OPTIMIZATION OF BIPOLAR PLATE DESIGN FOR FLOW AND TEMPERATURE DISTRIBUTIONS USING NUMERICAL TECHNIQUES

by

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ABSTRACT

Optimization of Bipolar Plate Design for Flow and Temperature Distributions Using Numerical Techniques

by

Kiran Mohan Veepuri

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Associate Professor of Department of Mechanical Engineering
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Although water is fed controllably into the flow channels in the bipolar plates surrounding the membrane electrode assembly (MEA), the complex flow geometry can lead to non-uniformity of the flow and temperature distribution inside the channels. In addition, non-uniform temperature distribution in the cell will affect the electrochemical process for hydrogen production or fuel cell applications. There are many studies on the theoretical analysis of fuel cells, but not many have been reported on the characteristics of the PEM electrolyzer.

In this thesis work, numerical simulations were carried out on the basic bipolar plate given by the Proton Energy Systems in the United States. A 3-D steady state, incompressible flow model was developed. Finite volume method was used to solve the model for flow and temperature distributions inside the channels of the bipolar plate.
A parametric study was performed based on number of inlets and outlets and an optimized bipolar plate design was selected. Later, the optimized model was again simulated for two-phase flow. The flow and temperature distributions inside the channels of the new bipolar plate design were found to be uniform even for two-phase flow. Again a parametric study was performed based on volumetric flow rate of water and mass flow rate of oxygen production. Results were tabulated and numerical values were compared with the back of the envelope calculations.
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NOMENCLATURE

\( C_p \) Specific heat at constant pressure, J·kg\(^{-1}\)·K\(^{-1}\)

\( D \) Hydraulic diameter, m

\( F \) Body force, N

\( g \) Acceleration due to gravity, m·s\(^{-2}\)

\( K \) Coefficient of thermal conductivity, W·m\(^{-1}\)·K\(^{-1}\)

\( n \) Number of phases

\( \Delta P \) Pressure drop, Pa

\( p \) Static pressure, Pa

\( Q \) Volumetric flow rate, m\(^3\)·s\(^{-1}\)

\( Re \) Reynolds number

\( S_h \) Heat of chemical reaction, kg·K·m\(^3\)·s\(^{-1}\)

\( T \) Temperature, K

\( u_i \) Mean velocity component (i = 1, 2, 3), m·s\(^{-1}\)

\( u_j \) Mean velocity component (j = 1, 2, 3), m·s\(^{-1}\)

\( u_k \) Mean velocity component (k = 1, 2, 3), m·s\(^{-1}\)

\( \bar{\text{g}} \) Velocity of the fluid

\( \bar{g}_m \) Mass-averaged velocity, m·s\(^{-1}\)

\( \bar{g}_{d,r,k} \) Drift velocity for secondary phase k
\( w_i \)  Length coordinate \( i \) \((x,y,z)\), m

\( w_j \)  Length coordinate \( j \) \((x,y,z)\), m

\( w_k \)  Length coordinate \( k \) \((x,y,z)\), m

\( \lambda \)  Thermal conductivity, \( W \cdot m^{-1} \cdot K^{-1} \)

\( \mu \)  Dynamic viscosity, \( kg \cdot m^{-1} \cdot s^{-1} \)

\( \mu_m \)  Viscosity of mixture, \( kg \cdot m^{-1} \cdot s^{-1} \)

\( \nu \)  Kinematic viscosity, \( m^2 \cdot s^{-1} \)

\( \rho \)  Density, \( kg \cdot m^{-3} \)

\( \rho_m \)  Mixture density, \( kg \cdot m^{-3} \)

\( \rho_k \)  Density of phase \( k \), \( kg \cdot m^{-3} \)

\( \alpha_k \)  Volume fraction
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CHAPTER 1

INTRODUCTION

1.1 Global Picture

One of the main reasons for many people doing research on Proton Exchange Membrane Electrolysis Cell (PEMEC) for production of hydrogen is “Global warming”. Global warming is the increase in the average temperature of the Earth’s near-surface air and oceans. Increasing global temperature will cause sea level to rise, and is expected to increase the intensity of extreme weather events and to change the amount and pattern of precipitation. In the past century, Earth’s temperature has risen about 1°F. The global sea levels have risen 4 to 8 inches [1]. The past 50 years of warming has been attributed to human activity. On Earth, the major greenhouse gases are carbon dioxide (CO$_2$), methane (CH$_4$) and ozone.

Human activity since the industrial revolution has increased the concentration of various greenhouse gases, leading to increased radiative forcing from CO$_2$, CH$_4$, tropospheric ozone, chloro flavo carbons (CFCs) and nitrous oxide. In all, methane is a more effective greenhouse gas than carbon dioxide, but its concentration is much smaller so that its total radiative effect is only about a fourth of that from carbon dioxide. Some other naturally occurring gases contribute very small fractions of the greenhouse effect. The atmospheric concentrations of CO$_2$ and CH$_4$ have increased by 31% and 149%
respectively since the beginning of the industrial revolution in the mid-1700s [2]. Fossil fuel burning has produced about three-quarters of the increase in CO$_2$ from human activity over the past 20 years. Fig.1.1 shows the increase in the global fossil carbon emissions in the last two centuries. The fossil carbon emissions in the beginning of the industrial revolution were in control. But, after 1850, it rose drastically and is expected to increase at a higher rate in the future.

![Global Fossil Carbon Emissions](image)

**Fig.1.1 Global fossil carbon emissions in the last two centuries [3]**

Another important reason for the increasing research work on production of hydrogen is, the above mentioned fuels are non-renewable energy sources. Non-renewable energy is energy that comes from the ground and is not replaced in a relatively short amount of time. Fossil fuels are the main category of non-renewable energy. Fossil fuels include;
coal, oil and natural gas. They currently provide more than 85% of all the energy consumed in the United States, nearly two-thirds of the electricity and virtually all of the transportation fuels [4]. Moreover, the demand for fuels is expected to increase in the next two decades. In an article written by Michael T. Klarke, in the weekly journal “The Nation”, he stated that “we are nearing the end of the petroleum age and have entered the age of insufficiency”. The Department of Energy in the United States indicated that the global output of fuels would increase from 84 million barrels of oil equivalent (mboe) per day in 2005 to a projected 117.7 mboe in 2030 which is barely enough to satisfy the anticipated world demand of 117.6 mboe [5].

