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Optimization of Tapering Angle of Flow Channels of Pemfuel Cell: A Numerical Study

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Abstract

Proton Exchange Membrane Fuel Cells (PEMFCs) are essential for the efficient operation of hydrogen-powered automobiles. In order to improve their performance, the researchers have proposed tapered flow channels as a possible solution. However, determining the optimal value for the tapering has not been explored in depth. In this work, a numerical investigation is conducted to optimize the tapering of tapered serpentine channels in PEMFCs. The results obtained show that while anode channel tapering has a negligible effect on performance, cathode channel tapering has a significant impact. The study finds that a flow channel geometry with an inlet of 0.8 mm and an outlet of 0.2 mm, with a gradual decrease in cross-section results in the maximum net output, with a 10.64% increase in net power output at 0.7 V. Additionally, the improved water management performance is observed. Based on these findings, tapering flow channels only on the cathode side could be utilized as an optimal design for achieving a higher performance. Overall, this study is significant as it provides valuable insights into optimizing the performance of PEMFCs, which can enhance their efficiency and utilization in hydrogen-powered vehicles. It highlights the importance of investigating the effects of flow channel geometry on performance, and can guide future research works in this area to improve the efficiency of PEMFCs.

Keywords: *Proton exchange membrane fuel cell, flow channel, tapered channels, optimization of flow, numerical analysis.*

1. Introduction

The vehicle business is moving at a furious pace these days. The automotive industry faces two major challenges: growing global warming and the concern of conventional energy supplies, such as crude oil, natural gas, and coal, being depleted. Electrification of car power trains using non-conventional or renewable energy sources is one of the most notable solutions to these difficulties. It can be accomplished in two ways. The first are battery-powered electric vehicles, while the second are fuel-cell-powered electric vehicles. The vehicle is suited for passenger cars in the event of battery-powered electric vehicles. However, due to the weight of the battery pack, it is not a viable solution for transportation, sea travel, or the aviation industry. PEMFC is preferred as an automotive power unit in fuel cell vehicles due to its higher efficiency, good transient qualities, and quick start-up properties. However, low power density and high flammability of hydrogen, as well as storage concerns, are the key roadblocks to bringing this technology to the automobile sector. Furthermore, hydrogen PEMFC cars necessitated the construction of a large and entirely new infrastructure for hydrogen replenishment and production. As a result, implementing hydrogen-powered vehicle technology is complicated and time-consuming. As a result, it is critical that PEMFC be as efficient as feasible [1].

Designing efficient flow channels is one of the areas where PEMFC performance may be improved. Thermal and water management, as well as pressure drop throughout the channels, are all factors that can be used to assess the efficiency of a flow channel design. The even distribution of reactants is dependent on the pressure drop in flow channels. In some cases, if the pressure drop is large enough, the fuel cell will run out of fuel. As a result, low pressure causes poor performance. In some circumstances, external pumping was required to solve the problem.

In the numerical investigations done on various channels, single serpentine channel design exhibited the best thermal, water and gas management as well as stack performance. But, pressure drop was high across it [2,3]. The single serpentine channel found to have higher power output with more pressure drop compared to double and triple serpentine channels whereas the performance in thermal, water and gas management were best in the case of single channel [4,5].

Hence, single serpentine channel proved to be best till now. In addition to that, providing a tapering angle to single serpentine channels improves performance. Tapering angle on cathode side on simple 2D model of PEMFC improved fuel cell performance at lower voltages also [6]. Similarly, Perng et.al employed a baffle plate in the channel and utilized a 2D half-cell model to replicate the findings. The application of a tapering angle to flow channels resulted in a greater fuel flow velocity and, a higher pressure drop. A considerable localized increase in current density was found at the baffle plates. Additionally, the pumping power required for baffle plates was determined to be greater. [7].

C. Wang *et al*. evaluated the effect of tapering a serpentine channel numerically and experimentally by lowering the height of the gas channel from 1 mm to 0.5 mm and reducing the number of channels by one at each turn towards the exit. Tapering increased the performance in high current density locations. Good water removal qualities were also discovered as a result of the enhanced flow velocity [8].

R. Ram Kumar *et al*. conducted a 5-hour experiment on serpentine and tapered channels, demonstrating that the maximum performance rose by 17% in the polarization curve for the tapered channel. After utilizing tapering to serpentine channel for 0.5 V loading, a 15% increase in current was also obtained [9].

