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Computational Evaluation of an Enhanced Serpentine Flow Field Design for PEM Fuel Cells

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Abstract: ***Fuel cell is a electro-chemical energy conversion system, which converts the chemical energy of fuel, directly into electrical energy. The ever increase in energy demand, non-polluting energy generation, and other environmental issues have persuaded many researchers to look for new efficient energy conversion technologies. Proton exchange membrane (PEM) fuel cells have many unique features compared with other types of fuel cell, such as relatively low operating temperature (around 80^{o}C), high power density, quick start, rapid response, and high modularity which makes them as the most promising system in the applications such as automotive, distributed power generation and portable electronic devices. In this work, a new compound serpentine flow field is introduced and conducted simulations to study its performance. A 3-D PEM fuel cell model of size 49 cm^2 and 84 cm^2 active area is developed. A conventional serpentine flow field is modified and the same is considered for the supply of reactants. Computational fluid dynamics (CFD) based simulations were conducted to analyse the pressure drop, distribution of reactants (H_2 and O_2), liquid water activity, current flux density and water content in the membrane.***

Keywords: CFD, Fuel Cell, Serpentine flow, PEM Fuel Cell

I. INTRODUCTION

Fuel cell (FC) is an electro-chemical energy conversion device, which converts chemical energy of fuel directly into electrical energy. The ever increase in energy demand, pollution free energy generation, and other ecological issues have persuaded many researchers to look for new efficient energy conversion technologies [1]. Within such perception FC systems may consider as promising alternative due to practical advantages such as high-energy density, less harm to the environment, good dynamic response, and lightweight. Depending on type of electrolyte material used FCs are categorized as polymer membrane, alkaline, phosphoric acid, molten carbonate, and solid oxide fuel cells [2]. Proton exchange membrane (PEM) fuel cell has unique features such as relatively low operating temperature (around 80^{o}C), high power density, quick start, rapid response, and high modularity make them as the most promising system for power generation in the applications such as automotive, distributed power generation and portable electronic devices [3,4].

In the early 1960s, PEM fuel cell (PEMFC) was first used in the Gemini space program, that FC was developed by General Electric based on the work of Grubb and Niedrach. Following the Gemini Program the FC was also used in the Apollo program, to produce electricity for life support and communications. These FCs were made by Pratt and Whitney based on the Bacon's patents. Due to their high cost, use of FC systems were limited in space applications and in some special applications. In 1990, Ballard Power systems started development of PEMFC systems. The strategy of Ballard was to reduce the cost of the fuel cell by using low cost materials and fabrication techniques, that FC turn out to be a real option for many applications. In 1993, Ballard Power Systems manifested fuel cell powered buses. Figure 1.1 illustrates the schematic of a PEMFC. Hydrogen (H2) comes into the anode flow channel and disperses into the anode gas diffusion layer (GDL) whereas oxygen (O2) enters into the cathode flow channel and disperses into the cathode gas diffusion layer (GDL). The membrane comprises catalyst usually platinum, on both sides and it is made from a material that only permits the hydrogen ions and offer resistance to the flow of electrons. When hydrogen and oxygen reaches the catalyst layers (CLs) through GDLs on the PEM, the following reaction takes place.

$$\text{Anode: } H_2 \rightarrow 2H^+ + 2e^- \quad (1.1)$$

$$\text{Cathode: } \tfrac{1}{2}\, O_2 + 2e^- + 2H^+ \rightarrow H_2O \quad (1.2)$$

At anode catalyst layer hydrogen splits into hydrogen ions and electrons. Hydrogen ions pass from anode side to cathode side, through the membrane and electrons flow out of the cell through an electrical circuit. At the cathode CL oxygen reacts with hydrogen ions and electrons flow into the cathode, completing an electrical circuit. The overall reaction in a hydrogen and oxygen fuel cell is given in Equation 1.3.