As a consequence, investigations of renewable energy strategies have recently become important, particularly for future world stability. The most important property of renewable energy sources is their environmental compatibility. In 2005 about 18% of global final energy consumption came from renewables [6]. Fig.1.2. shows the different kinds of renewable sources used to generate energy in 2005. From this pie diagram it can be found that more than 50% of the renewable energy that is used is generated from hydropower. Hydroelectricity is generated from hydropower and it does not produce greenhouse gases. But, hydroelectric projects can be disruptive to the surrounding aquatic ecosystems. The reservoirs of hydroelectric power plants in tropical regions may produce substantial amounts of methane and carbon dioxide due to plant material in flooded areas decaying in an anaerobic environment. Another important and serious reason is failure of large dams. The Banqiao Dam failure in southern China resulted in the deaths of 171,000 people and left millions homeless [7]. Other ways of producing energy from water is by electrolysis. This is a very simple process. When current is passed through water, the
water is split into hydrogen (H₂) and oxygen (O₂). The hydrogen thus produced can be used as energy carrier in many applications.

\[ 2H_2O(l) \rightarrow 2H_2(g) + O_2(g) \]  

(Eq. 1.1)

Since chemical (H₂) energy is being created, a minimum energy must be input to drive the process according to the laws of thermodynamics. In terms of electrical energy, this corresponds to a voltage greater than 1.23 V. In reality, the working voltage, generally known as the over voltage, represents a waste of energy or loss of efficiency. It has two main causes, one of which is the internal voltage drop loss due to the finite electrical resistance of the electrolyte, or the membrane in this case. The second is kinetic in origin, i.e., to do with the overall speed of the process at the electrode surface. [8]

---

**World Renewable Energy 2005**

![Pie chart](image)

- Large hydro: 58.23%
- Small hydro: 5.12%
- Wind power: 4.58%
- Biomass elec: 3.42%
- Geothermal elec: 0.72%
- Photovoltaic: 0.42%
- Other elec**: 0.05%
- Biomass heat*: 17.08%
- Solar heat: 6.83%
- Geothermal heat: 2.17%
- Biodiesel fuel: 1.21%
- Bioethanol fuel: 0.16%

Fig. 1.2. Renewable energies used in year 2005 [6]
1.2 Hydrogen

While the fossil-fuel era enters its sunset years, a new energy regime is being born that has the potential to remake civilization along radically new lines – hydrogen. Hydrogen is the most basic and ubiquitous element in the universe. It can be used as fuel in almost every application where fossil fuels are used. It never runs out and produces no harmful CO\textsubscript{2} emissions when burned; the only byproducts are heat and pure water. Hydrogen power will reduce the CO\textsubscript{2} emissions and mitigate the effects of global warming. In the long run, the hydrogen-powered economy will fundamentally change the very nature of our market, political and social institutions, just as coal and steam power did at the beginning of the Industrial Revolution.

Hydrogen can be produced from a diverse array of potential feedstocks, including water fossil fuels and organic matter. Commercial bulk hydrogen is usually produced by the steam reforming of natural gas. But, this method of hydrogen production is dependent on a potentially limited and volatile natural gas supply. On the other hand, this process results in moderate emissions of CO\textsubscript{2} and is not desirable. As discussed earlier, the better way of producing hydrogen is by electrolysis.

1.3 Electrolyzer

The electrolyzer is a device that generates hydrogen and oxygen from water through the application of electricity. It consists of a series of porous graphite plates through which water flows while low voltage direct current is applied. An electrolyzer stack consists of several cells linked in series. These cells are of two types namely monopolar and bipolar cell [9]. In the monopolar design the electrodes are either negative or
positive with parallel electrical connection of the individual cells (Fig. 1.3), while in the bipolar design the individual cells are linked in series electrically and geometrically (Fig. 1.4). One advantage of the bipolar cell design is that they are more compact than monopolar systems which give shorter current paths in the electrical wires and electrodes. This reduces the losses due to internal ohmic resistance of the electrolyte, and therefore increases the electrolyzer efficiency.

![Fig. 1.3 Monopolar design [9]](image)

![Fig. 1.4 Bipolar design [9]](image)
1.3.1 Alkaline Electrolyzer

Alkaline electrolyzers usually use an alkaline solution of sodium or potassium hydroxide (NaOH or KOH) that acts as the electrolyte, mostly with 20-30 wt% because of the optimal conductivity, they require using corrosion resistant stainless steel to withstand the chemical attack. These electrolyzers, generally, operate at a temperature of 70-100°C and at a pressure of 1-30 bar. The following are the two chemical reactions that take place at anode and cathode finally resulting in the production of hydrogen:

For the anode reaction it is:

\[
4H_2O(l) + 4e^- \rightarrow 2H_2(g) + 4OH^-(aq) \quad \text{(Eq. 1.2)}
\]

For the cathode reaction it is:

\[
4OH^-(aq) \rightarrow O_2(g) + 4e^- + 2H_2O(l) \quad \text{(Eq. 1.3)}
\]

And finally the overall electrolyzer reaction is:

\[
2H_2O(l) \rightarrow 2H_2(g) + O_2(g) \quad \text{(Eq. 1.4)}
\]

1.3.2 Solid Oxide Electrolyzers

Solid oxide electrolyzers, which use a solid ceramic material as the electrolyte that selectively transmits negatively charged oxygen ions at elevated temperatures, generate hydrogen in a slightly different way –

- Water at the cathode combines with electrons from the external circuit to form hydrogen gas and negatively charged oxygen ions;
- The oxygen ions pass through the membrane and react at the anode to form oxygen gas and give up the electrons to the external circuit.

