Numerical investigations on a proton exchange membrane fuel cell of active area 50 cm²

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Abstract. The present study focuses on the results of a numerical work carried out on a proton exchange membrane fuel cell with an active area of the bipolar plate as 50 cm². The investigations are employed on various operating conditions such as different flow rates of hydrogen and oxygen, cell voltage and temperature. Assumptions made in the study are steady state, single phase, laminar, compressible ideal gasses, the by-product water in liquid phase, transfer of heat in the cell only through conduction mode and so on. The landing to channel ratio employed in the present study is 1:1. The results obtained from the numerical investigations are validated with the help of an experimental study on a 50 cm² serpentine channel of a bipolar plate in a proton exchange membrane fuel cell with same operating parameters. Results show that mass flow rates and temperature have a significant effect on the performance of the fuel cell.

Keywords: Proton exchange membrane fuel cells, active area, serpentine channel

1. Introduction
Fuel cells are direct energy conversion devices which convert the chemical energy of the fuel into electrical energy. The PEMFCs (Proton Exchange Membrane Fuel Cells) are considered promising power sources and command attraction nowadays due to advantages such as low operating temperature (50-90°C), high efficiency (60-70%), low emissions and quick start up. Main application areas of PEMFCs are automobile, stationary and portable sector. A number of studies have been done on the numerical investigations on PEMFCs.

The numerical approach has become an effective tool to analyse the performance of the fuel cells. Cheddie et al. [1] do the three-dimensional modelling of a high temperature PEMFC. This model gives all transport and polarization phenomena. The model reveals that the oxygen depletion happens in the catalyst area under the ribs. Velocities of inlet gases and conductivity of membrane are numerically studied by Sezgin et al. [2]. They develop a three-dimensional, isothermal and steady state model. At sufficiently high flow rates for air, this model gives best results for mass transport region. At an inlet hydrogen gas velocity of 0.133 m/s and an inlet air velocity of 1.3 m/s, the fuel cell gives results closely matching with experimental data. Meng et al. [3] develop a three-dimensional numerical model to study current distribution and performance of the cell under a current density
boundary condition. Their results show that long channel direction gives rise to a difference in the electronic phase potential in the bipolar plate.

The numerical model of both parallel and serpentine flow field is done by Iranzo et al. [4]. The modelling results are calibrated with the help of exchange current density. Water in the channels produces a blockage effect that is difficult to model with this numerical analysis. An automotive application-based modelling of PEMFC is carried out by Haddad et al. [5]. Model responds to both low and high dynamics of power demand and the results show that membrane humidity has a considerable effect on the cell’s efficiency. Wong et al. [6] conduct a theoretical investigation of relative humidity control in PEMFC. Authors conclude that peak power of a PEMFC depends on the combination of anode and cathode humidification factors. Cooling flow field performance of a PEMFC is assessed by Asghari et al. [7]. They studied the thermal management of the cell. Results show that free convection from stack faces has a negligible role in heat removal, but the inlet and outlet manifolds of reactant gases have an influence on the temperature distribution within the bipolar plates. Yu and Jung [8] conduct thermal management strategy for a PEMFC system with a large active cell area. Automobile applications require PEMFCs with the large active area, which produces high temperature, so this model shows proper thermal management to handle the high temperature. A review of thermal management issues in a PEMFC stack is conducted by Kandlikar and Lu [9]. Authors review the basic heat transfer mechanisms at PEMFC at the component level.