In PEMFCs, the auxiliary devices like compressor and cooler are used to attain the inlet reactant condition. So, the net power outcome from PEMFC is power generated minus power required to run auxiliary devices. The compressor is used to get the air inlet flow at required pressure. When pressure of air is increased, the temperature is also getting increased. Thus to decrease the temperature, a cooler has to be used. From the outlet of the channel, some amount of energy can be gained back with the help of the turbine. Thus, the primary objective of this work is to get the optimized tapered angle to minimize penalties. Additional power required to run the auxiliary devices is the penalty to the performance [10].

Hence, net power output becomes:

$$\mathbf{Power_{Net} = Power_{Total} - Power_{Parasitic}} \tag{1}$$

$$\mathbf{Power_{Total} = I_{avg} \times V_{cell} \times A_a} \tag{2}$$

$$\mathbf{Power_{Parasitic} = P_c - P_t + P_{cool}} \tag{3}$$

There are three distinct regions of polarization curve of PEMFC, based on the causes of potential loss, as follows:

1. Activation polarization region (energy absorbed by electrochemical reactions happening at catalyst surface).
2. Ohmic polarization region (potential drop due to ohmic resistances of various parts of fuel cell, i.e. bipolar plates, GDLs, CLs catalyst layers and membrane).
3. Concentration polarization region (Potential drop caused by lesser diffusion of reactant in GDL due to water flooding).

The activation polarization area is determined by the catalyst material. The design of reactant flow channels has a significant impact on the ohmic and concentration polarization areas [11]. The beneficial impact of a tapering angle applied to channel geometry on the second and third regions is obvious from the literature, but the negative effect on pressure drop cannot be overlooked.

Serpentine channel shape is the best due to improved water management, current density, and power generation. Yet, it has a detrimental influence on pressure drop across the channel. Thus, to overcome this drawback, literature may be used to understand the qualitative influence of tapering angle on performance. However, there is a limited quantity of material available in the field of quantitative effect.

Excessive tapering might also result in a higher pressure decrease [12]. Thus to compensate for channel pressure losses, the tapering angle should be optimized in order to produce the maximum net power.

2. Methodology

The ANSYS Fluent simulation programme is utilized to simulate the tapered geometries. The PEMFC add-on module in Fluent allows the users to simulate the PEMFC for a variety of geometries and boundary conditions. The boundary conditions for each simulation are kept similar to keep all simulations on the same footing. Therefore, it is possible to compare the change in simulation output for a single change in geometry. The flowchart of steps involved in this study is given figure 1.

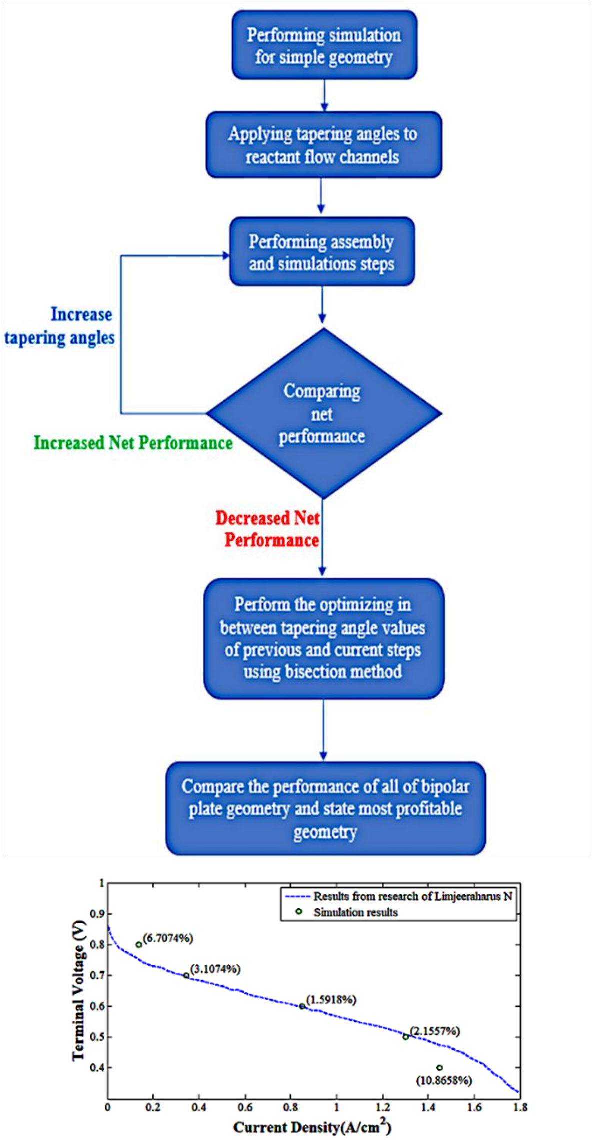


Figure 1. Process of optimizing the tapering angles of both reactant flow channels of PEMFC.

