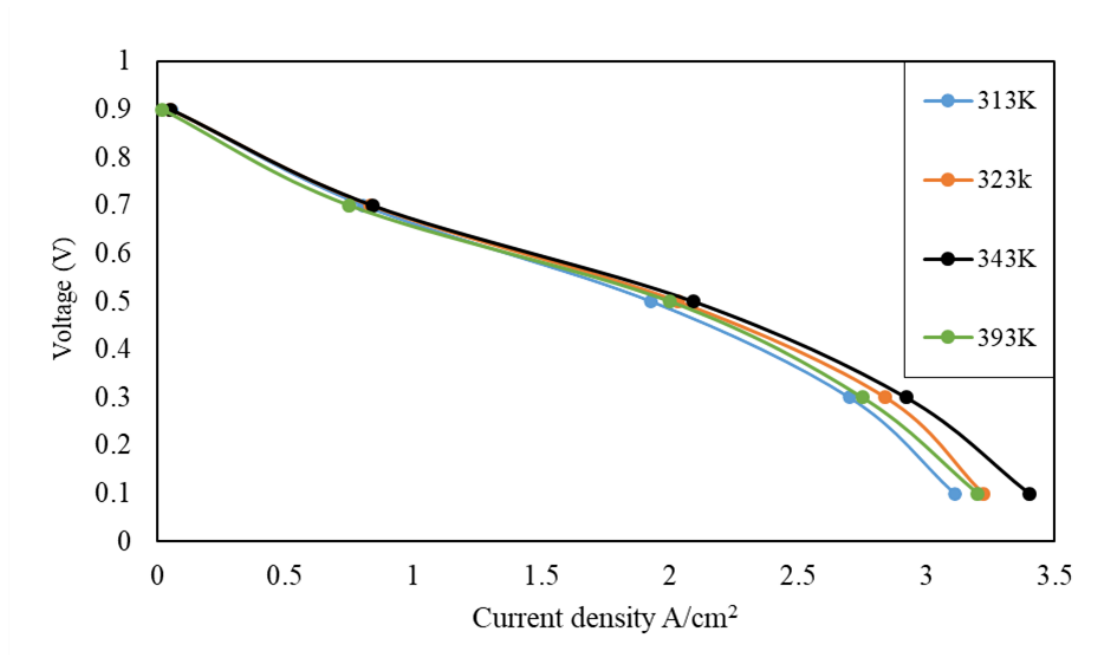


Fig ٦. Effect of operating temperature on Polarization curve

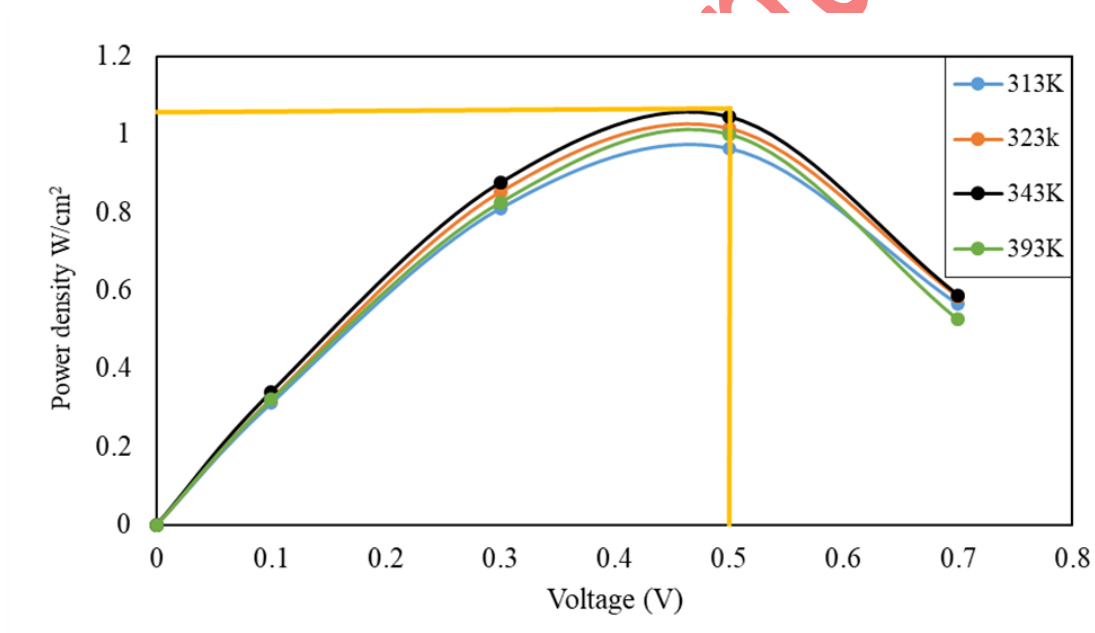


Fig ٧. Effect of operating temperature on power density curve

To find an optimum feed composition, the mass fraction of hydrogen (anode inlet) is varied, and its effect on the power density, power density, and fuel utilization efficiency are analyzed ($P = ٣ \text{ atm}$ and $T = ٣٤٣ \text{ K}$). This is shown in Table ٧. Its effect on the magnitude of current and