$$\text{Overall: } H_2 + 1/2\, O_2 \rightarrow H_2O \quad (1.3)$$

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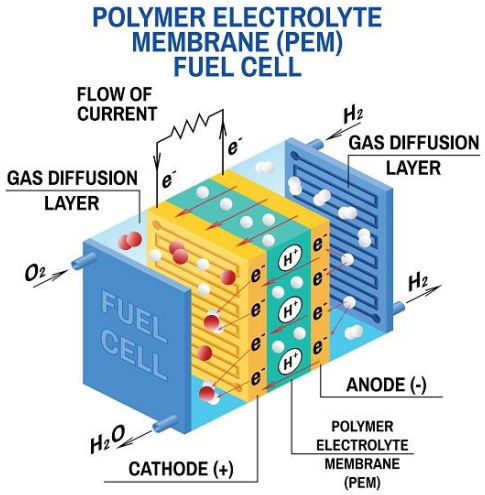

Figure 1.1 Schematic of a PEM fuel cell

Being enthralled with Grove's invention, Bacon began working on FCs in 1939 and successfully constructed a FC stack of 6 kW output power 1959. Later FCs have been used in the U.S. Space Program for the first time. Furthermore, the FCs were used in the Apollo Space Program to produce power for life support and communications. Based on Bacon's patents, Pratt and Whitney made the fuel cells. General Motors made trials with a FC operated van by the mid-1960s, in the meantime the U.S. Space Program has continued to effectively make use of FCs up to today. In the 1960s many industries recognised that the FCs can be used in different applications, but because of their high manufacturing cost and technical difficulties, FCs were not have the capacity to monetarily focused with other energy conversion devices. In the 1980s, the Canadian Government sponsored the preliminary development work of FCs which was supported by Ballard Power Systems. Later in 1989, the company decided to concentrate on FC systems for transportation and stationary applications.

II. METHODOLOGY

Computational evaluation of PEM fuel cell performance includes three major steps. The first step is modeling the geometry of the PEMFC by means of computer-aided design software. The geometrical model forms the basis for creating a computational mesh.

The second step involves generating the mesh from the geometry. In order to solve the numerous of equations associated with a fuel cell simulation, the entire cell is split into a finite number of discrete volume elements or computational cells. The relevant equations are then solved in each individual cell and integrated over the computational domain to give a solution for the entire domain. Generating a good mesh is one of the challenging steps. It needs a careful balance of generating adequate computational cells to capture the geometry without exceeding the available memory of the meshing computer. Many other factors must also be considered in order to create a computational mesh which delivers archetypal results when simulated.

The third and final step involves inputting the various physical and operating parameters of the simulation. Some of these include thermal and electrical properties of the various materials, operating temperatures and pressures, inlet gas flow rates, open circuit voltage, porosity, and humidification among many others. The flow chart of the computational methodology can be seen in Figure 2.1.

A. Modeling Assumptions

The developed models were assumed as 3-D, steady and isothermal. The reactants at inlet to the channel assumed as perfect gases, the flow is laminar, incompressible and the porous layers assumed as isotropic and the thermo-physical properties assumed as constant.

B. Governing Equations

Fundamental conservation equations such as conservation of mass, momentum and charge were used to develop a mathematical model for PEMFC. Conservation of energy equation was not considered as the model was assumed as isothermal. The PEMFC was examined in four parts: flow channels, GDLs, CLs and the membrane.