Cozzolino et al. [10] analyse the theoretical and experimental investigations on thermal management of a PEMFC stack. Micro cogeneration applications have been investigated through experimental and numerical investigations. Results show that electrical efficiency decreases as the current intensity rises, due to higher ohmic losses and that thermal efficiency always increases from partial to full loads. Huang et al. [11] show the interaction between heat and water transport in PEMFCs. Authors also address the economic factor of the cell due to the use of platinum metal. Results show the influence of porosity gradient and enhancement of performance of the cell. Jang et al. [12] conduct both experimental and numerical investigations on spiral flow field channels. In this study, authors focus their attention on spiral channel design which produces secondary vortices, that can improve the heat and mass transfer characteristics and reduce the large pressure thereby enhancing the fuel cell performance. Due to the presence of secondary vortices in the spiral channel flow field design, the current density of spiral flow field channel is 11.9% higher than the conventional serpentine channel. Roshandel et al. [13], conduct a numerical study on a bio inspired pattern for fuel cells. Authors suggest a new bipolar design inspired from the existing biological fluid flow patterns in a plant leaf. From the results obtained, they find that bio inspired flow channel design shows 26% higher power density than the serpentine channel and 56% more than parallel flow design. But this power density shown by bio inspired flow channel design does not consider the liquid water formation, temperature variations and other minor losses. As a result, there will be a decrease in the power density of the bio-inspired flow channel when these factors are taken into account.

Damain, et al. [14] present a numerical analysis of channels with a design based on the leaf like flow field design. Numerical investigations are conducted at 9 cm² active area fuel cell. To find the leaf like arrangements of the flow field design, authors investigate thirty most common trees in Mexico region and 20 leaves from each tree are photographed. From these observations, they statistically identify two most repetitive configurations. They find that the increase in the inlet humidity causes an increase in the current density. The best fuel cell performance is obtained from flow field channel with two levels of sub-branches. They observe that increasing the number of sub branches gives more uniform gas distribution, hence it will enhance more uniform current density production.

The main contributions of the current work are:
1) Numerical investigations on the serpentine flow field (Landing to Channel ratio, L:C=1:1) of bipolar plates with area 50 cm²
2) Mesh sensitivity analysis and validation of numerical results with experimental results.
3) Effect of electrical performance of the fuel cell with respect to various operating conditions such as flow rates, cell voltage and temperature.
2. Numerical modelling

Numerical modelling involves three major steps. The first step is the creation of fuel cell geometry. Solidworks 2017 is used for this purpose. The second step is the creation of mesh, ICEM meshing module available in ANSYS Fluent 15.0 is used. The last step is the analysis part. A block diagram depicting this sequence is shown in figure 1.

\[ F_i = \sum_{i\neq j} \xi_{i,j} x_j (u_i - u_j) \]

where, \( F_i \) is the driving force on \( i \), at a given \( T \) and \( p \), \( F_i = -\frac{RT}{x_i} \frac{dx_i}{dz} \), \( \xi_{i,j} \) is the friction coefficient between \( i \) and \( j \), \( x_i \) is mole fraction of \( j \), \( u \) is velocity.

For the multiphase mixture flow in the GDL, Darcy’s Law is used for momentum transport modelling

\[ \frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla P + \nabla \cdot (\nabla \cdot \mu u) - \frac{\mu}{K} (\rho u) \]

The energy conservation equation for the multiphase mixture is

\[ \varepsilon \frac{\partial}{\partial t} (\rho C^u) + \nabla \cdot (\gamma_a \rho u C^u) = \nabla \cdot (\varepsilon \rho \nabla C^u) + \nabla \cdot \left[ \rho_s \xi_k D_k^a (\nabla C_k^u - \nabla C_k^u) \right] - \nabla \cdot \left[ \sum_k C_k^u j_k \right] \]

Boundary and initial conditions at the interface between the membrane and the cathode are:

\[ u(x = 0) = u_m, \ v(x = 0) = 0, \ \frac{\partial C^{H_2}}{\partial x} (x = L) = C^{H_2}_{in}, \ C^{H_2}(x = L) = \frac{P_{H_2}}{\rho_g} \frac{RH_{H_2}}{\rho_g} \]

Figure 1. Flow diagram of modelling.