2.1. Description of the steps involved in optimizing tapering angle of flow channel

1. Firstly, the simulation of the geometry without tapering is done and results are obtained.
2. Then the tapering angle of flow channels is increased such that outlet heights of channels are decreased by 0.2 mm, and the assembly and simulation steps are carried out.
3. The results of current steps are compared with the previous step results. If net performance increases, then again, the second step is carried out as performance can still be increased or if net performance decreases, it indicates that the optimized tapering angle value is in between values taken for the previous step and current step.
4. Then the optimization step is carried out between these two values by using the bisection method approach. Bisection method is a mathematical method for getting the root of the equation, when there is one root in a given interval. No. of iterations required to achieve required tolerance $\varepsilon = 1$ mm and ε_0 (initial interval) = 2 mm are,

$$n = \log_2\left(\frac{\varepsilon_0}{\varepsilon}\right) = \log_2\left(\frac{2}{1}\right) = \log_2(2) = 1 \quad (4)$$

Thus accuracy of answer, i.e. optimized channel outlet thickness is 1 mm.

These steps are carried out for two cases, tapering of both anode-cathode flow channels and tapering on only cathode side.

2.2. Modelling of geometries

For the development/construction of geometry, CAD software CATIA (Computer Aided Three-Dimensional Interactive Application) has been used in this work. The following geometric parameters are constant for every geometry in this study:

Table 1. Model geometry dimensions (common for all geometries).

	Parameters	Ref.
1.	L = 24.8 mm, B = 23.6 mm	[3]
2.	D_{bp}= 1.6 mm	
3.	D_{ci} = 0.8 mm	
4.	D_{gd} = 0.19 mm	
5.	D_{cat} = 0.015 mm	
6.	D_m = 0.05 mm	

The values of the flow channel tapering angle are modified on these geometries, and then the assembly phase for new components is completed. The impact of changing the tapering angle of channels on the anode-cathode side and just on the cathode side on the performance of PEMFC is then calculated using this redesigned assembly.

2.3. Procedure to apply tapering angles to both reactant flow channels

For providing tapering angles to the flow channels, Pocket up to plane operation in CATIA software is used. The steps involved are as follows:

1. Set the channel inlet and outlet heights, for which the tapering angle is to be determined.
2. Determine the tapering angle value for whole channel by using following formula.

$$\text{Tapering angle} = \tan^{-1}\left(\left[\frac{\text{difference in heights of channel at inlet and outlet}}{\text{Total length of channel}}\right]\right)$$

3. Create a line, which is making required angle with reference horizontal line.
4. Create a plane passing through that line.
5. Draw the top view of geometry of flow channel in XY plane.
6. Perform Pocket operation on geometry up to newly created plane for bipolar plates.
7. Use Fill command in ANSYS Design-modeler to model flow channels.

2.4. Validation

The present work outcomes are compared with the literature in this stage. The parameters of the numerical study might be altered after validation to conduct future research.

For validation, Nuttapol Limjeerajarus, *et al.* (2015) work has been considered as a reference. Numerical validation is carried out using identical geometry and boundary conditions. The simulation findings closely match this study for a 1.1 stoichiometric ratio of reactants. The polarization curve produced in prior study is validated in Figure 2. In terms of the root mean squared error of current density at various terminal voltages, the value is 5.999%, which makes the CFD model considered to be sufficiently accurate [3].

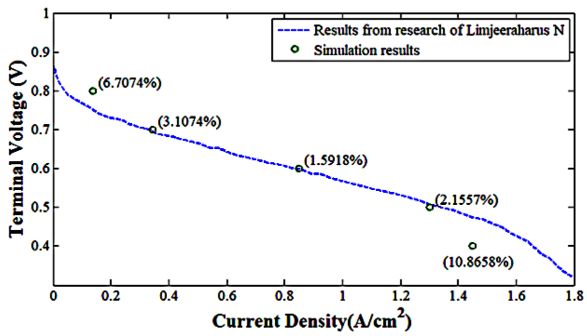


Figure 2. Model validation by comparing simulated results with the research carried out by Nuttapol Limjeerajarus, *et al.* (2015).

2.5. Gird independence and iterative independence

The geometry is studied both using grid and in iterative independence measures. Figure 3(a) shows that the results with the required accuracy were obtained by using 7 divisions of the components of the MEA.

The errors in the case of simulation with 7 number of divisions of components of MEA with respect to simulation with 8 number of divisions is 0.44769%, which can be considered as negligible for grid independence. Iterative independence can be observed from Figure 3(b), after 5000 iterations the change in the results with respect to the result of 10100 iterations is 1.668%. After performing these studies, the finalized mesh is shown in Figure 4.