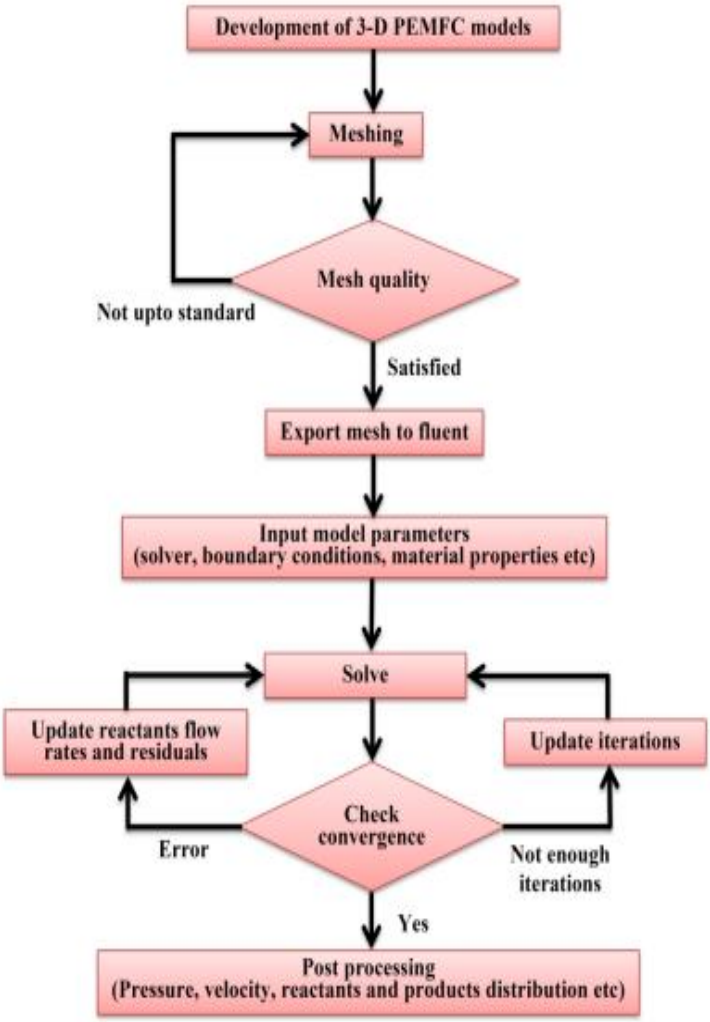

Figure 2.1 Flow chart of computational methodology

C. Development PEM fuel cell models

The first step in the development of FC model is modeling of individual parts of the three active area PEMFCs such as current collector, gas diffusion layer, catalyst layer (for anode and cathode) and a membrane (PEM) in SOLIDWORKS 2015. These parts have been assembled to get the complete fuel cell assembly. The geometric dimensions of these components have been given in Table 2.1. The exploded view of the PEMFC with proposed serpentine flow fields is shown in Figure. 2.2.