Solid oxide electrolyzers must operate at temperatures high enough for the solid oxide membranes to function properly (about 500 – 800°C; compared to PEM electrolyzers,
which operate at 80-100°C, and alkaline electrolysers, which operate at 100-150°C). The solid oxide electrolyser can effectively use heat available at these elevated temperatures to decrease the amount of electrical energy needed to produce hydrogen from water. [10]

1.3.3 Proton Exchange Membrane Electrolyzer

Polymer electrolyte membranes (PEMs) were first developed for the chlor-alkali industry. These specialized materials, also known as ionomers, are solid fluoro-polymers which have been chemically altered to make them electrically conductive. The fluorocarbon chain has typically a repeating structural unit, such as \(-[\text{CF}_{2\text{m}}\text{CF}_{2}]_n\)-, where \(n\) is very large. Treatments like sulphonation or carboxylation, insert ionic or electrically-charged pendant groups, statistically spaced, into some of these base units giving, e.g., \([\text{CF(SO}_3\text{H})\frac{1}{4}\text{CF}_{2}]_m\)-, where \(m\) can range from \(n/5\) to \(n/20\) depending on the properties most suited for the application. Nafion, made by Du Pont, is the most commercially successful of such materials, and is available as thin pre-formed membranes in various thicknesses, or as a 5% solution which may be deposited and evaporated to leave a polymer layer of customized shape. The electrolysers that are based on polymer electrolyte membrane separators are mostly used for industrial purposes because they can achieve high efficiencies. These devices anticipate the imminent development of a renewable energy economy based on electricity and H\(_2\) fuel as complementary energy vector. [8]

A PEM electrolyzer is shown in Fig.1.5. Its efficiency is a function primarily of the membrane, electrocatalysts and the bipolar plate. This becomes crucial under high-current operation, which is necessary for industrial-scale application. The following reactions occur in a PEM electrolyzer:
Reaction at anode:

\[ 2\text{H}_2\text{O}_{(l)} \rightarrow 4\text{H}^+_{(aq)} + 4\text{e}^- + \text{O}_2(g) \]  
(Eq. 1.5)

Reaction at cathode:

\[ 4\text{H}^+_{(aq)} + 4\text{e}^- \rightarrow 2\text{H}_2(g) \]  
(Eq. 1.6)

Overall electrolyzer reaction:

\[ 2\text{H}_2\text{O}_{(l)} \rightarrow 2\text{H}_2(g) + \text{O}_2(g) \]  
(Eq. 1.7)

---

Fig. 1.5 Schematic diagram of a PEM electrolyzer [9]
1.3.3-1 Membrane

The membrane consists of solid fluoro-polymer which has been chemically altered in part to contain sulphonic acid groups, SO$_3$H, which easily release their hydrogen as positively-charged atoms or protons [H$^+$] [8]:

\[
\text{SO}_3\text{H} \leftrightarrow \text{SO}_3^- + \text{H}^+ \quad \text{(Eq. 1.8)}
\]

These ionic or charged forms allow water to penetrate into the membrane structure but not the product gases, molecular hydrogen (H$_2$) and oxygen (O$_2$). The resulting hydrated proton, H$_3$O$^+$, is free to move whereas the sulphonate ion (SO$_3$) remains fixed to the polymer side-chain. Thus, when an electric field is applied across the membrane the hydrated protons are attracted to the negatively charged electrode, known as the cathode. Since a moving charge is identical with electric current, the membrane acts as a conductor of electricity. It is said to be a protonic conductor. A typical membrane material that is used is called “Nafion”. Because “Nafion” is a solid, its acidity is self-contained and so chemical corrosion of the electrolyzer housing is much less problematic. Furthermore as it is an excellent gas separator, allowing water to permeate almost to the exclusion of H$_2$ and O$_2$, it can be made very thin, typically only 100 microns. This improves its conductivity so that the electrolyzer can operate effectively even at high currents.

1.3.3-2 Electrocatalyst

A solid catalyst speeds up chemical reactions due to its surface action. As a simple example, two H atoms held loosely on a surface are much more likely to collide and make H$_2$ gas than if they are dispersed in a liquid with billions of water molecules in-between. This is a spatial or localized concentration effect. The case of O$_2$ evolution is
much more complex. Two water molecules must be broken into their constituent atoms; then the two O atoms must combine. The electrocatalyst at the anode is a special catalyst, which facilitates this process by withdrawing electrons from the water such that the H atoms are ejected as protons, which enter the membrane. Water is said to be activated by charge-transfer. The OH or O atoms are very reactive in their free state. However, when fixed at the surface by chemical bonds they are much more stable. When more water encounters the surface, its protons are ejected in turn and O atom are accumulated. These are then able to combine easily by surface diffusion just as described for hydrogen. It is said that the surface provides a low-energy pathway, which is intrinsically much faster because the speed of the reaction is related exponentially to the energy difference.

It is easy to visualize that if the cathode and anode surfaces, respectively, attract H or O atoms too strongly, the surfaces will become completely covered with these intermediates and the catalytic process stops. On the other hand, if protons or water are not attracted strongly enough, the process never gets going. Only when there is a moderate strength of binding of reactants and intermediates at the electrode surfaces, the right balance will be obtained. This is the key factor in determining if a solid catalyst will work efficiently. It is also obvious that the larger the catalyst surface area available, the more H₂ and O₂ will be produced in a given time, i.e., a higher current will flow in the electrolyzer.

Platinum is long known to be the best catalyst for water electrolysis due to its moderate strength of adsorption of the intermediates of relevance. It has the lowest over-voltage of all metals. However due to its cost, and the preferred operation of the electrolyzer at high current, ingenious ways have been devised to deposit ultra-fine Pt
particles either on the electrode support plate, or directly onto the membrane, which is then clamped for good electrical continuity. A current of 1-3 A/cm² can be obtained from as little as milligrams of Pt spread over the same area. [11]

1.3.3-3 Bipolar Plate

The bipolar plates are in weight and volume the major part of the PEM electrolyzer cell stack, and are also a significant contributor to the stack costs. The bipolar plate is therefore a key component if power density has to increase and costs must come down. Bipolar plates have to accomplish many functions in the electrolyzer cell stack. Main functions are:

- Distribution of water uniformly over the active areas;
- Uniform thermal distribution to water from the membrane;
- Conduction of current from cell to cell;
- Preventing leakage of gases and coolant.