The assumptions made in the numerical modelling are: steady state, single phase, laminar flow, gases are compressible ideal gasses, the by-product water is in liquid phase and heat transfer inside the cell is only through conduction. The physical phenomena occurring in a fuel cell can be represented by solutions of conservation equations like mass, momentum, energy, species and current transport. In addition, equations that deal specifically with a phenomenon in a fuel cell may be used where applicable such as Darcy’s equation for fluid flow in porous media, Fick’s law of diffusion, Stefan-Maxwell equation for multispecies diffusion, Faraday’s law, Butler-Volmer equation, Ohms law and so on.

2.1. Governing equations
The dimensions employed for this work are shown in table 1.

**Table 1.** Dimensions of the fuel cell model for 50 cm² active area

| Component Name        | Width (mm) | Height (mm) | Thickness (mm) |
|-----------------------|------------|-------------|----------------|
| Current collector     | 100        | 100         | 10             |
| Gas Diffusion Layer   | 100        | 100         | 0.3            |
| Catalyst Layer        | 100        | 100         | 0.06           |
| Membrane              | 100        | 100         | 0.15           |

Model is shown in figure 2.

![Bipolar plate, L:C ratio = 1:1 (50 cm² active area).](image)

A Dell Optiplex PC with the i7 processor having 8 GB ram and graphics card of 4 GB is used for the numerical analysis. CPU time for 1 simulation is 8 hours.

3. **Mesh sensitivity analysis**

The present model is discretized into 10,22,547 elements, 17,18,652 elements and 20,51,432 elements and the results are evaluated and are shown in table 2.

**Table 2.** Current density at various no. of discretized elements

| No. of discretized element | Current density(A/cm²) @ 0.4 V |
|----------------------------|---------------------------------|
| 10,22,547                  | 1.0121                          |
| 17,18,652                  | 1.0186                          |
| 20,51,432                  | 1.0188                          |

From table 2 it is observed that the results predicted with the numerical code are grid independent after 17,18,652 elements.

4. **Validation**

The numerical investigations of the PEMFC with an active area of the bipolar plate 50 cm² are carried out to study how close the predicted results match with experimental work. Experimental work conducted by the same research group is used for validation purpose [15]. Figure 3 shows the comparison of power density against cell voltage for experimental and numerical work. The numerical
The results of power density obtained for 50 cm² PEMFC is quite close to the experimental work as shown in figure 3. The percentage deviation between experimental and numerical results are shown in table 3. The deviation between the predicted results and that of the experimental work for the power density is between 4.70 -14.20 %. It is found that the numerical results achieved by CFD technique resemble the experimental work. Thus, the CFD code ANSYS Fluent 15.0 can be extended further with confidence to study the fuel cell characteristics at other operating conditions.

![Figure 3. Validation of power density of 50 cm² PEMFC model](image)

Moreover, the cost and time required for machining a scaled up PEMFC for experimental studies are quite high, and hence numerical study with CFD technique gives an opportunity to optimize qualitatively the flow channel design of scaled up PEMFCs.

Table 3. Percentage deviation between experimental and numerical work

| Voltage (V) | Power Density (W/cm²) | Percentage deviation (%) |
|------------|----------------------|--------------------------|
|            | Experimental | Numerical |                        |
| 0.40       | 0.3891       | 0.4074     | 4.70                    |
| 0.45       | 0.3416       | 0.3729     | 9.16                    |
| 0.50       | 0.2243       | 0.2456     | 9.49                    |
| 0.55       | 0.1557       | 0.1757     | 12.85                   |
| 0.60       | 0.0966       | 0.1100     | 13.91                   |
| 0.65       | 0.0608       | 0.0691     | 13.67                   |
| 0.70       | 0.0246       | 0.0281     | 14.20                   |

5. Results and Discussion

Results obtained from the work are shown below. The various input parameters used in the present investigations are shown in table 4.