power density is insignificant. However, it significantly affects fuel utilization efficiency. Its value is found to be high when the mass fraction ratio of H_2 to H_2O is 0.2:0.8 (optimum)

Table 3. Effect of mass fraction on the performance of PEMFC

Mass Fraction $H_2 : H_2O$	Fuel utilization (%)	Current density (A/cm ²)	Power density (W/cm ²)	Pressure drop (pa)
0.2:0.8	56.62	2.17	1.080	2.6
0.4:0.6	52.06	2.21	1.100	2.4
0.6:0.4	48.22	2.24	1.120	2.4
0.8:0.2	43.32	2.18	1.090	2.2
1.0:0.0	39.41	2.10	1.000	2.2

To improve the performance of PEMFC, various inlet configurations such as convergent-divergent and divergent are proposed and compared with straight channel inlets, as depicted in Fig 8. The calculated current and power density are analyzed. This is shown in Table 3. The magnitude of current and power density is observed to be almost identical. However, these modifications affect the fuel utilization efficiency with increased pressure drop values for the proposed inlet configurations, such as convergent-divergent and divergent. Hence, instead of using different inlet configurations at the inlet of the fuel cell, geometric modifications at the flow channel of the fuel channel were proposed (i.e., serpentine channel) to improve the cell performance.

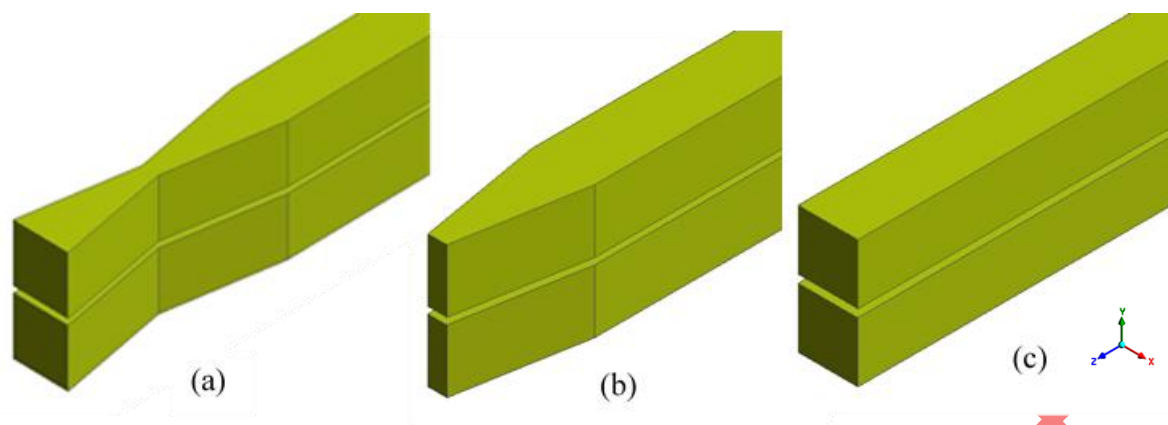


Fig 8. Geometric modification at the inlet of PEMFC with (a) Convergent divergent (b) Divergent (c) Straight

Table 3. Effect of different inlet configuration on performance of PEM fuel cell

Inlet configuration	Fuel utilization (%)	Current density (A/cm ²)	Power density	Pressure drop (pa)
Convergent divergent (0.0 mm)	48.25	2.23	1.115	2.08
Divergent (0.0 mm)	48.27	2.21	1.105	2.07
Straight (0.0 mm)	48.22	2.24	1.120	2.04
Convergent divergent (1.0 mm)	96.41	2.27	1.135	3.25
Divergent (1.0 mm)	96.47	2.28	1.140	3.24
Straight (1.0 mm)	96.35	2.26	1.130	3.21

