The performance of flow field channel in direct methanol fuel cell

P V Sachin¹, Asha Sathish² and T S Boopathi³

¹ Dept of Electrical and Electronics Engineering, Amrita School of Engineering, Coimbatore, 641112, Tamil Nadu, India.
² Dept of Science, Amrita School of Engineering, Coimbatore, 641112, Tamil Nadu, India
³ Dept of Science, Amrita School of Engineering, Coimbatore, 641112, Tamil Nadu, India

E-mail: s_asha@cb.amrita.edu

Abstract. A 3D computational fluid dynamics (CFD) model is developed to examine the impact of flow field design on the performance of direct methanol fuel cells (DMFCs). Effect of three various type flow fields is investigated in this study: single, double serpentine and honeycomb models. The distribution of velocity and temperature are simulated in 3D models. According to simulation studies, the honeycomb flow field has made uniform flow velocity distribution and minimum temperature change on plate surface. This could result better on DMFC performance. The experimental studies emphasize the performance of a single cell DMFC with different flow field channel designs as well as exhibit maximum power density and open circuit voltage. In subsequent study, electrodeposited Ni-Co alloy on stainless steel mesh surface is utilized to oxidize methanol and the electrode performance has been tested using cyclic voltammetry in alkaline conditions to replace expensive and sensitive platinum and platinum alloy catalysts

Keywords: Single DMFC, Computational simulation, Honeycomb flow field channel

1. Introduction

The consumption of electricity is increasing each year in the world because of population progress. According to the survey of US Department of Energy the energy demand would rise dramatically in future and is expected to rise by 44% between 2006 and 2030. However, due to a rise in fossil fuel combustion, pollutant emissions, and the greenhouse effect, fossil fuels will be less dependable in the coming year [1]. Furthermore, fossil fuel sources are depleting, and significant price increase can be projected in the future. Subsequently, the depletion of fossil fuel and the degradation of the environment are major issues in modern society. This leads to the need of a clean and sustainable energy resource. The fuel cell produces electricity by working under an electrochemical reaction. Different type of fuel cell is available based on their components, functions and purposes. The efficiency of the fuel cell is increased by incorporating new designs in various components like electrodes, electrolytes, flow field and changes in working conditions such as temperature, the reactants flow rate, and treatment of heat [2]. DMFC and PEMFC are the major employed cells which can be used in low-temperature applications. Unlike PEMFC, which uses H₂, DMFC uses liquid methanol, which removes the essential H₂ cylinder storage [3]. The DMFC can be worked as a very hopeful portable energy sources as it offers
higher energy density, a quick start-up time, simple in design, and produce low emission. Nevertheless, numerous technological challenges in the practical application of DMFCs are the catalytic activity of anode portions, methanol crossover, water management and stability issues. Temperature, pressure and methanol velocity are mutually essential factors in the operation of DMFCs, as they assess the system's efficiency and durability [4]. In the single fuel cell, the design is not suitable for direct monitoring of these factors. In this regard another approach is made to utilize computational simulation to estimate fuel cell performance under a variety of operating situations, and then design a better fuel cell system based on the CFD results [4].

2. Methodology

2.1. Theory in DMFC

The electrochemical reaction that occurs in the anode and cathode catalyst layers of the DMFC are given as follows:

\[ CH_3OH + H_2O \rightarrow CO_2 + 6H_+ + 6e^- \]  \hspace{1cm} (1)

\[ \frac{3}{2}O_2 + 6H_+ + 6e^- \rightarrow 3H_2O \]  \hspace{1cm} (2)

Net reaction \[ CH_3OH + \frac{3}{2}O_2 \rightarrow CO_2 + 2H_2O \]  \hspace{1cm} (3)

It is critical to understand the amount of heat developed by electrochemical process. The heat flux is mainly produced in two ways of electro-catalytic process and electro chemical process [4]. Thus, its numerical studies are important. The heat generated per unit time (Q) is calculated using the reaction enthalpy due to the chemical reaction and methanol consumption rate from following equation:

\[ Q = \text{mol}_{MeOH}(\Delta H_f - nF\Delta E_{cell}) \]  \hspace{1cm} (4)

Where \( \text{mol}_{MeOH} \) is the number of moles of methanol, F is Faraday constant and n denotes the number of electrons transferred. At steady state, the heat flux q can be represented as:

\[ q = \frac{Q}{A} = \frac{nI(-\Delta H_f / 6F - V)}{A} \]  \hspace{1cm} (5)