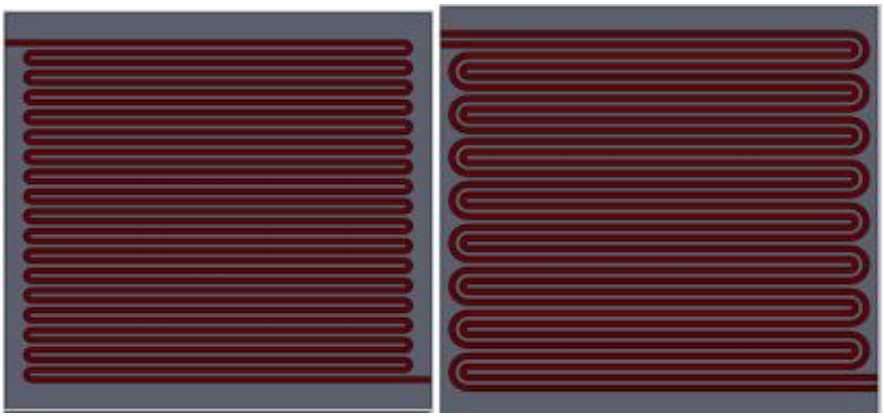

Figure 2.2 7 cm x 7 cm size single, double serpentine flow field designs

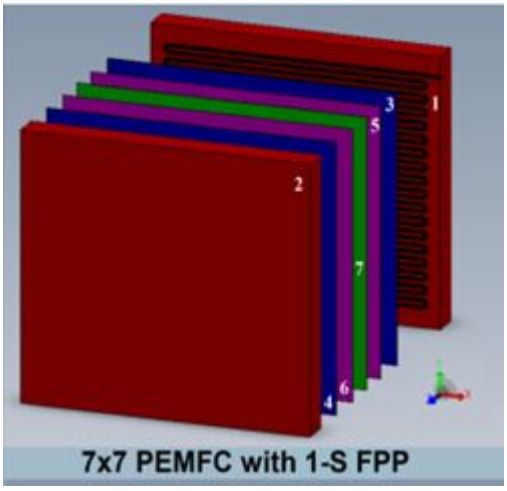

Figure 2.3 Exploded view of active area PEMFC with serpentine flow fields

Where
1. Anode flow field 2.Cathode flow field 3.Anode gas diffusion layer 4.Cathode gas diffusion layer 5.Anode catalyst layer 6.Cathode catalyst layer 7.Membrae (PEM)

Table 2.1 Geometric dimensions of PEM fuel cell

Cell	Part	Length (cm)	Width (cm)	Height (cm)
PEMFC 1 (7x7 cm^2)	Gas diffusion layers (GDL)	7	7	0.025
	Catalyst Layer (CL)	7	7	0.005
	Membrane	7	7	0.00175
	Channels	7	0.1	0.1
	Rib	7	0.1	0.1

D. Computational Procedure

The simulation setup is initiated by loading fuel cell module. This is accomplished by typing the following command into the Text User Interface (TUI) and pressing the Enter key./define/models/addon-module 3. Once the module is loaded, it is important to test the mesh with the default settings first. The basic parameters have to be set first. To set operating parameters and material properties, open the Fuel Cells & Electrolysis– PEMFC module.

III.RESULTS AND DISCUSSION

Computational investigations on the performance of PEMFC using single (1-S), double (2-S) and triple (3-S) serpentine flow field configurations has been completed. Numerically predicted pressure drop, mass fraction distribution of hydrogen, oxygen, and liquid water activity along the channel at peak power performance with three flow fields presented.

A. Pressure Drop

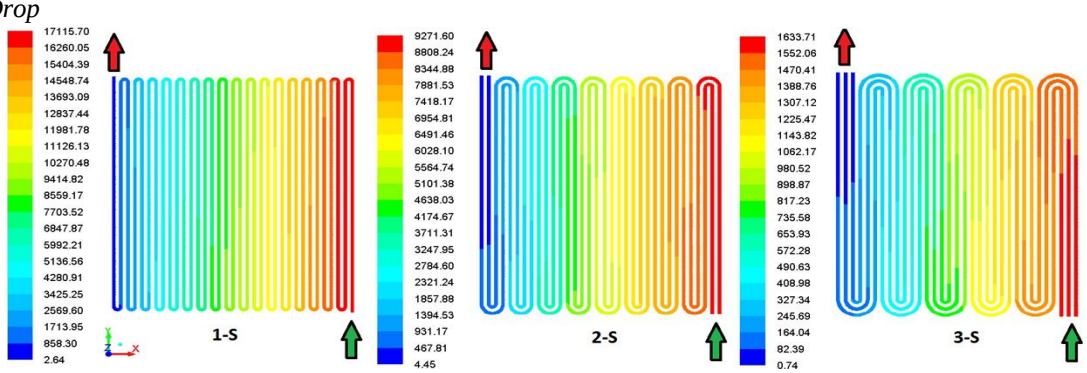

Figure 3.1 Variation of Pressure in cathode channel of PEMFC 1

CFD analysis was carried out on 1-S, 2-S and 3-S flow field models to study the pressure drop from inlet to outlet. From Figures 3.1 it is observed that pressure drops are maximum at the inlets and gradually reduced towards the outlets. It is also observed that highest-pressure drops are observed in 1-S flow channels and lowest pressure drops in 3-S flow channels of PEMFC, pressure drop for 1-S, 2-S and 3-S are 17105, 9125 and 1620 Pa.