CFD simulations were performed at an optimum operating condition (343 K, 1 atm) by maintaining the flow channel length as 0.0 cm with five, seven, and nine bend configurations. The schematic of the proposed design configurations is depicted in Fig 9. The predicted

contours of velocity magnitude for the corresponding design configuration are shown in Fig 10. It is observed that the magnitude of velocity is high for the flow channel with nine bends. To quantify this, predicted polarization and current density curves are analyzed. This is shown in Fig 11 and Fig 12. The current and power density magnitude is high when nine bends are used. This is further verified by calculating fuel utilization and pressure drop. This is reported in Table 4. The fuel utilization efficiency of reactant gases is high when a flow channel with nine bends is used. This is due to increased gaseous reactant residence time over the catalyst layers and for electrochemical reactions. Thus, the proposed design configuration supports improving the cell performance. It has also been noticed that serpentine channels cause a considerable pressure drop in comparison with straight channel PEMFC. In addition, serpentine flow channels lead to water formation at the cathode side of the flow channel. The predicted contours of water saturation at the cathode side of the flow channel (Fig 13) and at the GDL/CL interface (Fig 14) are analyzed. The water formation is observed to occur near the bends of the serpentine flow channel and accumulates over the period. Thus, there is an increase in the magnitude of pressure drops in the fuel cell.

Table 4. Effect of serpentine flow channel configuration on performance of PEMFC

Channel Type	Fuel utilization (%)	Current density (A/cm ²)	Power density	Pressure drop (pa)
Straight	41.22	2.24	1.120	2.04
Channel with 5 bends	52.00	2.31	1.190	2.27
Channel with 7 bends	59.62	2.43	1.280	2.40
Channel with 9 bends	60.62	2.72	1.360	2.74

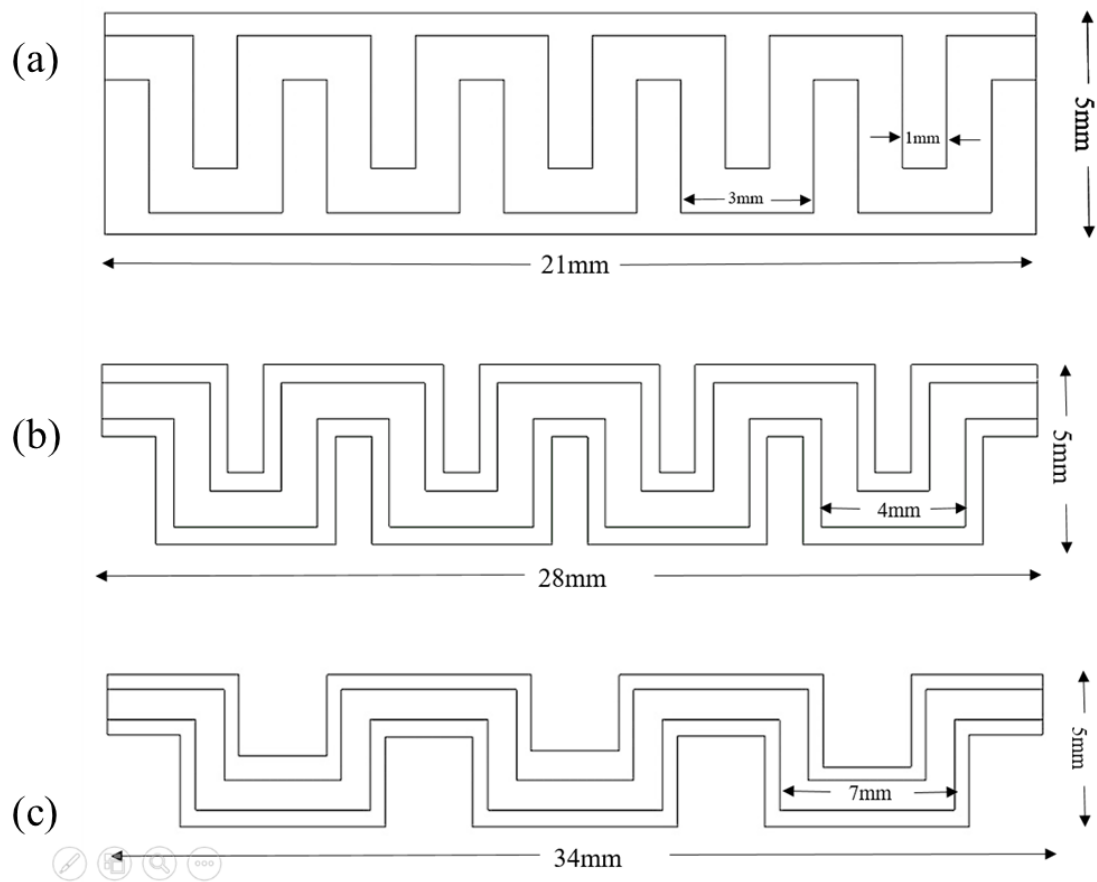


Fig 9. Schematic of serpentine flow channel with (a) 90° bends (b) V bends (c) U bends