For uniform fluid flow distribution inside the channels of the bipolar plate, tight tolerances on channel dimensions have to be met. Small deviations lead to reduced efficiency, poor utilization of the catalyst and reduced hydrogen output and should therefore be avoided. Uniform thermal distribution of water in the channels is achieved only if the flow distribution is achieved. To minimize the ohmic losses the material needs to have low bulk resistance and low contact resistance [12]. Today several materials are being used in bipolar plates.
1.4 Literature Review

Hydrogen production from water electrolysis using proton exchange membranes has been studied to some degree since the development of the first PEM water electrolyzer by the General Electric Company [13]. Barbir [14] discussed the difference between the electrical grid independent and grid assisted hydrogen generation. It is also shown that electrolytically generated hydrogen from an integrated system of both grid connected and grid independent is stored and then via fuel cell converted back to electricity when needed. Grigoriev et al. [15] discussed the effects of the operating temperature and pressure on the volt-amperic curves of the electrolysis cell. The volt-amperic curves of electrolysis cell with different catalyst at 90°C were presented.

A theoretical model was proposed by Choi et al. [16], to explain the current-potential characteristics of PEM electrolysis cell based on the involved charge and mass balances as well as Butler-Volmer kinetics on the electrode surfaces. It is found that the reduction kinetics at the cathode is relatively fast while the anodic overpotential is mainly responsible for the voltage drop.

A technology where the membrane itself is catalytically effective, splitting water into protons and hydroxyl ions is described by Balster et al. [17]. A mature electromembrane technology was reviewed. In addition, bipolar, ion-exchange membrane technology was extensively described. The catalyst and absorbent technologies under development for the extraction of hydrogen from the natural gas to meet the requirements from the PEMFC were discussed by Farrauto et al. [18]. Electrochemical characterization of the various electrocatalytic powders was conducted in 0.5M H$_2$SO$_4$ electrolyte at room temperature, by supporting the powders on titanium plates using a spraying technique.
The performance of the various anode electrocatalysts were evaluated in a single PEM water electrolysis cell up to current densities of 2 A cm$^{-2}$ with the total (anode and cathode) noble metal loadings less than 2 mg cm$^{-2}$.

Millet et al. [20] discussed the design and performance of a PEM water electrolyzer. High cell voltages were contributed to poor electrical connections which introduced a significant ohmic loss. Rasten [21] provided a study of various electrocatalysts for water electrolysis using proton exchange membrane. A solid polymer electrolyzer was developed using IrO$_2$ as the anode catalyst and Pt black as the cathode catalyst at loading of 3 mg/cm$^2$ [22].

Since 1987 Mitsubishi Heavy Industries, Ltd. has been developing solid polymer water electrolyzer technology [23]. A chemical plating technique was used to plate iridium metal onto each side of the Nafion membrane. A 50 cm$^2$ solid polymer electrolyte electrolyzer was developed using a hot press method to adhere the catalyst film to the membrane [24]. Based on the results mentioned above, a 2500 cm$^2$ solid polymer electrolyte electrolyzer was developed [25]. A high pressure solid polymer electrolyte water electrolyzer was developed with Pt and Ir black serving as the anode catalyst and Pt black as the cathode catalyst [26]. The development of membrane electrode assemblies (MEAs) for a reversible solid polymer fuel cell was examined using Pt, Rh, Ir, and Ir-Ru mixed oxides, as the oxygen evolution electro-catalyst [27]. Millet [28] provided an experimental study for an electrode membrane electrode (EME) cell operated at high current densities. From their experimental work, the electric potential across the cell and membrane alone were computed, since the determination of anodic and cathodic over-voltages usually requires the use of a membrane strip [29, 30]. They also determined if a
membrane strip can be used as a reference potential to measure separately each term of the cell voltage.

A micro-scale model was developed by Zhou et al. [31] to predict the contact resistance between the bipolar plate and the gas diffusion layer (GDL) in PEMFC. Bipolar plate surface topology is simulated as randomly distributed asperities and gas diffusion layer modeled as randomly distributed cylindrical fibers. Heinzel et al. [32] discussed the method of production of low cost bipolar plates for PEM cells. Materials with low cost and high availability, high chemical resistance and good mechanical properties were chosen for manufacturing of bipolar plates. It was found that the cost for production of bipolar plate by injection moulding is very low. Injection moulding of composite bipolar plates for PEMFC compared with moulding technologies and the production feasibility of polypropylene based composites at different temperatures was tested by Muller et al. [33]. Electrical and chemical stability of the plates at different temperatures was tested.

Barreras et al. [34] demonstrated that the flow distribution inside a bipolar plate can be visualized by applying laser-induced fluorescence in an optically accessible model. A parallel-channel commercial bipolar plate with a transparent plastic plate cover was investigated. A three-dimensional transient numerical model of PEMFC was developed and the effect of gas flow-field design in the bipolar plates tested by Atul et al. [35].

Most of the research on the PEM electrolyzer cell so far, focused on the experimental studies and numerical analysis of the catalyst, electrolytic membrane and membrane electrode assembly. Even though a little amount of research work was done on
bipolar plate, no numerical analysis was done on the design optimization to obtain uniform flow and temperature distribution. The main aim of this thesis is to design a bipolar plate which gives uniform flow and temperature distribution of the fluid in the channels.