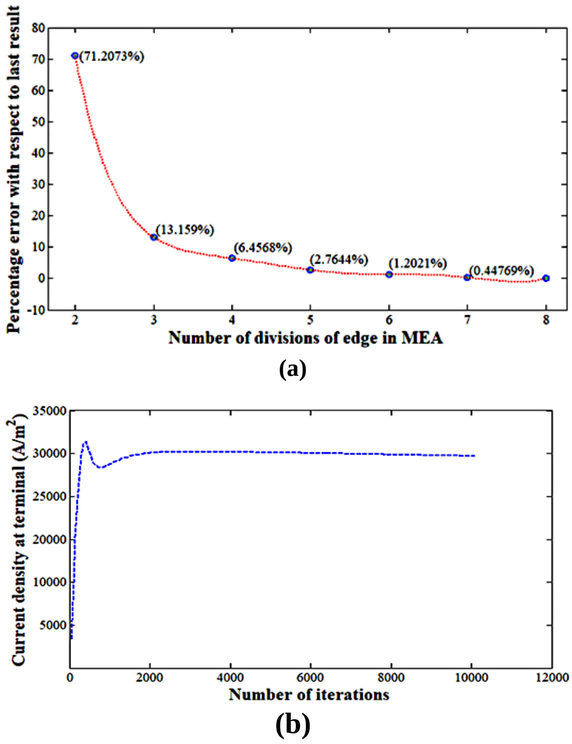


Figure 3. (a) Grid independence study and (b) Iterative independence study at 0.5 V.

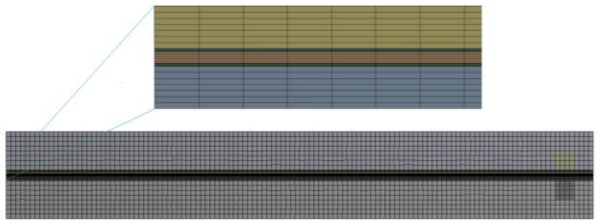


Figure 4. Structured meshing of PEM Assembly after grid independence.

2.6. Simulation of tapering channel geometries

After validation, the validated CFD model is used further. PEMFC add-on module in ANSYS Fluent is used for numerical study. The assumptions considered are as follows:

1. The fuel cell is operated at isothermal condition (333 K).
2. The reactant gases behave as ideal gases.
3. The flows of reactant gases are laminar, steady, and incompressible, and impurities are neglected.
4. Materials of catalyst layer, gas diffusion layer, and proton exchange membrane are isotropic.

5. Contact resistance between two layers is negligible.
6. For all solid boundaries, no slip boundary condition is maintained.
7. The effect of gravity on fuel cell operation is neglected.

The values of material properties of all components of PEMFC used in study are listed in table 2.

PEMFC efficiency improves as the working temperature rises. However, drying of the proton exchange membrane is a possibility at high temperatures. Consequently, ohmic losses increase, and performance suffers. To solve these issues, the fuel cell was operated at a higher temperature with 100% humidified reactants. The parameters and boundary conditions, which are used in the simulation of PEMFC geometries, are listed below in the table 3.

Table 2. Material properties used in the numerical study.

Properties	Catalyst and GDL	Current collector	Membrane	Tab	Units	Ref.
Density	2719	2719	1980	2719	kg/m^3	[13]
Specific heat	871	871	2000	871	$J/(kg \times K)$	
Thermal conductivity	10	100	2	202.4	$W/(m \times K)$	
Electrical conductivity	5000	1×10^6	10^{-16}	3.541×10^7	$1/(\Omega \times m)$	
Porosity	0.5	-	-	-	-	
Permeability	10^{-12}	-	-	-	m^3	

Table 3. Parameters used in the numerical study.

Parameters	Location	Value	Units
Operating pressure		2	bar
Operating temperature		60	℃
Fuel cell current density		1	A/cm^2
Reactant flow rate	Anode channel	3 times stoichiometry	kg/s
	Cathode channel	3 times stoichiometry	kg/s
Relative humidity		100	%
Open circuit voltage		1.19	V
Voltage at tab	Anode	0	V
	Cathode	0.3-1.1	V
Reference current density	Anode	10,000	A/cm^2
	Cathode	20	A/cm^2
Reference concentration	Anode	1	$kmol/m^3$
	Cathode	1	$kmol/m^3$
Concentration exponent	Anode	0.5	-
	Cathode	1	-
Exchange exponent	Anode	1	-
	Cathode	1	-
Reference diffusivity	-	3×10^{-5}	-
Membrane Equivalent weight	-	1100	$kg/kmol$
Membrane Protonic conduction coefficient	-	1	-
Membrane protonic conduction exponent	-	1	-
Surface to volume ratio of catalyst layer	Both-catalyst layers	1.127×10^7	m^2/m^{-3}