B. Hydrogen and oxygen distribution

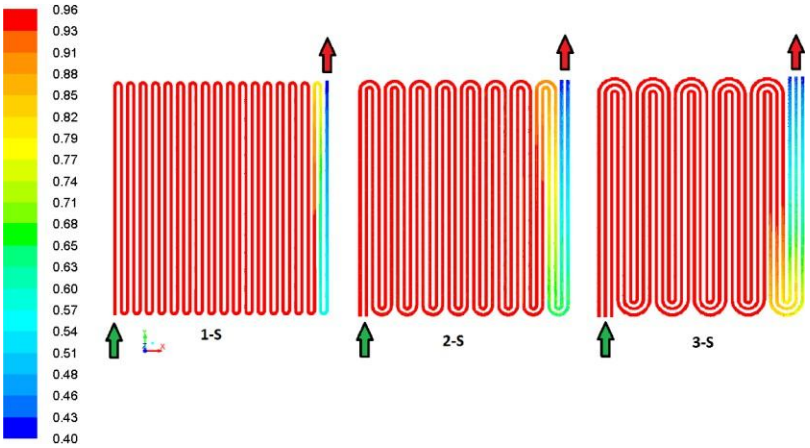

Figure 3.2 H_2 mass fraction distribution in anode channel of PEMFC 1 at 0.5 V

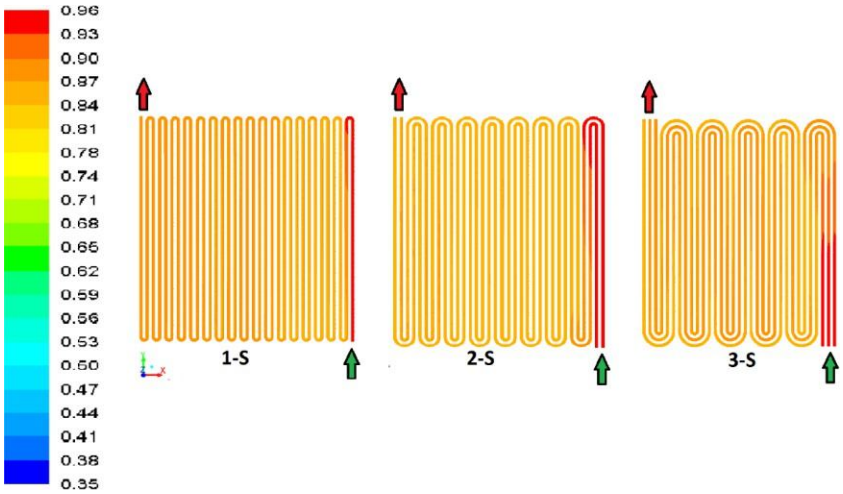

Figure 3.3 O2 mass fraction distribution in cathode channel of PEMFC 1 at 0.5V

Figure 3.3 shows the oxygen mass fraction distribution along the cathode flow channels (1-S, 2-S and 3-S) of PEMFC1 at cell potential of 0.5 V. From Figures it is observed that oxygen mass fractions are high at the channel inlets, decreased along the flow channel, and become low at the channel outlets. It is also observed that oxygen mass fraction distribution is more uniform than hydrogen mass fraction distribution. The reduction of species concentration along the channels is due to consumption of reactants in the reaction.

C. Current flux density distribution

Figure 3.4 shows the current flux density distribution over the cathode catalyst layer of three flow field configurations (1-S, 2-S and 3-S) of PEMFC at a cell potential of 0.5 V. The simulation results showed that the current densities are the maximum in the region close the anode inlet and decreased along the direction of the flow. The drop in the local current densities is because of the reactant depletion. It is also observed that the current flux density distribution over the CL of 3-S flow fields PEMFC is better than 1-S and 2-S flow field PEMFC.