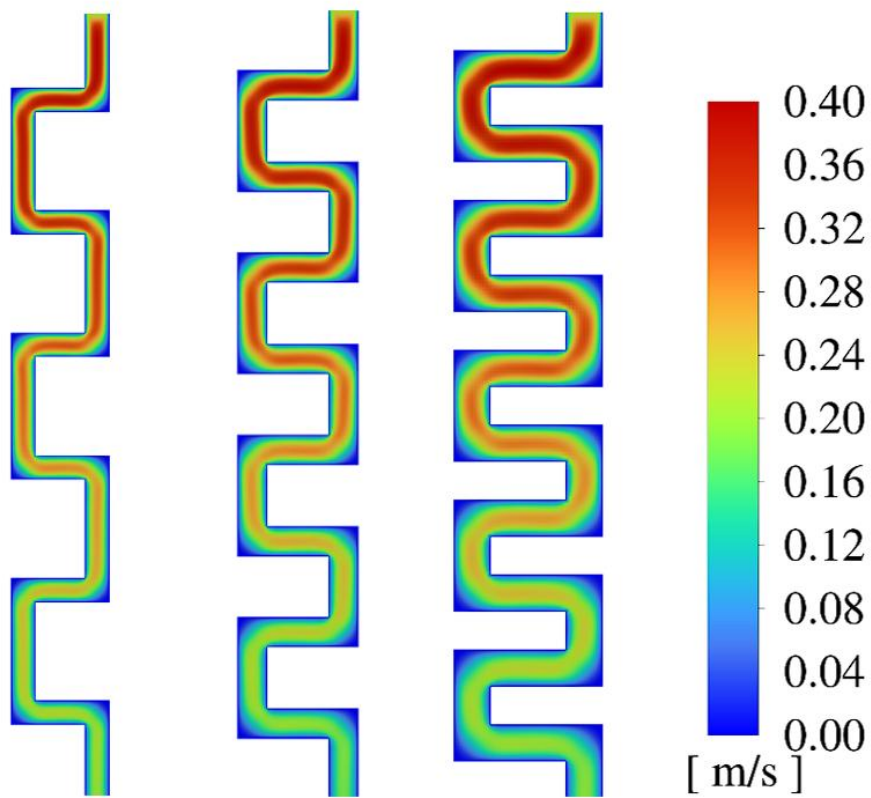


Fig 10. Contours of velocity magnitude for serpentine channel flow configuration

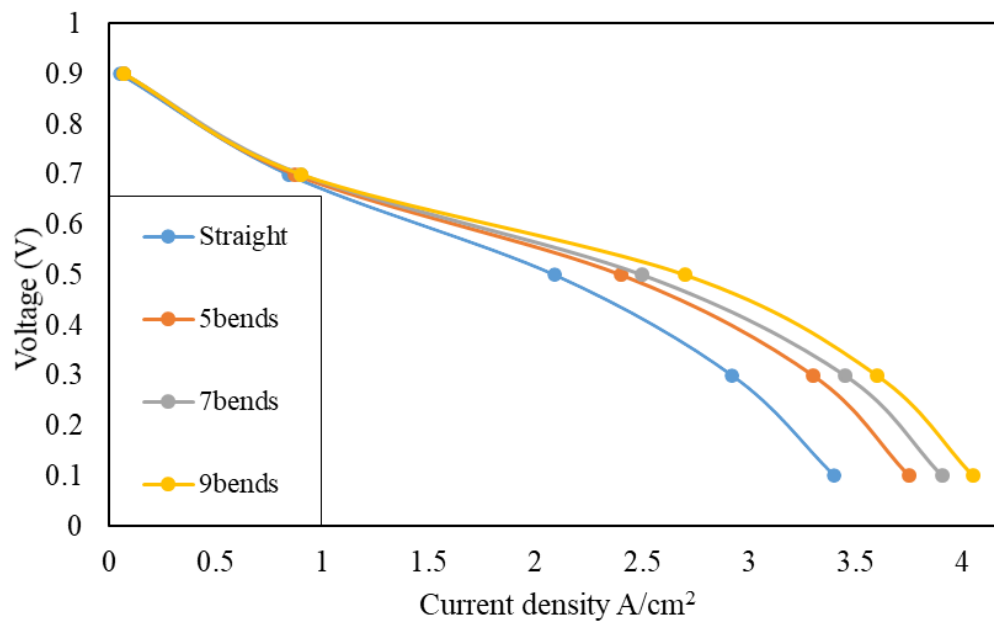


Fig 11. Effect of serpentine channel flow configuration on polarization curve