Simulations are preceded by the SIMPLE algorithm to solve the CFD model. Navier-Stokes equations, Maxwell-Stefan equation, Darcy law, charge balance equation, Butler-Volmer equation, and conservation equation of water saturation are employed in the analysis. Too many equations increase the complexity of the CFD model. This may lead to divergence in solution. Thus the under-relaxation factors for all equations are kept 0.8 at the starting of the simulation [14]. After 500 iterations, those factors are increased to attain convergence at a faster rate. The solution is considered as converged, when the residues of all the equations are reached to the value 10^{-6}. From the research work of R. Ram Kumar *et al*., it can be seen that the effect of tapering of the channels is maximum at 0.5 V loading voltage. Thus the geometries of tapered channel PEMFC are simulated at 0.5 V [9]. After finding optimized tapering angle, the whole polarization curves for PEM fuel without tapered channel and with optimized tapered channel are drawn.

3. Results and discussion

The numerical study's results are assessed by taking into account elements such as reactant species consumption, current density, net power production, water content, liquid saturation, and reactant velocity in reactant flow.

3.1. Consumption of reactant species

The consumption of hydrogen and oxygen in a Proton Exchange Membrane Fuel Cell (PEMFC) is calculated by analyzing the concentration of species at each outlet. It has been observed that the species consumed by the PEMFC increases as the flow channel is tapered. Figure 5 illustrates the difference in consumption when both the anode and cathode sides are tapered compared to when there is no tapering at anode or tapering at cathode alone. The results obtained show that hydrogen consumption decreases significantly when only the cathode side is tapered, whereas oxygen consumption remains similar in both cases.

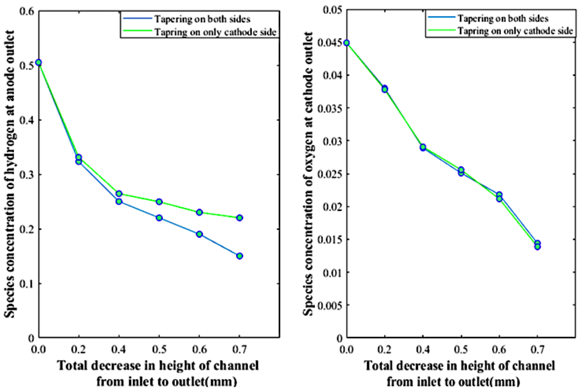
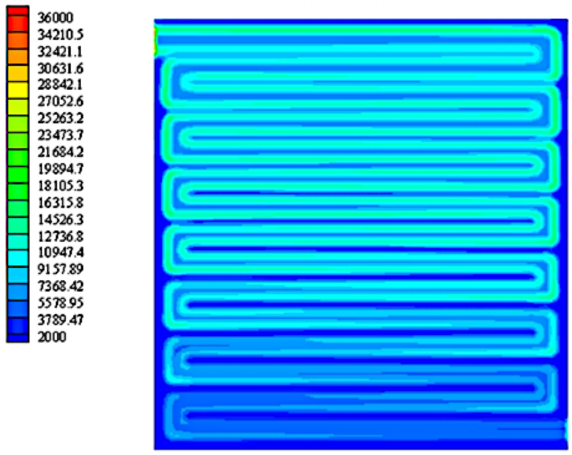


Figure 5. Species concentration of hydrogen and oxygen at anode and cathode outlet respectively at 0.5 V.

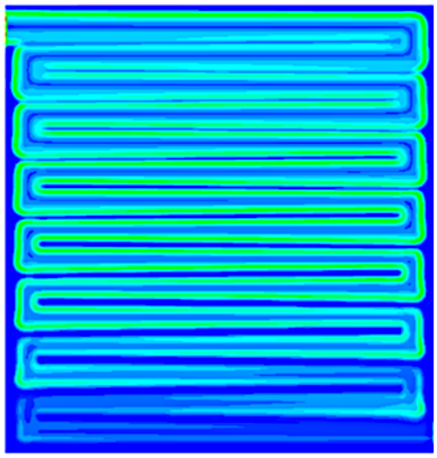
Increasing the tapering angle on the cathode side resulted in increase in hydrogen consumption up to 0.4 mm decrease in channel height at outlet. However, after this point, while consumption continued to increase, the rate of increase decreased. Conversely, tapering on the anode side also increased consumption but it led to more pumping losses due to the narrowing of flow channels. Therefore, to effectively calculate the effect of tapering on net power, only the tapering on the cathode side was considered for further analysis. The benefits of tapering in enhancing species consumption are evident but it iss crucial to consider the cost of pumping losses as well. To fully comprehend this trade-off, refer to Figure 8.