Where I is the current, V is the output voltage, A is the surface area of the electrode, \( \Delta H_f \) is the enthalpy of methanol formation. The methanol enthalpy value at gas and liquid state are 201 kJ mol\(^{-1}\) and 239 kJ mol\(^{-1}\) respectively. The thermal efficiency is taken as nearly 50% [4,5] and hence the cell power, output cell power and heat flux generated within in the DMFC would be compared.

\[ D_h = \frac{4S}{L} \]  \hspace{1cm} (6)

\[ Re = \frac{\rho_u u_{in} D_h}{\mu_m} \]  \hspace{1cm} (7)

The equation (7) is used to calculate Reynolds range (Re), \( D_h \), \( U_{in} \), hydraulic diameter and inlet velocity, respectively. In this simulation work, the heat flux developed on two sides of the flow field by electrochemical reaction in catalyst layer is considered. In equation (5) the constant heat flux boundary condition is assumed. As the maximum power density of DMFC is around 20-50 mWcm\(^{-2}\) at ambient temperature and its thermal efficiency is about 50%, the heat flux formed at inner side of the cell is around 200-500 Wm\(^{-2}\) [6-9]. The q value is assumed as 500 Wm\(^{-2}\) for the DMFC simulation. The fuel used is methanol solution.
2.2. Assumptions and Physical domains

The simulation is done with the ANSYS fluent (2020R2) programme, and the CAD software provides the correct dimensions and geometry. For the CFD modelling, the following assumptions are formulated.

- Steady state mass transfer and heat transfer
- Gravity is disregarded.
- Isothermal flow
- Incompressible laminar flow
- Methanol crossover is ignored
- Constant thermal conductivity of materials
- No-slip condition on flow channel
- Differential thermal energy conservation equations are used to model the thermal energy
- Standard outlet atmospheric pressure

In this work three flow field channels are used the study the performance of the DMFC. They are single serpentine, double serpentine and honeycomb channels. The model has executed in ANSYS fluent with the following steps:

- Geometric assembly with AutoCAD software
- Meshing with ANSYS software
- Suitable placing of structural shape, parameters, and domains
- Numerical analysis
- Final step to visualize the result and analysis

The number of mesh elements ranges various with geometry. In this work, the whole meshes are formed in hexahedral elements

2.3. Geometric model

The direct methanol fuel cell consists of flow field plates, catalyst layer, membrane and diffusion layer. The function of each component decides the performance of DMFC. The membrane electrode assembly and flow field channel are the major component of DMFC. Besides, in this work five-layer MEA containing nafion 117 membranes has been used. The main roles of membrane are to transfer the proton from anode to cathode and helps in diffusion of water. While, the fuel flow through the channel a few amounts get disperses into the diffusion coating and catalyst coating. However, the diffusion coating control the rate of flow of fuel into the catalyst coating [10,11]. In addition the diffusion coating should have some qualities such as high thermal, electrical conductivity and corrosion resistance. The 3D model of DMFC shown in figure 1

2.4. Governing equations

Using some assumptions such as incompressible fluid, flow is laminar and fluidic characteristics is constant, the mass conservation of the three-dimensional structures has been stated as follows:

$$\frac{\partial (\varepsilon \rho u)}{\partial t} + \nabla \cdot (\varepsilon \rho u) = S_m$$  \hspace{1cm} (8)

The first term in equation (8) represents unsteady state \(\varepsilon \rho u\) represent convection and \(S_m\) represent source of mass.
The simplified term for calculating the steady state mass transfer and mass conservation is written as:

$$\frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$

(9)

Equations (9) and (10) indicate the momentum and energy conservation.

$$\frac{\partial (pu_i)}{\partial x_i} = \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial u_i}{\partial x_i} \right)$$

(10)

Where \( P \) and \( \mu \) are the pressure and viscosity factor, respectively,

$$\frac{\partial (pu_iT)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{k}{c_p} \frac{\partial T}{\partial x_i} \right) + S_T$$

(11)

Where \( c_p \), \( k \), \( T \), \( S_T \) represent specific heat capacity under constant pressure condition, effective heat coefficient, temperature and source of temperature respectively.