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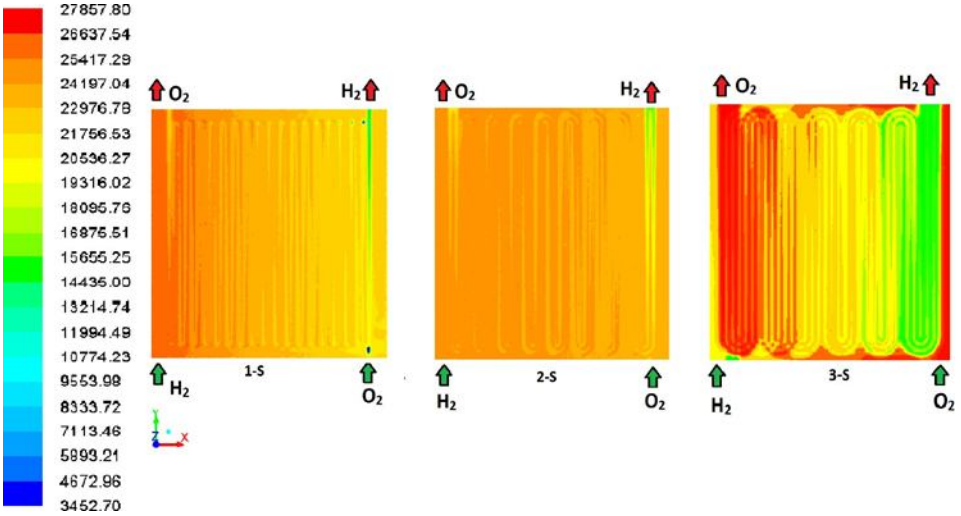

Figure 3.4 Current flux density distribution on cathode CL of PEMFC1 at 0.5 V

D. Effect of Membrane Thickness

Effect of membrane thickness on cell performance is analysed with three membranes having different thickness namely N212 (50 µm), N112 (51 µm) and N117 (178 µm). Figure 3.5 shows the effect of the membrane thickness on the performance of three active area PEM fuel cells. The analysis is done at 70°C cell temperature and 1 bar pressure. The highest power output of 16 W and 23 W have been obtained when N212 membrane was used in PEMFC 1 and PEMFC 2. The peak power delivered by the PEMFC loaded with N112 and N117 membrane are less than PEMFC loaded with N212 membrane because the ohmic resistance of N112 and N117 is higher than N212. From these results, it is concluded that a thin membrane (N212) offers less ohmic resistance and gives high performance.

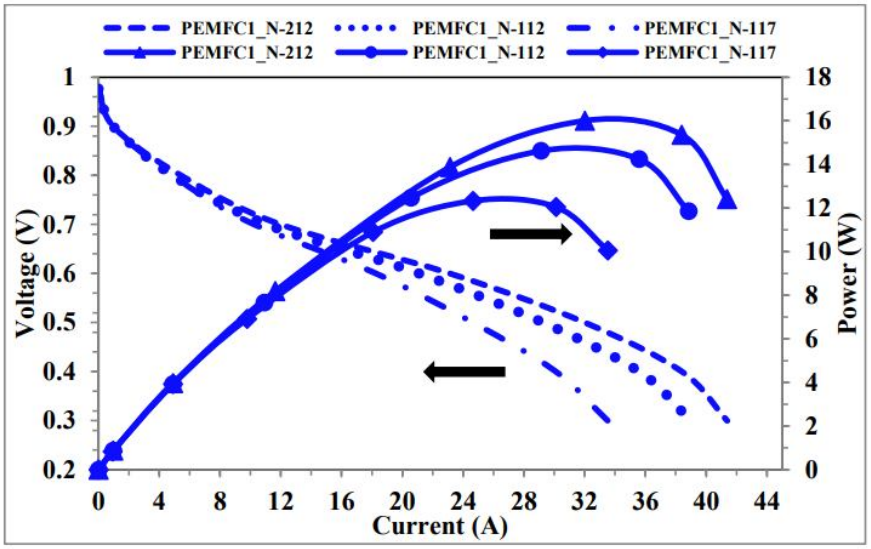

Figure 3.5 Effect of membrane thickness on performance of PEMFC 1

E. Effect of catalyst (Pt) loading

The effect of catalyst (Pt) loading on the performance of PEMFCs with an active area of 49 cm^2 were analysed by incorporating N212 membrane. The platinum loading on the cathode side is taken as 0.6, 0.8 and 1.0 mg/cm^2 and on anode side is 0.4 mg/cm^2. The catalyst loading is more critical on the cathode side due to the significant activation polarization/kinetic loss for the oxygen reduction reaction (ORR).