3.2. Current density

The contours of the Figure 6 (a & b), shown that tapered channel PEMFCs have a higher current density distribution than non-tapered ones, resulting in a higher power output. The tapered channel design increases the consumption of species in the electrochemical reactions, leading to higher current density. This is because the tapered channel design promotes a more uniform distribution of the reactants, allowing for more efficient and effective electrochemical reactions.
Towards the end of the flow channel, the increase in current density with tapering can observed. This is because the tapered channel design leads to a lower concentration of residual species in the flow channel. As species are consumed in the electrochemical reactions, there are fewer residual species available down the line in the channel, which limits the additional current that can be generated. Thus tapered channel designs can lead to higher current density and power output.



(a) No taper



(b). 0.6 mm decrease in height of channel (tapering of only cathode channel)

Figure 6. Contours of current density (A/cm^2) at the interface of cathode catalyst layer and gas diffusion layerat 0.5 V.

3.3. Pressure drops and net power output

As the tapering angle increases, the flow channel becomes narrower. Due to decrease in cross-section area of flow channel, the flow velocity of reactant increases. Resultantly, higher pressure drop is observed for tapering channels. From Figure 7, the trend of increasing pressure drop with higher tapering of flow channels can be observed. To counteract the higher pressure drop, higher power will be required to run the compressor. This adversely affects the net power output of the fuel cell.
Figure 8 depicts the values of produced power and net power output for two cases: tapering on both sides and tapering exclusively on the cathode side. The power output is increased in both cases as tapering of channels is increased. The power

required to run auxiliary devices is also continuously increasing with increasing tapering of channels. At higher tapering, the pressure drop is observed to be increasing exponentially. Therefore, the rate of increase in net power is observed to be decreased at higher tapering angle of channels.

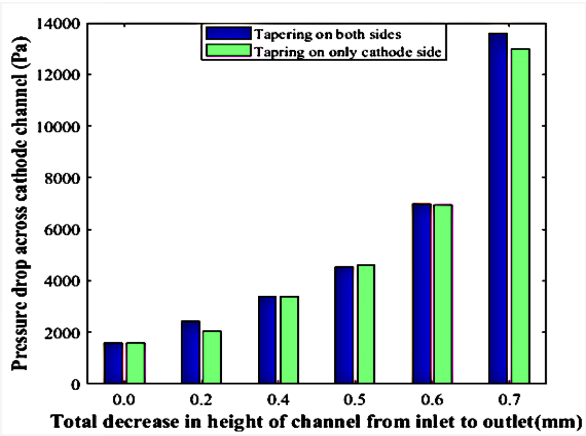


Figure 7. Pressure drops (Pascal) across cathode channels at 0.5 V.

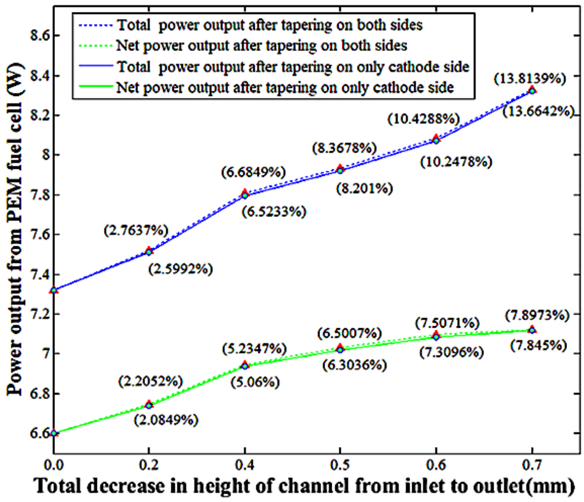
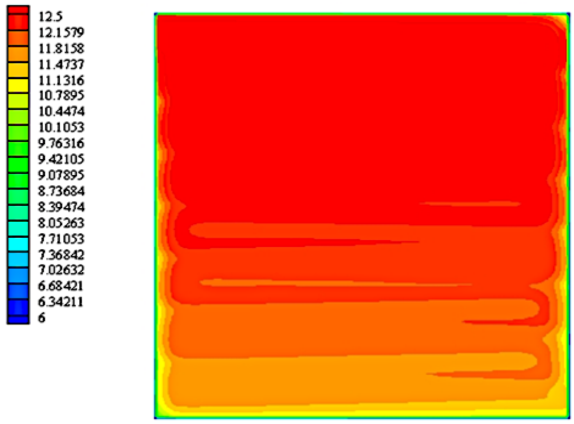


Figure 8. Power outputs (W) from PEMFCs at 0.5 V.