**Table 1. Parameters for simulations**

| Parameters/symbol                  | Values                        |
|-----------------------------------|-------------------------------|
| Inlet fluid temperature, \( T_{in} \) | 298.15 K                      |
| Outside pressure, \( P_{out} \)   | \( 1.01325 \times 10^5 \) Pa  |
| Inlet velocity, \( u_{in} \)      | 0.006, 0.01, 0.03 ms\(^{-1} \) |
| Heat exchange coefficient, \( k \) | 10 Wm\(^{-2}\)K\(^{-1} \)   |
| Heat flux, \( q \)                | 500 Wm\(^{-2} \)             |
| Flow field dimension, \( l_p \times w_p \times h_p \) | 50mm × 50mm × 10mm |
| Width of channel                  | 1.5 mm                        |
| Depth of channels                 | 1.5 mm                        |
| Width of rib, \( W_{rib} \)       | 2 mm                          |
| Density of graphite               | 2330 Kgm\(^{-3} \)           |
| Methanol concentration, \( C_{MeOH} \) | 980.97 Kgm\(^{-3} \)         |
| Methanol viscosity, \( \mu_m \)   | 0.001 Pa s                    |
| Methanol thermal conductivity, \( k_m \) | 0.5743 W m\(^{-1}\)K\(^{-1} \) |

2.5. Experimental section of single DMFC

To learn more about the impact of flow field structure on single DMFC performance, two different types of anodic flow fields have been designed and fabricated by CNC machines. The flow field plate is
fabricated with graphite material. The single DMFC shown in Figure 2 is created in the same dimension as the simulated model in order to verify the simulated studies. The total length of the plate is 70 mm, width is 70 mm and thickness are 10 mm. The active area of MEA is 250 mm². This study compares the open-circuit voltage and power density while using the different two type flow fields in DMFC at the same conditions.

In the test analysis of DMFC, 5 layers MEA are used. The gas diffusion layer is developed with carbon cloth (MPL-w151010) coated with 4.0 mg/cm² platinum black on the cathode, and 4 mg/cm² on the anode. The Nafion N-117 TM is used as the membrane with 183 micrometres thickness. The PTFE tape and gaskets are used to prevent the potential leaks from the DMFC. Besides, the open circuit voltage and power varies with respect to the fuel flow rates and methanol concentration in DMFC. The methanol solution is supplied through the anode region at various flow rates and air-breathing technique is used to operate the cathode. The open-circuit voltage and power density is measured using the single serpentine and honeycomb flow field in the single DMFC [12]. On increasing the load on the single DMFC the voltage drop may increase the current of the single DMFC.

2.6. Experimental section of Ni-Co alloy deposition on SS mesh
A stainless-steel mesh of 0.5x0.5 cm² area is thoroughly cleaned and coated with Ni-Co alloy. The Ni-Co solution is prepared in a 1:1 ratio, and the pH level of the solution should be kept at 3. The galvanostatic approach has been used to deposit Ni-Co on the SS mesh while maintaining a constant current of -0.02A. The modified electrodes are properly washed in water after deposition and then used. Throughout the experiment, newly deposited electrodes are used. The CHI608d workstation is used to conduct electrochemical studies [13-15]. The electrochemical cell employed in this study is just a three-electrode standard cell. The working electrode is Ni-Co coated SS mesh, reference electrode is Ag/AgCl and the counter electrode is Pt foil. The chemical reagents used in this experiment are NiSO₄.7H₂O, CoSO₄.8H₂O, H₃BO₃, NaOH, and methanol solution which are used as such.

3. Result and discussion

3.1. Simulation principles
Table 1 explain the parameters for simulation studies. In this study, various conservation, heat loss and heat transfer with the surroundings are considered. The various operating parameters such as fuel velocity distribution, temperature distribution, pressure drops are monitored to study the relation between flow field structures and cell output. The continuity equation, Eq. (9), the Navier-Stokes equation, Eq. (10), and the energy conservation equation, Eq. (11) are all solved using the SIMPLE algorithm.

3.2. Velocity distribution in different flow field structures
The different color codes helps to understand and analyze the simulation results. The fuel entering and leaving sides of the three structures are diagonally opposite to each other, with a 250 mm² active area.
The figures 6, 7 and 8, indicates the flow rate of fuel at an inlet velocity of 0.01 ms\(^{-1}\) on three flow fields. From the simulation results, the honeycomb flow field exhibits an uniform flow of fuel throughout the channel when compared to the other two flow field channels. This might be due to the larger fuel storage area in honeycomb flow field channel. Moreover, the uniform velocity flow aids in removing the heat and forming CO\(_2\) in the flow channel. Since the fluid motion is not uniform in single and double serpentine flow fields exhibit higher velocity distribution. The Figures 3, 4 and 5 represents the pressure drops in various channels at an intake velocity of 0.01 ms\(^{-1}\). When the pressure gradient increases the velocity of fuel also increases in the channel. The following equation shows the relation between \(dP\) and \(v\):

\[
dP = \rho_m |V - V_{in}|^2
\]  

(12)

The pressure drop between intake and output can be measured as well as analyzed. The low-pressure drop is more favourable for saving the external fuel pump supply energy. However, the lower pressure drops leads to decrease in the velocity of fuel. From the simulation studies the honeycomb flow field indicates a suitable pressure drop favourable for good performance of DMFC.