From figure 4 it is clear that maximum power output obtained is between the voltage range of 0.4 and 0.6 V. From numerical investigation it is observed that power output has a significant influence on the increase in flow rates of hydrogen and oxygen. Maximum power is obtained when the hydrogen flows at 600 and oxygen at 1200 SCCM (Standard Cubic Centimetre per Minute) respectively and its value is 23.79 W at 0.5 V. Meanwhile the maximum power obtained at 300 and 450 SCCM of hydrogen and oxygen respectively is 22.57 W at 0.5 V. Increased mass flow rate improves the mass transport between the anode and cathode side which results in the enhancement of reaction rate and hence both reactions at anode and cathode side increase and give better current.
density. But an increase in oxygen supply beyond 1200 SCCM will significantly degrade the performance of the cell because of the formation of water flooding.

Table 4. Input parameters used in the present study

| Varying Parameter   | Values                          |
|---------------------|--------------------------------|
| Hydrogen flow rate  | 300, 600 SCCM                  |
| Oxygen flow rate    | 450, 1200 SCCM                 |
| Temperature variation| 50, 60, 65, 70°C               |
| Voltage variation   | 0.40, 0.42, 0.45, 0.48, 0.50, 0.52, 0.55, 0.57, 0.59, 0.60, 0.63, 0.65, 0.68, 0.70, 0.72, 0.75, 0.78, 0.80, 0.83, 0.85, 0.88, 0.90, 0.92, 0.95 V |

Figure 4. Variation of power at various flow rates of hydrogen and oxygen

After finding the better flow rates of fuel and oxidant, next results show the best operating temperature of the cell under 600 and 1200 SCCM of hydrogen and oxygen. Following are the four temperatures taken into account: 50, 60, 65, 70°C. Results are shown in figure 5. From the figure 5, it is clear that maximum power is obtained at 65°C and its value is 24.49 W at 0.5 V. Further increase in temperature reduces the performance of the cell. It is observed that 70°C gives a performance level lower than at 50°C and 60°C. Two temperature regions which gives better results are 60 and 65°C.

Figure 5. Variation of power at various temperatures
Temperature is acting as a catalyst in the reaction, since further increase in the temperature value also improves the rate of reaction which in turn improves the product formation rate. Since water is one of the by-products of this reaction between anode and cathode side, water formation rate will increase with increase in temperature value. So, it is observed that temperatures above 65°C will improve the rate of reaction and hence the water accumulation rate will increase. This water accumulation degrades the performance of the cell.

Figure 6 shows the performance of the cell at 600 and 1200 SCCM of hydrogen and oxygen respectively with temperature at 65°C. Fuel cell operates between 0.2 and 0.8 A/cm² range which gives voltage in the range of 0.52 to 0.67 V. Regions of operation of a fuel cell is shown in figure 6. In activation region current density becomes very low which is due to the presence of activation losses. Activation losses arise because of the losses due to electrochemical reaction. Ohmic region is the region in which fuel cell operates. Reduction in voltage in this region is due to ohmic losses because of ionic and electronic conduction. Last is the mass transport region, in which further reduction in voltage occurs due to the losses arising during mass transport and these losses are known as concentration losses.

6. Summary and conclusions
In the present work, numerical studies are conducted on a 50 cm² active area PEMFC. The conclusions made from this investigation are as follows:

- Various flow rates of hydrogen and oxygen are used. The flow rates 600 SCCM of hydrogen and 1200 SCCM of oxygen give the best results.
- Numerical investigations establish the influence of temperature and its significance in the performance of the cell. 65°C gives the best performance, further increase in temperature reduces the performance of the cell. This is because of the water flooding the cell.
- Performance of a fuel cell can be assessed by current density – voltage curve, i.e. the polarisation curve of the fuel cell. Activation region, ohmic region and mass transport region are the three operating regions of the fuel cell. Among these, the major operating region of the fuel cell is the ohmic region. Figure 6 reveals the ohmic region is between 0.2 and 0.8 A/cm² with cell voltage between 0.52 and 0.67 V.

The key factors affecting the performance of PEMFC are flow rates of hydrogen and oxygen, temperature and cell voltage. This study can be extended further to predict the performance of the cell when it is a part of a more complex energy conversion system.
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