According to methodology, the outlet height of the channel is decreased in steps of 0.2 mm. After performing three steps, i.e. 0.6 mm decrease in channel height from inlet to outlet, further decrease of 0.2 mm is not possible as total thickness is 0.8 mm. At the third step, the increase in net power is significant. Thus to get optimized tapering angle, according to the bisection method, the next step should be performed with halving the step interval. Thus the step decrease in height becomes 0.2/2 = 0.1 mm. Therefore, simulations for 0.5 mm and 0.7 mm decrease in channel height from inlet to outlet are carried out. Comparing 0.5 mm and 0.6 mm decrease in height, simulation for the case of 0.6 mm decrease shows higher net output, while for 0.7 mm decrease in height, the increase in net power is less than 0.5% compared to that of the case of 0.6 mm decrease. Thus 0.6 mm decrease in flow channel height is observed to give best performance. Also, the difference in performance improvement in the case of tapering on both sides i.e. anode-cathode side channels and that of the case of tapering on only cathode side channel is observed to be less than 0.5% in all cases, which can be considered to be negligible.

3.4. Water content and liquid saturation

For the membrane's longevity, it is important to keep the water content consistent. However, high water content, particularly14 units of saturation, causes water flooding, which reduces the PEMFC's power output [15]. As tapering is applied to flow channels, the maximum value of water content decreases while uniformity increases, as indicated by the contours in figure 9. Because the cross section area is reduced, the flow velocities rise. As a result, the water is washed away with the reactant flow, and there is minimal water build-up.

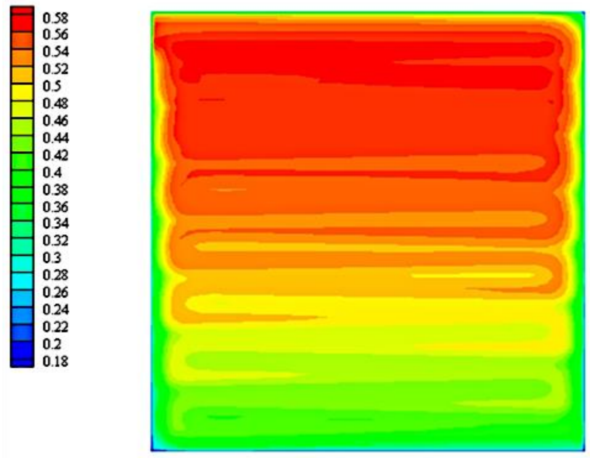


(a) No taper

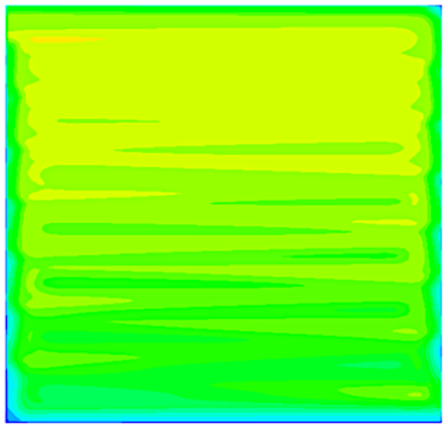
(b). 0.6 mm decrease in height of channel (tapering of only cathode channel)

Figure 9. Contours of water content (%) at the interface of cathode catalyst layer and membrane at 0.5 V.

Another important aspect of PEMFC water management is liquid saturation. The higher the liquid saturation, the more channels will be flooded. As a result, reduced liquid saturation is sought for improved performance over lengthy periods of time. The lower value of liquid saturation is found for tapered shape in the contours illustrated in Figure 10.



(a) No taper



(b). 0.6 mm decrease in height of channel (tapering of only cathode channel)

Figure 10. Contours of liquid saturation at surface of gas diffusion layer at 0.5 V.

3.5. Velocity of reactant flow

The velocity of reactant flow increases as the tapering angle increases. This has a positive impact on liquid saturation and water content [16]. Simultaneously, it has a negative impact on the gas diffusion layer's durability. GDL is eroded when velocity rises owing to increased shear forces on the GDL surface [17–19] . As a result, a trade-off between gas diffusion layer velocity and durability must be made.

Figure 11 shows the value of maximum velocities for various tapering geometries. At 0.7 mm decrease in channel height from inlet to outlet, the maximum value of velocity is around 45 m/s, which is unfavorable for durability of gas diffusion layer [18], whereas, for 0.6 mm decrease in height, maximum velocity is around 28 m/s, which would have less impact on erosion of GDL.