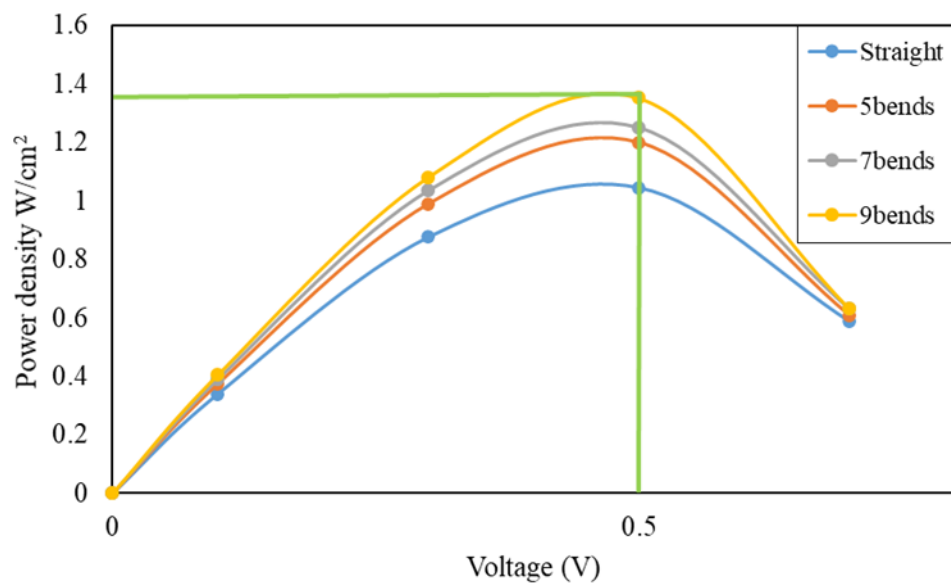


Fig ١٢. Effect of serpentine channel flow configuration on power density curve

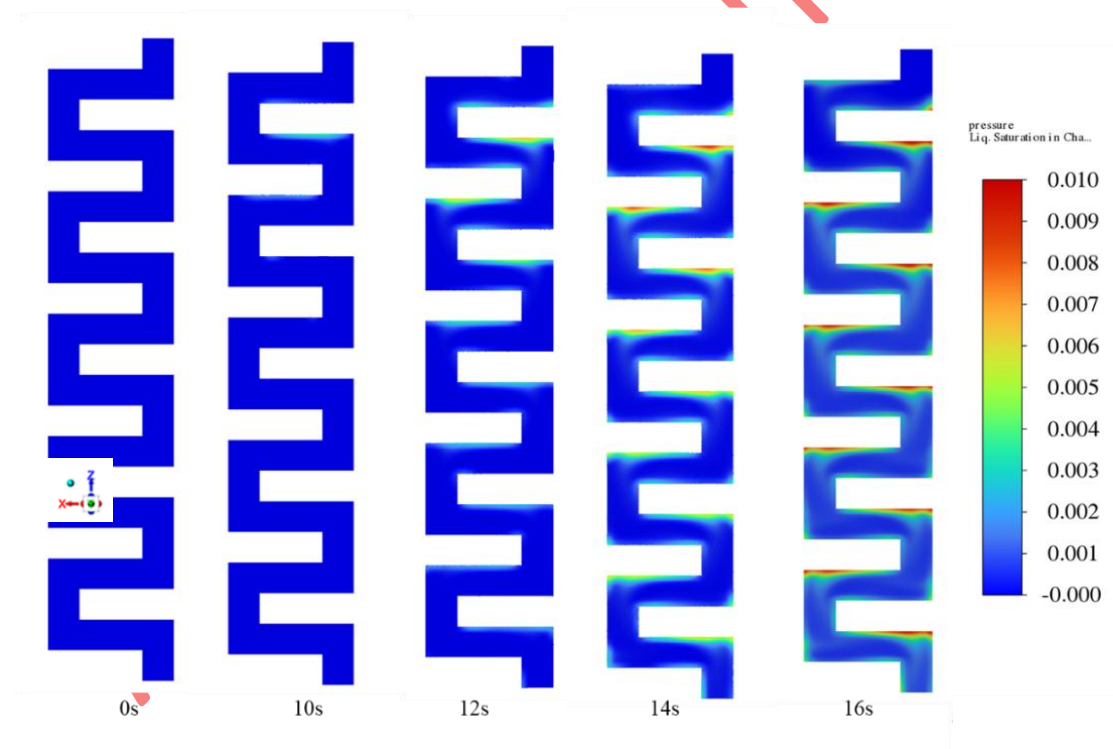


Fig ١٣. Contours of water saturation inside the nine-bend serpentine cathode flow channel