1.5 Objective of Research

The present work is funded by the Department of Energy of the United States under award DE-FG36-03GO13063. Some of the research objectives are outlined as follows:

- To develop a computational model for the bipolar plate of the PEM electrolyzer;
- To analyze the flow and temperature distribution of the fluid inside the channels of the above developed bipolar plate;
- To redesign the bipolar plate so as to obtain homogeneous flow and temperature distribution;

In the next chapter, the design of the bipolar plate is described. The numerical model and the operating and boundary conditions that will be used are also discussed. Computational meshing and the mesh independent study will be discussed in Chapter 3. After mesh independent study, the design optimization of the bipolar plate in order to achieve uniform flow and temperature distribution will be discussed in Chapter 4. The new bipolar plate that is designed in Chapter 4 is again simulated for two-phase flow. The results are shown in Chapter 5. In Chapter 6, the numerical experiment performed for this thesis is concluded and future work that can be done in order to achieve a good design in other aspects also are pointed out.
CHAPTER 2

PROBLEM DESCRIPTION AND NUMERICAL MODELING

2.1 Problem Description

The PEM electrolysis cell is used to produce hydrogen from the water flowing through the bipolar plate as discussed earlier in Chapter 1, when water comes in contact with the catalyst surface. Fig. 2.1 shows the basic two-dimensional schematic picture of the PEM electrolysis cell. The well known catalyst that is used in this process is platinum. This increases the cost of hydrogen produced by this process. To improve the cost efficiency of this process, the platinum catalyst must be used in a much more effective way.

Fig. 2.1 PEM Electrolysis cell [36]
The effective use of platinum is achieved by the uniform flow of water in the channels of the bipolar plate. From the experiments done by Barreras et al. [34] and Atul et al. [35], it can be found that the flow distribution of water inside the channels of the bipolar plate is not uniform. Fig. 2.2 shows the distribution of water inside the channels of the bipolar plate. The flow rate in the end side channels is more when compared with the middle side channels. In this case the platinum catalyst is more effective in the ends channels when compared with the middle channels. This results in low efficiency of hydrogen production.

To improve the efficiency of the PEM electrolysis cell and to make maximum use of the platinum catalyst, a new bipolar plate has to be designed which gives uniform flow of water in the channels.

Fig. 2.2 Flow distribution of water in channels of the bipolar plate [34]
The geometry of the bipolar plate of the PEM electrolysis cell that is considered is shown in Fig. 2.3.

The above shown bipolar plate consists of 60 channels, each with a width of 0.08 inches and a height of 0.035 inches. The length of each channel is 9.52 inches. The channels are connected to one inlet and one outlet with the header section, which is one inch in width and 9.52 inches in length. The inlet and outlet are circular in cross-section with 1 inch diameter. The header is designed with cylindrical pellets in it. This changes the flow direction of water and helps to flow into the channels.
The water is fed into the bipolar plate from the inlet with a volumetric flow rate of 0.3 liters per minute (lpm). The velocity of the water is assumed to be uniform at the entrance of the inlet along the cross-sectional area. The properties of water like density and viscosity etc. are considered at a temperature of 80°C. The bottom surfaces of all the channels will be in contact with the catalyst layer. This surface is known as active region as shown in Fig. 2.3. A constant heat flux of 2500 W/m² is applied to the surfaces at the bottom of the bipolar plate.

To know whether the flow inside the bipolar plate is laminar or turbulent, the Reynolds number is calculated. The Eq. 2.1 below shows the formula to calculate the Reynolds number (Re):

\[
\text{Re} = \frac{\rho \bar{u} D}{\mu}
\]  
(Eq. 2.1)

Here “\(\rho\)” and “\(\mu\)” are the density and viscosity of the water. “\(\bar{u}\)” is the velocity of the water at the inlet and “\(D\)” is the hydraulic diameter of the inlet. In this case the hydraulic diameter is simply the diameter of the inlet area. The value of the Reynolds number for the above boundary conditions is 172. This value is much less than 2400. Therefore this model falls in the laminar flow region. Thus, laminar, incompressible flow model was used for further calculations.

2.2 Governing Equations

The steady state governing equations for continuity, momentum and energy for laminar flow can be expressed as follows:

\[
\frac{\partial}{\partial \tilde{w}_i}(\rho \tilde{u}_i) = 0
\]  
(Eq. 2.2)
\[
\frac{\partial}{\partial x_i} (\rho u_i u_k) = \frac{\partial}{\partial x_i} (\mu \frac{\partial u_i}{\partial x_k}) - \frac{\partial p}{\partial x_k} \quad \text{(Eq. 2.3)}
\]

\[
\frac{\partial}{\partial x_i} (\rho u_i T) = \frac{\partial}{\partial x_i} \left( \frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \right) + S_h \quad \text{(Eq. 2.4)}
\]

2.3 Numerical Method

The flow of water through the micro channels of the bipolar plate and the complex geometry of the bipolar plate make the study of the flow distribution difficult. To simplify the analysis, the physical model is replaced by infinite points and 3-D elements. The points are known as grid-points or nodes. The 3-D elements are of three types: hexahedrals, tetrahedrons and prisms. These elements are known as grid elements or cells. These nodes and cells define the entire geometry and this model is known as finite element (FE), finite volume (FV) or finite difference (FD) model depending on the type of numerical method used. For the current numerical experiment, finite volume method (FVM) is followed. When the above mentioned mathematical governing equations will be solved for this model, it gives very close results of pressure, temperature, velocity distributions etc when compared the actual physical device. The governing equations will be solved only at the grid points representing the geometry.

The computational mesh model of the geometry is obtained from the commercial software HYPERMESH 7.0 and is solved in the Cartesian coordinate system using the general purpose CFD code FLUENT 6.3.26 which is based on finite volume method. FLUENT is powerful commercial software for solving fluid flow, heat transfer and chemical reaction problems [37].
2.3.1 Finite Volume Method

The finite volume method (FVM) is one of the most versatile discretization techniques used in computational fluid dynamics (CFD). Based on the control volume formulation of analytical fluid dynamics, the first step in the FVM is to divide the domain into a number of control volumes (elements) where the variable of interest is located at the centroid of the control volume. The next step is to integrate the differential form of the governing equations over each control volume. Interpolation profiles are then assumed in order to describe the variation of the concerned variable between the cell centroids. The resulting equation is called the discretized or discretization equation. In this manner, the discretization equation expresses the conservation principle for the variable inside the control volume.

The most compelling feature of the FVM is that the resulting solution satisfies the conservation of quantities such as mass, momentum, energy and species. This is exactly satisfied for any control volume as well as for the whole computational domain and for any number of control volumes. Even a proper coarse grid solution may exhibit similar integral balances. It is also preferred while solving partial differential equations containing discontinuous coefficients.