Figure 3.6 shows the effect of catalyst (Pt) loading on the i-V characteristics of two PEMFCs. It is observed that the cell performance has increased with increase in platinum loading. A larger catalyst loading facilitates higher surface area for electrochemical reactions, as a result, more reactant species involve in the reactions, generate more current and decrease the activation loss. It is also observed that the rate of increase in performance is more when the platinum loading increased from 0.6 to 0.8 mg/cm^2 than 0.8 to 1.0 mg/cm^2.

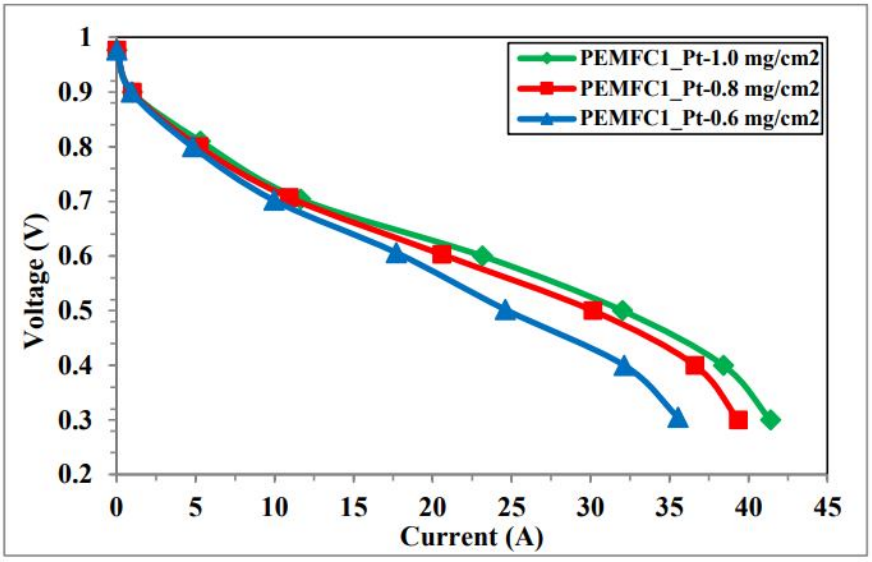

Figure 3.6 Effect of catalyst loading on performance of PEMFC 1

IV. CONCLUSIONS

First, a computational fluid dynamics study on two active area PEMFCs with three types of serpentine flow fields (1-S, 2-S and 3-S) has been carried out and key parameters such as pressure drop, reactants mass fraction, liquid water activity, the membrane water content, polarization and performance of the PEMFC were presented.

The following conclusions were drawn from this study.

1) Highest pressure drops were observed in single (1-S) and lowest pressure drops were observed in triple (3-S) serpentine flow fields. Therefore the 3-S flow field is considered for further investigations.
2) Oxygen mass fraction distributions were more uniform than hydrogen mass fraction distributions.
3) Liquid water activity in the cathode channels is less at inlet and increases gradually towards outlet and 3-S flow field has the better water removal capability
4) PEMFCs with triple serpentine flow field performs better than PEMFCs with single and double serpentine flow fields.
5) A thin membrane (N212) offers less ohmic resistance than thick membrane (N112 and N117) and results in improvement in the cell performance.
6) Fuel cell performance was increased with increase in platinum loading from 0.6 to 1.0 mg/cm^2. Rate of increase in performance is more when the platinum loading increased from 0.6 to 0.8 mg/cm^2 than 0.8 to 1.0 mg/cm^2.