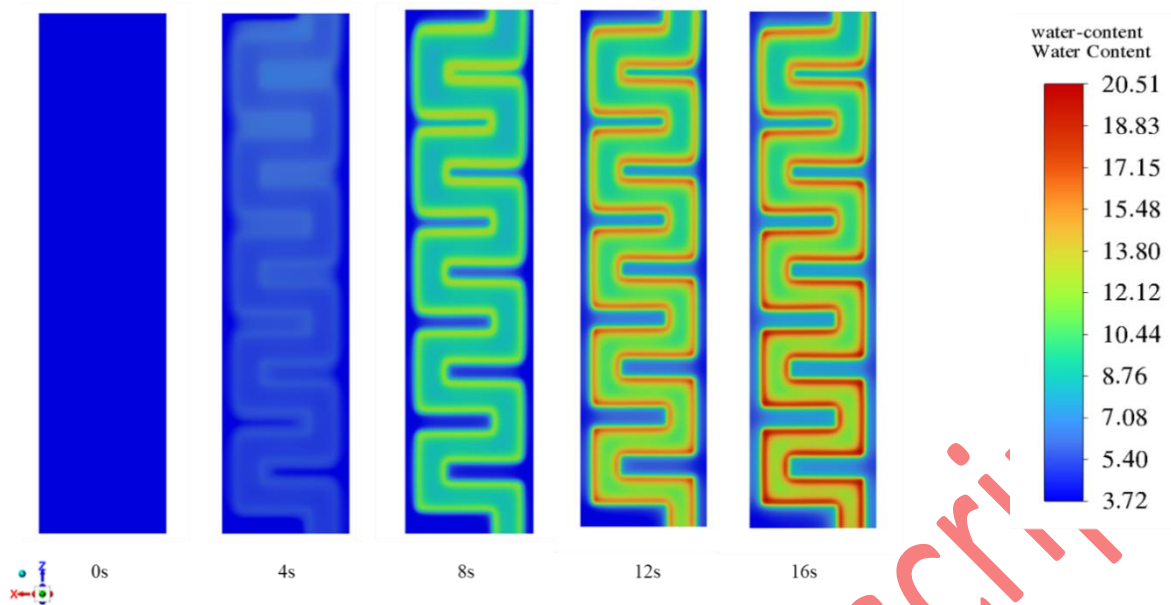


Fig 14. Contours of water content in GDL/CL interface of serpentine channel with nine bends

To overcome this problem and enhance the performance of PEMFC, a fraction of hydrogen from the outlet of PEMFC is recirculated. The proposed hydrogen recirculation system is depicted in Fig 15. The percentage of hydrogen recirculation is varied (20 to 30 %), and the current density distribution at the GDL/Catalyst interface is shown in Fig 16. The predicted current density is observed to be high with the H₂ recirculation system. This is due to the proposed design configuration maintaining a significant amount of H₂ at the anode side of PEMFC. It is quantitatively analyzed by calculating fuel utilization efficiency and pressure drop. This is depicted in Table 6. The calculated utilization efficiency is high when using a straight-channel fuel cell with a recirculation system. Also, the magnitude of pressure drop is observed to be less in comparison with serpentine flow channels (nine bends). This is due to the H₂ recirculation system allowing the amount of fuel at the anode side of the fuel cell and transport of reactants to the catalytic sites, which support increasing reaction rates, hence improving system performance. Therefore, PEMFC with a hydrogen recirculation system is a necessary design configuration to enhance fuel cell performance without increasing pressure drop values.

Table 9. Effect of hydrogen recirculation on the performance of PEMFC

Channel Type	Fuel utilization (%)	Current density (A/cm ²)	Power density	Pressure drop (pa)
Straight	48,22	2,24	1,120	2,04
Straight Channel with 20 % recirculation	56,51	2,31	1,152	2,30
Straight Channel with 30 % recirculation	61,60	2,41	1,345	2,48
Channel with 9 bends	60,62	2,72	1,360	2,74