2.3.2 Segregated Solution Algorithm

The segregated solver was used to solve the governing integral equations for the conservation of mass, momentum and energy equations. The numerical scheme that is used in this study is first order upwind scheme and SIMPLE (semi-implicit method for pressure-linked equations) algorithm is used to resolve the coupling between pressure and velocity. The discrete and nonlinear governing equations are linearized using an implicit
formulation with respect to a set of dependent variables in every computation cell. The resulting algebraic equations are solved iteratively using an additive correction multi-grid method with Gauss-Seidel relaxation procedure.

2.4 Boundary Conditions

2.4.1 Velocity Inlet Boundary Condition

The velocity inlet boundary condition is used to define the flow velocity, along with all other relevant scalar properties of the flow, at the flow inlets. User can define the inflow velocity by specifying the velocity magnitude and direction, the velocity component, or the velocity magnitude normal to the boundary. If the cell zone adjacent to
the velocity inlet is moving, the user can specify either relative or absolute velocities. In this case, the velocity magnitude and direction type was used.

2.4.2 Pressure Outlet Boundary Condition

Pressure outlet boundary conditions require the specification of a static (gauge) pressure at the outlet boundary. The value of the specified static pressure is used only while the flow is subsonic. If the flow becomes locally supersonic, the specified pressure will no longer be used; pressure will be extrapolated from the flow in the interior. All other flow quantities are extrapolated from the interior. A set of “backflow” conditions is also specified should the flow reverse direction at the pressure outlet boundary during the solution process. Convergence difficulties will be minimized if the user specifies realistic values for the backflow quantities.

2.4.3 Thermal Boundary Condition

This type of boundary condition is defined only when the energy equation is chosen to solve. At flow inlets and outlets, the temperatures are set. At the walls the following thermal conditions can be used:

- Specified heat flux
- Specified temperature
- Convective heat transfer
- External radiation
- Combined external radiation and external convective heat transfer

In the current study case, specified heat flux is specified at the walls that come in contact with the platinum catalyst and the inlet temperature is also set.
2.4.4 Wall Boundary Conditions

This type of boundary conditions are used to bound the fluid and solid regions. In viscous flows (which is considered in the current numerical experiment), the no-slip boundary condition is enforced at the walls. Several other pieces of information that can be given under the wall boundary condition are shear conditions, wall roughness etc. But, for this numerical experiment all these conditions are neglected.
CHAPTER 3

NUMERICAL MODELING FOR THE FLOW AND TEMPERATURE DISTRIBUTION IN THE BIPOLAR PLATE

3.1 Baseline Design Analysis

The purpose of the numerical analysis of the bipolar plate of PEMEC is to check the flow distribution of the water inside the channels and also the temperature distribution in the fluid due to the constant heat flux supplied to channels from the bottom of the channels. The analysis is done on the baseline design of the bipolar plate and then studied. If the flow and temperature distribution inside the channels is not uniform then it has to be redesigned so as to achieve uniform distribution of flow and temperature. For analysis, as mentioned in the earlier chapters, meshing is done using the powerful commercial software HYPERMESH 7.0 and then simulation is done using the FLUENT software. Different zones like inlet, outlet, walls etc. are set up in HYPERMESH and then the boundary conditions are incorporated using FLUENT. The different boundary conditions specified for the current model are:

- Inlet volumetric flow rate : 0.3 lpm
- Inlet temperature : 80°C
- Operating pressure : 1 atm
- Heat flux : 2500 W/m²
All the walls that bound the fluid, other than the walls that come in contact with the catalyst, are assumed to be adiabatic. The properties of water like density, viscosity, etc. are taken at 80°C. From the calculations of Reynolds number (Re=172) it is known that water flow falls into laminar flow range; so laminar, incompressible flow model is set up for the analysis. Once the model is set up, it is simulated for several iterations until the solution is converged according to the absolute iterative convergence criterion. The absolute convergence criterion is used by setting the absolute criteria to $10^{-6}$. After the simulation, the results are plotted and the conclusions are made. But in this whole process, the results obtained need to be mesh independent. This is done by performing a mesh independent study.

3.2 Mesh Independent Study

A mesh independent study otherwise known as grid independent study plays a very important study in the finite element analysis (FEA), finite difference method (FDM) and finite volume method (FVM). After the given CAD model is divided into finite elements and simulated, the obtained results are plotted. When the same model is refined and simulated it gives different results. This variation is because of the fact that the results obtained after simulation depends on the grid. In order to avoid this, a grid independent study is performed through which the percentage of error can be minimized. Once the percentage error is within the tolerance limit, it can be said that the model with that mesh is grid independent.

In the current numerical experiment, the grid independent study is done for fluid flow analysis alone. Since the aim of this experiment is to achieve uniform flow
distribution inside the channels, the grid independent study is also done by varying the number of elements across the width of the channels. Fig. 3.1 (a) shows the computational mesh model and Fig 3.1 (b), (c) and (d) show different number of mesh elements inside the channels.

Fig 3.1(a) Computational mesh model of the bipolar plate
Fig 3.1 (b), (c) & (d) Closer images of the grid inside the channels with element density 4, 6 and 8, respectively
The grid independent study is carried out by plotting the pressure at a point inside the channels against the number of elements. The results are obtained at Cartesian coordinates (0.1148, 0.0005, -0.03) which is approximately at the centre of the middle channel.

![Mesh Independent Study](image)

**Fig 3.2** Mesh independent study plot

Fig 3.2 above shows the mesh independent study plot. In this plot, it can be seen that the percentage error between the 8 elements model and the 10 elements model is much smaller (0.3%) when compared to differences of the other models. By considering the percentage error differences between the models and the computational time taken to run the model for simulation, the model with 8 elements across the channel is selected as a baseline model. This model will be used for further studies.
3.3 Velocity Distribution

As mentioned earlier, the mesh independent study was carried out for fluid flow analysis. After the mesh independent study was done and the baseline model was selected, the fluid flow distribution inside the channels was studied. The velocity distribution inside the channels is plotted for the baseline model and is shown in Fig 3.3.