**Figure 3.** Pressure drops through single serpentine flow field channel at an intake velocity of 0.01 ms\(^{-1}\)

**Figure 4.** Pressure drops through double serpentine flow field channel at an intake velocity of 0.01 ms\(^{-1}\)

**Figure 5.** Pressure drops through honeycomb flow channels at an intake velocity of 0.01 m s\(^{-1}\).
3.3. Temperature distribution on flow field on surface

The temperature change on the surface of flow-field should be uniform and minimum for enhance the performance of DMFC. The irregular temperature distribution disperses the catalyst very quickly in MEA. Figure 6 shows the temperature ranges on varying the inlet velocity from $0.006 \text{ ms}^{-1}$ to $0.05 \text{ ms}^{-1}$. The increase in flow velocity of fuel reduces the temperature changes on the flow field surface. Moreover, temperature distribution on the surface is high at an inlet velocity of $0.006 \text{ ms}^{-1}$. Besides on increasing the flow velocity the temperature distribution in each flow field is reduced gradually. Thus, from the simulation studies the honeycomb flow field surface shows uniform and minimum temperature change. In the same operational condition, the temperatures in the single and double flow field channels are very high which will reduce the performance of DMFC. The temperature distribution with various velocity results in figure 9, 10 and 11.

![Velocity distribution through single serpentine flow channels at an intake velocity 0.01 ms$^{-1}$](image1)

![Velocity distribution through double serpentine flow field channel at an intake velocity 0.01 ms$^{-1}$](image2)

![Velocity distribution through honeycomb flow field channel at an intake velocity 0.01 ms$^{-1}$](image3)
Figure 9. Top surface temperature distribution in (a) serpentine, (b) double serpentine and (c) honeycomb flow fields at an intake velocity of 0.006 m s$^{-1}$.

Figure 10. Top surface temperature distribution in (a) serpentine, (b) double serpentine and (c) honeycomb flow field channel at an intake velocity of 0.01 m s$^{-1}$.

Figure 11. Top surface temperature distribution in (a) serpentine, (b) double serpentine and (c) honeycomb flow fields at an intake velocity of 0.05 m s$^{-1}$.
3.4. Experimental evaluation of single DMFC

In the experimental studies, the performance of DMFC is analyzed using the honeycomb and single serpentine flow field channel. The figures 12 and 13 show the variation of power density and open circuit voltage with methanol flow rate. On increasing the methanol flow rate an increase in open circuit voltage and power density is observed. From the polarization curve studies, the honeycomb flow field channel exhibits higher power density and better open circuit voltage than single serpentine flow field channel. The better performance is obtained at a methanol flow rate of 3 mL/min.

![Figure 12. Polarization curve of DMFC with honeycomb flow field channel at 2M methanol concentration](image)

![Figure 13. Polarization curve of DMFC with double serpentine flow field at 2M methanol concentration](image)

3.5. Experimental evaluation of Ni-Co solution deposited on SS mesh

The electrocatalytic activity of Ni-Co alloy deposited SS mesh is analysed using cyclic voltammogram studies. Two electrodes with varying deposition time of 10 minutes and 20 minutes are prepared using 1:1 Ni-Co solution. The finest methanol oxidation and less oxidation voltage are observed in 10 minutes electrodeposited electrode. When the time of deposition increases the thickness of the electrode also increases which may cause the non-uniform deposition on the electrode. During the oxidation reaction,
the formation of Co (OH)$_2$ helps to improve the charge absorption of Ni and formation of γ-NiOOH disable the Ni catalyst activity. The figure 14 indicating the oxidation rate of CH$_3$OH in 0.5M NaOH and the figure 15 shown the oxidation rate of CH$_3$OH at two different time deposition.

![Figure 14](image1.png)

Figure 14. CH$_3$OH Oxidation in 0.5 M NaOH (0.1 mL to 0.5 mL) CH$_3$OH at the scan rate of 0.1 V s$^{-1}$ using 10 minutes coated electrode

![Figure 15](image2.png)

Figure 15. 10 and 20 minutes electro catalytic activity analyse of Ni-Co deposited electrode in presence of 0.5 mL methanol and 0.5 M NaOH at a scan rate of 0.1 V s$^{-1}$.