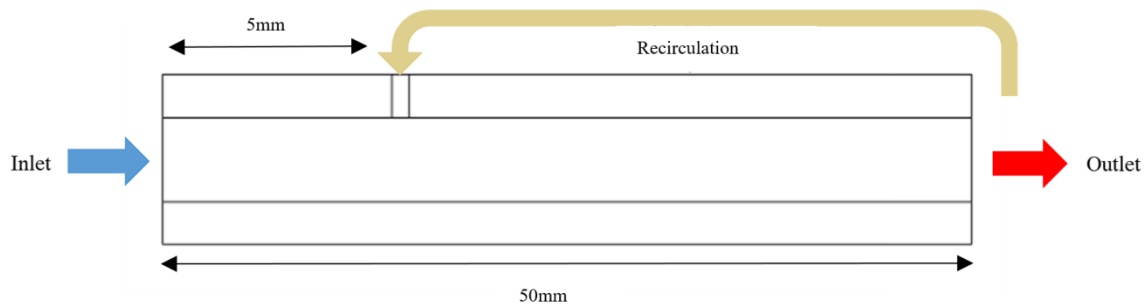


Fig 10. Proposed hydrogen recirculation system in straight channel PEMFC

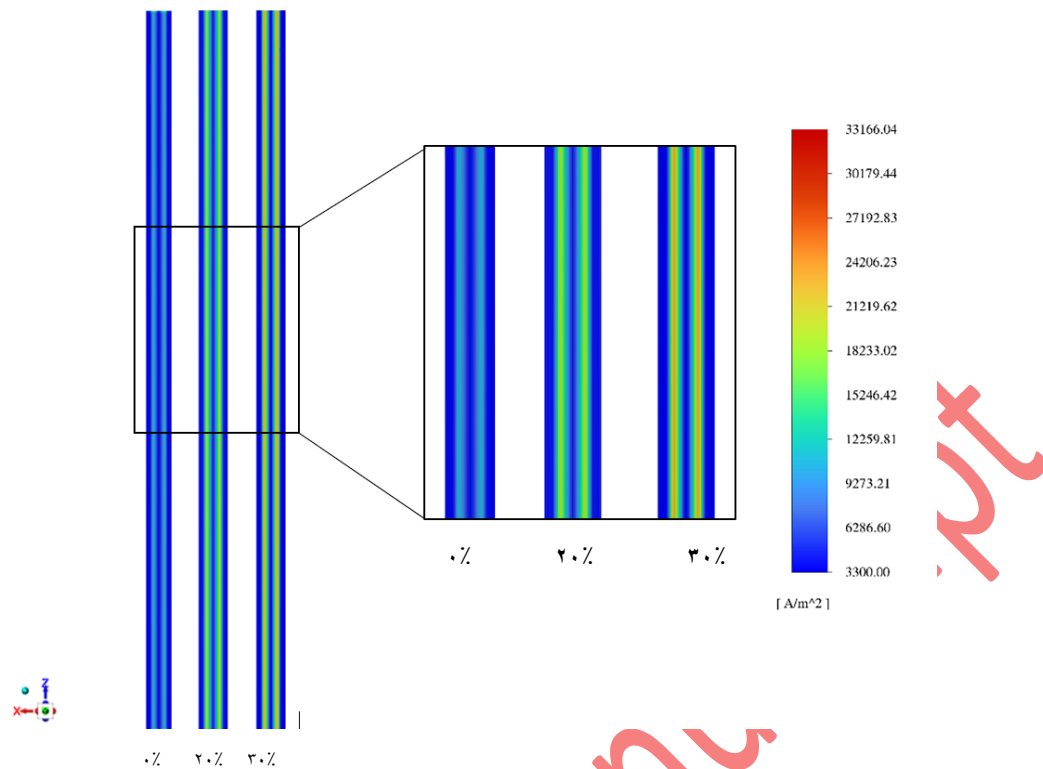


Fig 16. Contours of Current density distribution at GDL/Catalyst interface at different Recirculation

9. Summary and Conclusions

The performance of fuel cells is investigated numerically using CFD. The simulations are performed for a range of operating conditions. The power density and polarization curves are analyzed to find an optimum condition (343 K and 3 atm) for the operation of PEMFC. To enhance the performance of PEMFC, the geometry of the flow channel is modified as a serpentine configuration with bends (five, seven, and nine). The simulation predictions are compared with straight-channel fuel cells. The serpentine flow channel with nine bends increases the cell performance by 14% compared to the straight flow channel. This is due to the rise in residence time of gaseous reactants in the fuel cell. However, these serpentine channels cause a considerable increase in pressure drop. To overcome this, H₂ gas leaving from the fuel cell has been recirculated into the flow channel. The performance of the hydrogen recirculation system is comparable with that of the serpentine channel configuration and offers less pressure drop. Hence, the hydrogen recirculation fuel cell system improves fuel cell performance.