Fig 3.3 Velocity distribution inside the channels of the bipolar plate & CAD model showing plane of cut AA & BB
The CAD figure shown in Fig 3.3, along with the velocity plot shows the plane of cut where the slice is taken to plot the results with help of the AA and BB. The plane BB is along the channel at a half the height of the channels. From this figure it is clear that the flow distribution inside the channels is not uniform. In the end channels, where the velocity is very high, the water molecules might not stay in contact with the catalyst layer for sufficient amount of time for the reaction to take place. And in the middle channels, where the movement of water molecules is very slow, if the time taken by the water molecules to move on the catalytic surface is more than the reaction time it leads to the shortage of water for the reaction to take place at the surface. This leads to the improper use of the catalyst. And since the catalyst that is generally used in a PEM electrolysis cell is platinum, which is very costly, the production cost goes up. This indirectly means the efficiency of the PEM electrolysis cell is less which is undesirable.

To reduce the production cost of the hydrogen using a PEM electrolysis cell, a new bipolar plate has to be designed which gives a uniform flow distribution inside all the channels.

In Chapter 4, several configurations of bipolar plates that are designed and simulated to achieve uniform flow will be discussed. These designs will also be studied for the thermal distribution inside the channels. For a good bipolar plate the uniform distribution of temperature is also very important. Finally, optimized design of the bipolar plate will be chosen from those designs. This design will be used as the new bipolar plate for further analysis.
CHAPTER 4

DESIGN OPTIMIZATION OF THE BIPOLAR PLATE FOR UNIFORM FLOW AND TEMPERATURE DISTRIBUTION

4.1 Reason for Non-Uniform Flow

In the previous chapter, it is shown that the baseline design of the bipolar plate gives the non-uniform flow distribution inside the channels. In this chapter, the design will be changed and simulated to achieve uniformity. But, to change the design, one should first know the reason for the non-uniformity. If that is known, then it’ll be easy to rectify it by changing the design in the areas where it is required.

The isometric view of the baseline design along with the coordinate axes is shown in Fig 4.1. This figure helps in understanding the flow of water inside the bipolar plate along with the direction. The water is fed into the bipolar plate from the inlet duct in negative y-direction flows into the header along the 7 intermediate channels that connect inlet duct and the header. Because of this, the flow direction is changed to negative x-direction. Here, one should make a note that the velocity vector is not exactly in the negative x-direction. There will be non-zero y and z components of the velocity of the water. Due to the z-component velocity vector, as soon as the water enters the header, some amount of the water is diverted in z direction and enters the initial channels. In the later section of the header, the water is deflected because of the cylindrical pellets inside
the header. Even though the water is deflected, the major component of the velocity vector will be in the $x$-direction. So, the water moves completely to the end of the header in the negative $x$-direction and when it is blocked by the wall, it changes its direction and enters the end channels with high velocity. Due to the deflection because of the pellets some amount of water enters the middle channels, but the amount of water that enters the end channels is more when compared with the amount that enters the middle channels.

Fig 4.1 CAD model of the baseline design (Isometric view)
In order to achieve the uniform flow, changes should be made in the header in such a way that same amount of water is fed into the middle channels as in the end channels. In the next few sections, several modifications made in the design will be discussed as different cases.

4.2 Design Modification

4.2.1 Case-1

Since the flow direction in the channels is positive z-direction, it is better if the water in the header also flows in the z-direction. Taking this point into consideration, a new bipolar plate is designed which is shown in Fig 4.2.

Fig 4.2 New bipolar plate design: Case-1
The new bipolar plate designed has 6 inlets and 6 outlets as shown in Fig 4.2. The number six for inlets and outlets was selected randomly. As the total number of channels is sixty, it was assumed that one inlet duct should supply water sufficiently to 10 channels. The centers of the inlet and outlet ducts are at a distance of 1.5 inches from the entrance and exit of the channels respectively. Even though the number of inlets and outlet is changed, the diameter of the ducts still remains the same (1 inch). All the inlet and outlet ducts are placed at equal distances, such that each duct covers 10 channels. The Mesh was generated for this geometry with 8 elements across the channels and then simulated to study the flow and temperature distribution inside the channels.

In this case, the energy equation is solved to know the temperature distribution inside the channels when a constant heat flux is supplied. The model is run for the same operating conditions and in the boundary conditions, a constant heat flux of 2500 W/m² is supplied to the channels from the bottom surface. Even though the volumetric flow rate is not changed (0.3 lpm), the inlet velocity which is defined in FLUENT is reduced since the number of inlet ducts increased. Thus the Reynolds number is dropped to 114. After the model is run for the mentioned boundary and operating conditions, a velocity distribution plot and a temperature distribution contour were plotted. The slice was taken at the same place as mentioned earlier in Chapter 3. Fig 4.3 shows the velocity distribution and pressure distribution and Fig. 4.4 shows temperature distribution inside the bipolar plate.
Fig 4.3 Velocity distribution plot and pressure contour: Case-1

Fig 4.4 Temperature contour: Case-1
The velocity profile drawn in Fig 4.3 shows that the velocity in each channel. The mean velocity of was found to be 0.083 m/s and the percentage deviation of velocities in each channel was found to be 3.87%. With this it can be said that there is uniform flow distribution inside the channels and the pressure distribution reads the pressure drop between the inlet and outlet around 100 Pa. From Fig 4.4 it is clear that even the temperature distribution inside the bipolar plate is uniform.

Even though uniform flow and temperature distribution is achieved using the new bipolar plate design of Case-1, it cannot be said that this design is the optimized model. Thus, a parametric study is done by changing the number of inlets and outlets. If similar results are obtained with less number of inlets, then it can be considered as optimized bipolar plate design. A Parametric study is carried out for number of inlets 1, 2 and 4 on the top of the header similar to the new bipolar plate design of Case-1.

4.2.2 Case-2

In this case study, the bipolar plate was designed with one inlet and one outlet. The centre of the inlet and outlet are located at 1.5” away from the entrance and exit of the channels similar to the design in Case-1 and exactly at the middle of the whole width of the bipolar plate as shown in Fig 4.5.