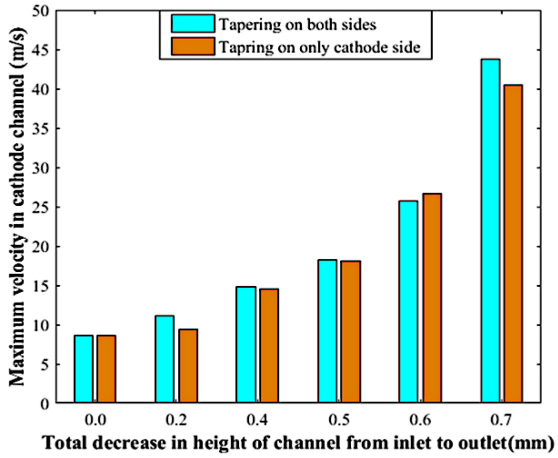


Figure 11. Maximum magnitude of flow velocity (m/s) across cathode channels at 0.5 V.

3.6. Polarization characteristics

Figure 12 shows the polarization and power density curves for a PEMFC with no taper channels and an optimal tapering configuration (0.6 mm drop in channel height from intake to outlet) based on the preceding comparisons [20]. With the narrowing of channels, the concentration loss region has expanded, as has the power density. The graph shows how fuel usage has improved when current density has increased.

As a result, channel tapering is shown to increase performance when compared to a PEMFC with no taper, particularly after tapering on the cathode side alone.

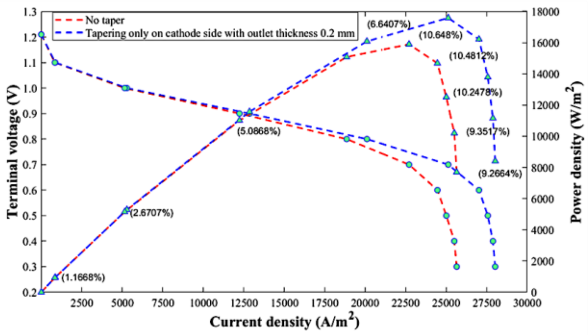


Figure 12. Polarization and power density curve for no taper channel and optimized tapered channel geometry.

4. Conclusions

In this work, a numerical analysis on PEMFC was carried out to investigate the influence of increasing tapering angle on fuel cell performance. The following conclusions may be derived from the findings:

1. Tapering the flow channels improves the fuel cell's ability to operate at greater current densities, as well as the consumption of reactant species and uniform water distribution. However, because of the greater power required to run the auxiliary devices, the rate of improvement in net power production is seen to decrease at higher tapering angle values.
2. Due to the negative effects of channel tapering on pressure drop, parasitic losses, and the durability of the gas diffusion layer, a 0.6 mm reduction in cathode channel height from inlet to outlet (0.8 mm inlet and 0.2 mm outlet height), and a uniform height for the anode channel was determined as an optimized tapering arrangement to improve overall performance.
3. Tapering only the cathode side channel improves performance almost as much as tapering both the anode and cathode side channels. Furthermore, the little gain in net power generation due to anode tapering is not justified by the increased production cost. Therefore, only tapering the cathode side channel is found to be more cost effective.
4. The maximum increase in power generation for optimized tapering arrangement is observed to be 10.648% at 0.7 V terminal voltage.

In comparison to PEMFCs without taper channels, the optimized shape of PEMFC may be employed to achieve better current density and net power production, uniform water content, and lower liquid saturation.

5. Nomenclature

Nomenclature	
A_a	Active area (m^2)
I_{avg}	Average current density (Ampere/m^2)
B	Breadth of fuel cell (mm)
V_{cell}	Cell voltage (V)
D_{bp}	Depth of bipolar plate (mm)
D_{cat}	Depth of catalyst layer (mm)
D_{ci}	Depth of gas channel at inlet (mm)
D_{co}	Depth of gas channel at outlet (mm)
D_{gd}	Depth of gas diffusion layer (mm)
D_m	Depth of proton exchange membrane (mm)
L	Length of fuel cell (mm)
P_t	Power generated by turbine (W)
P_{cool}	Power required to run air cooler (W)
P_c	Power required to run compressor (W)

Abbreviations	
CL	Catalyst Layer
CFD	Computational Fluid Dynamics
CAD	Computer Aided Design
CATIA	Computer Aided Three Dimensional Interactive Application
GDL	Gas Diffusion Layer
MEA	Membrane Electrode Assembly
PEMFC	Proton Exchange Membrane Fuel Cell

Greek symbols	
ε_0	Initial tolerance
ε	Required interval
n	Number of the iteration

6. References

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