Nomenclature

$\frac{\partial C}{\partial z}$	concentration gradient
C_{cl}	concentration in catalyst layer
$C_{channel}$	concentration in channel
S	cross sectional area
ρ	density of the gas
D_i	diffusion coefficient of species i
$\vec{J}_i$	diffusive flux of species i
D	Diffusion coefficient, $m^2 s^{-1}$
K_{eff}	effective conductivity
K	Effective conductivity, $W m^{-1} K^{-1}$
μ^{eff}	effective viscosity (gas mixture)
h	Enthalpy, J
j	Exchange current density, $A m^2$
F	Faraday constant, $96,485 C mol^{-1}$
J	Flux diffusion, $kg m^2 s^{-1}$
μ	gas viscosity ($kg m.s^{-1}$)
L	length of conductor
y	Mass fraction species
K	Permeability (catalyst layers & gas diffusion layers)
k	Permeability, m^2
p	Pressure, Pa
r	resistivity
p	static pressure

S_m	source term
S_i	source term for species i
T	Temperature, K
δ_{gdl}	thickness of gas diffusion layer
E	total energy
R	Transfer current, A m^{-3}
R	Universal gas constant, $8.314 \text{ J K}^{-1} \text{ mol}^{-1}$
$\vec{v}$	velocity of gas
v	Velocity, ms^{-1}
a	Water activity

Greek letters

$\emptyset$	Cell potential, V
γ	Concentration coefficient
ρ	Density, kg m^{-3}
μ	Dynamic viscosity, $\text{kg m}^{-1} \text{ s}^{-1}$
σ	Electric or ionic conductivity, $\text{ohm}^{-1} \text{ m}^{-1}$
η	Over-potential, V
α	Transfer coefficient
λ	Water content

Subscripts/superscripts

an	Anode
ca	Cathode

eff	Effective
m	Mass
mem	Membrane
p	Porous
ref	Reference
sol	Solid

Conflict of Interest

The authors declare no competing financial interests.

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Excel Source Data for Figures

Fig ٤: Effect of operating pressure on Polarization curve

Voltage (V) vs Current density (A/cm ²) data			
Voltage (V)	1 atm	2 atm	3 atm
0.1	1.974	3.12	3.38
0.3	1.902	2.66	2.92
0.5	1.48	1.89	2.09
0.7	0.44	0.7	0.84
0.9	0.018	0.038	0.053

Fig 5: Effect of operating pressure on power density curve Voltage (V) vs Power density (W/cm ²) data			
Voltage	Current density for 0 bends	Current density for 2 bends	Current density for 3 bends
0	0	0	0
0.1	0.370	0.390	0.40
0.3	0.99	1.030	1.08
0.5	1.2	1.20	1.30
0.7	0.609	0.63	0.63

*in (W/cm²)

Fig 6: Effect of operating temperature on Polarization curve Voltage (V) vs Current density (A/cm ²) data						
Voltage (V)	313K	323K	333K	343K	353K	393K
0.1	3.11	3.22	3.2	3.4	3.37	3.2
0.3	2.7	2.84	2.9	2.92	2.93	2.70
0.5	1.927	2.03	2.08	2.09	2.1	2
0.7	0.806	0.834	0.84	0.84	0.80	0.70
0.9	0.056	0.0520	0.053	0.053	0.054	0.02

Fig 7: Effect of operating temperature on power density curve Voltage (V) vs Power density (W/cm ²) data						
Voltage (V)	313K	323K	333K	343K	353K	393K
0	0	0	0	0	0	0
0.1	0.311	0.322	0.33	0.34	0.337	0.32
0.3	0.81	0.802	0.87	0.876	0.879	0.820
0.5	0.9630	1.010	1.04	1.040	1.00	1
0.7	0.0642	0.0838	0.088	0.088	0.090	0.020

Fig 11: Effect of serpentine channel flow configuration on polarization curve Voltage (V) vs Current density (A/cm ²) data			
Voltage (V)	0 bends	2 bends	3 bends
0.1	3.70	3.90	4.0

٠,٣	٣,٣	٣,٤٥	٣,٦
٠,٥	٢,٤	٢,٥	٢,٧
٠,٧	٠,٨٧	٠,٩	٠,٩
٠,٩	٠,٠٧	٠,٠٧	٠,٠٧

Fig ١٢: Effect of serpentine channel flow configuration on power density curve Voltage (V) vs Power density (W/cm ^٢) data			
Voltage (V)	١ atm	٢ atm	٣ atm
٠	٠	٠	٠
٠,١	٠,١٩٧٤	٠,٣١٢	٠,٣٣٨
٠,٣	٠,٥٧٠٦	٠,٧٩٨	٠,٨٧٦
٠,٥	٠,٧٤	٠,٩٤٥	١,٠٤٥
٠,٧	٠,٣٠٨	٠,٤٩	٠,٥٨٨