4. Conclusion

To increase the efficiency of DMFC, three types of flow fields are analysed computationally and two flow fields are compared experimentally. From the computational studies of DMFC using three parameters of pressure drops, velocity and temperature distribution. The honeycomb flow field channel exhibit better functioning than single and double serpentine flow field channels. For experimental studies, the best two models of single serpentine and honeycomb flow field channels are selected. From the experimental studies, the honeycomb flow field channel with 3 mL/min flow rate exhibits higher power density and better open circuit voltage than single serpentine flow field channel. As a result, the honeycomb design is thought to be the optimal flow field structure, with an optimized flow rate of 3 mL/min.
The Ni-Co solute on deposited SS mesh has been examined for electrocatalytic activity of methanol with the help of cyclic-voltammetry. The studies showed that 10 minutes deposited SS mesh exhibits better electrocatalytic activity of methanol in 0.5M NaOH until 0.5 mL methanol addition. The SS deposited electrode can be used instead of the Pt alloy catalyst. This can reduce the overall cost of DMFC.

Acknowledgements

The authors are grateful to express their gratitude and indebtedness to all who, directly or in directedly had an impact on the execution of work.

References

[1] EG&G Technical Services 2004 Inc., Fuel Cell Handbook, seventh ed. U.S. Department of Energy West Virginia pp.2-1.
[2] Oliveira V B, Rangel C B and Pinto A M F R 2010 Effect of anode and cathode flow field design on the performance of a direct methanol fuel cell Chemical Engineering Journal, 157 174–180.
[3] Leonardo K.K Maia, and Ruy de Sousa Jr Three-dimensional CFD modeling of direct ethanol fuel cells: evaluation of anodic flow field structures J Appl Electrochemical DOI 10.1007/s10800-016-1013-6.
[4] Hima Sharifi, Rahbar Rahimi, Davod Mohebbi-Kalhori, and C Ozgur Colpan 2020 Coupled computational fluid dynamics-response surface methodology to optimize direct methanol fuel cell performance for greener energy generation energy 198 117293.
[5] Sheng-Jun Wang, Wei-Wei Huo, Zhi-Qing Zou, Yong-Jin Qiao and Hui Yang Computational simulation and experimental evaluation on anodic flow field structures of micro direct methanol fuel cells Applied Thermal Engineering 31(14-15):2877–2884.
[6] Kablou Y, Matida E and Cruickshank C Two-Phase Flow Modelling of Direct Methanol Fuel Cell Anode Compartment fuel cells DOI: 10.1002/fuce.20190002.
[7] Pradeep A, Raveendran J, Dr. Ramachandran T, Dr. Bipin Nair G, and Dr. Satheesh Babu T G 2016 Computational simulation and fabrication of smooth edged passive micromixers with alternately varying diameter for efficient mixing Microelectronic Engineering vol. 165, pp. 32-40.
[8] Dyer C K 2002 Fuel cells for portable applications, Journal of Power Sources 106 31-34.
[9] Guo Z, and Faghri A 2008 Development of a 1W passive DMFC, International Journal of Heat and Mass Transfer 35 225-239.
[10] Yu S H, Sohn S, Nam J H, and Kim C J 2009 Numerical study to examine the performance of multi-pass serpentine flow fields for cooling plates in polymer electrolyte membrane fuel cells, Journal of Power Sources 194 697-703.
[11] Aricò A S, Baglio V, and Antonucci V 2009 Direct Methanol Fuel Cells: History, Status and Perspectives. Wiley pp. 8-10.
[12] Wu W, and Lin Y T 2010 Fuzzy-based multi-objective optimization of DMFC next term system efficiencies, International Journal of Hydrogen Energy 35 9701-9708.
[13] Durgadevi N, Sunitha M, Dr. Asha Sathish, Guhan S and Dr. Ramachandran T 2016 Electro Oxidation of Methanol on Ni/Ni-Co Coated SS mesh Electrode. Indian Journal of Science and Technology vol.9.
[14] Sunitha M, Sathish A and Dr. Murali Rangarajan 2019 Ni-Zn-P catalyst supported on stainless steel gauze for enhanced electrochemical oxidation of methanol for direct methanol fuel cell application Materials Research Express, vol. 6.
[15] Rajamani A R, Jothi S, Datta M and Dr. Murali Rangarajan 2018 Electrodeposition of tin-bismuth alloys: Additives, morphologies and compositions Journal of the Electrochemical Society, vol. 165, pp. D50-D57.