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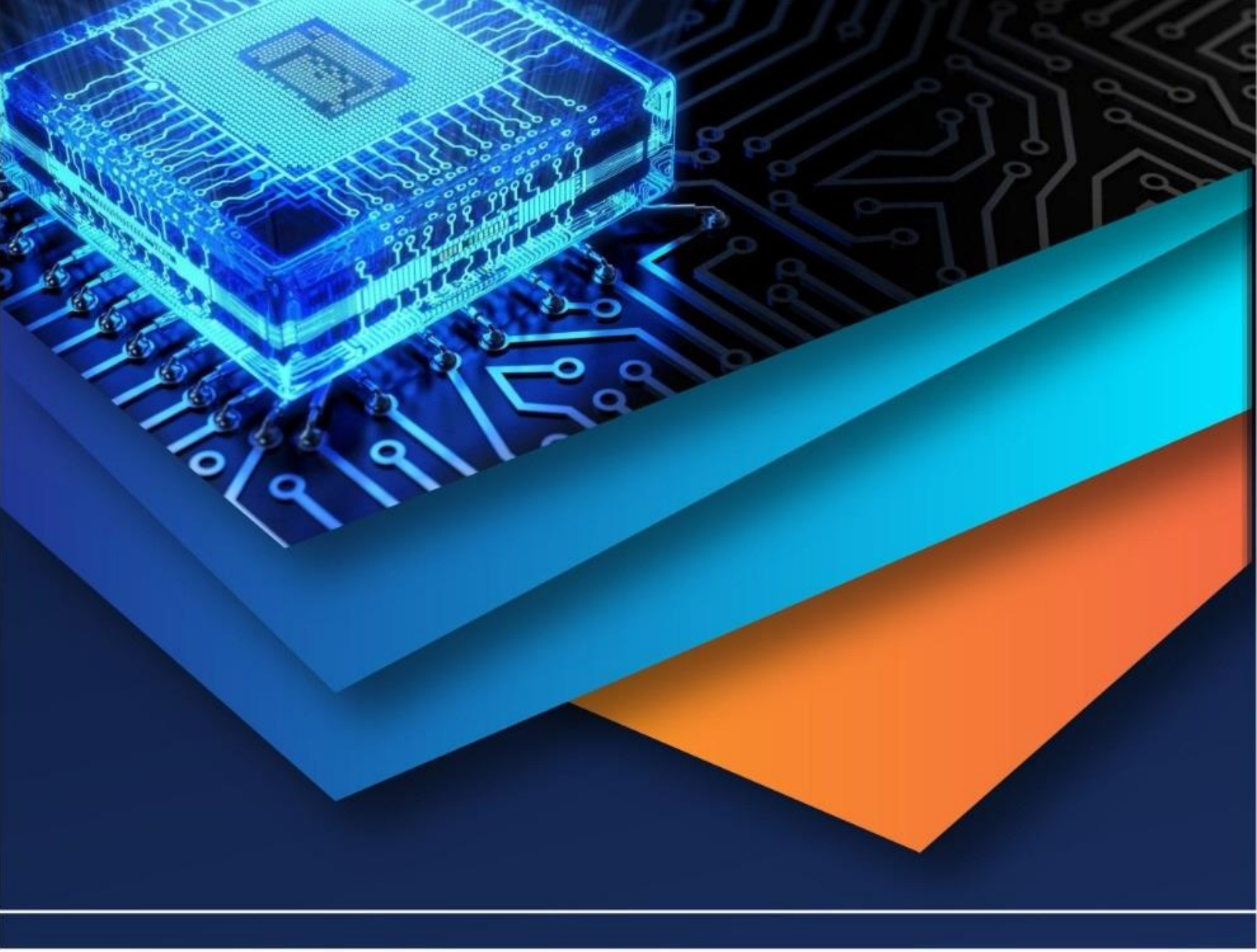

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