The operating and boundary conditions are the same as for the Case-1. The mass flow rate is same as the Case-1, but since there is only one inlet duct with a radius of 1 inch, the inlet velocity increases and thus the Reynolds number is increased to 687. Even though the Reynolds number is increased it is still in the laminar flow region.
Fig 4.5 CAD model of bipolar plate with one inlet and outlet: Case-2

Fig 4.6 Velocity distribution plot and pressure contour: Case-2
In this case, the water rushes into the middle channels as they are closer to the inlet duct. The mean velocity was found to be 0.02 m/s and the percentage deviation of velocities in each channel was found to be 47.84%. The mass flow rate in the end channels is almost negligible. As a result, even the temperature contour is also not uniform. The temperature is more in the end channels and less in the middle channels. Thus, it can be said that this is not a good bipolar design. Thus, Case-3 is run with a new bipolar plate design with 2 inlets and 2 outlets.
4.2.3 Case-3

This case also has all the conditions similar to the previous cases except the velocity is slightly less than that for case-2 and the Reynolds number is calculated as 343. The CAD model is shown in Fig 4.8 and the numerical results are shown in Fig 4.9 and Fig 4.10.

Fig 4.8 CAD model of the bipolar plate with two inlets and outlets: Case-3
Fig 4.9 Velocity distribution plot and pressure contour: Case-3

Fig 4.10 Temperature contour: Case-3
The bipolar plate design with two inlets and two outlets gave a good velocity profile when compare with the results obtained in Case-2. But, the results are not as good as of Case-1. The mean velocity of was found to be 0.083 m/s and the percentage deviation of velocities in each channel was found to be 12%. Even though the velocity profile is comparable to some extent, the pressure distribution inside the bipolar plate as shown in Fig 4.9 is not uniform. Even the temperature distribution, shown in Fig 4.10 is not uniform. Thus, this cannot be considered as an optimized bipolar plate design.

4.2.4 Case-4

This case is run with a new bipolar plate design with four inlets and four outlets. The operation and boundary conditions are still the same except the velocity is lower than that in the Case-3 and the Reynolds number is calculated as 172. Fig 4.11, 4.12 and 4.13 show the CAD model and simulated results, respectively.
Fig 4.12 Velocity distribution plot and pressure contour; Case-4

Fig 4.13 Temperature contour: Case-4
The velocity profile obtained in this is very similar to that obtained in Case-1 with 6 inlets and 6 outlets. Even though the pressure distribution inside the bipolar plate is slightly non-uniform, it is comparable with that obtained in Case-1. The mean velocity of was found to be 0.083 m/s and the percentage deviation of velocities in each channel was found to be 4.58%. The temperature contour is also uniform, and the temperature rise is also similar to Case-1.

4.3 Conclusion

From the above four cases it is found out that the bipolar plate design with 1 and 2 inlets are not good designs and that with 6 inlets and outlets gives very good results. The bipolar plate design with 4 inlets and 4 outlets also gives good results and these results are very much similar to those obtained for 6 inlets. Thus one of these two has to be chosen as an optimized design and will be used for further analysis. Taking material usage for the manufacturing of the bipolar plate and the manufacturing costs, it can be said that bipolar plate with 4 inlets and outlets is the optimized design. This design uses less material when compared with bipolar plate with 6 inlets and outlets. Thus the bipolar plate with 4 inlets and 4 outlets will be used for further analysis.

In the next chapter, the new optimized bipolar plate which was selected earlier will be simulated to study the flow distribution inside the channels with multi-phase flow.
CHAPTER 5

HYDRODYNAMIC ANALYSIS ON TWO-PHASE FLOW

5.1 Need for Two-Phase Flow Analysis

In the previous chapters, the fluid flow inside the bipolar plate was discussed and the model was developed which gave uniform flow and temperature distribution. For this kind of analysis water was used as the fluid that flowed through the plate. But, in reality, the water flows through the inlet ducts and enters the channels and there it is split into hydrogen ions (H\(^+\)) and hydroxide ions (OH\(^-\)) when it comes in contact with the bottom surface of the bipolar plate where constant heat flux is supplied. Then, the reduction reaction occurs and the hydroxide ions combine with electrons and give water and oxygen gas. This chemical equation was shown earlier in Chapter 1. Then the hydrogen ions flow through the gas diffusion layer (GDL) and membrane electrode assembly (MEA) and then enter another bipolar plate the other side. During entering another plate it gains electrons from the cathode and becomes hydrogen gas.

In the first bipolar plate, where water is split, the remaining amount of water which is not split flows out of the bipolar plate along with the oxygen gas produced. Thus there is a two-phase flow inside the channels. The oxygen bubbles might result in non-uniform flow inside the channels. Thus hydrodynamic analysis for two-phase flow must
be done to make sure that the new bipolar plate gives uniform flow. If it does not give uniform flow distribution, a new geometry must be developed. This chapter briefly gives the introduction to two phase flow and discusses about which approach to follow, assumptions made and finally the simulation and results.

5.2 Introduction to Two-Phase Flow

There are currently two approaches for the numerical calculation of two-phase flow:

1. Euler-Lagrange approach
2. Euler-Euler approach

In Euler-Lagrange approach, the fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles or droplets through the calculated flow field. The dispersed phase can exchange momentum, mass and energy with the fluid phase. In this approach, the fundamental assumption made is that the dispersed second phase occupies a low volume fraction. Thus, this approach is inappropriate for the models where volume fraction of the second phase is not negligible. In the current model, the second phase is oxygen and its volume of fraction is not neglected. Thus this approach is inappropriate for the current experiment.

In Euler-Euler approach, the different phases are treated mathematically as interpenetrating continua. Since the volume of a phase cannot be occupied by the other phase, the concept of phasic volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. In
the commercial software FLUENT that is being used for the simulation, three different Euler-Euler models are available:

1. The volume of fluid model (VOF Model)
2. The Eulerian model
3. The mixture model

VOF model is a surface-tracking technique applied to a fixed Eulerian mesh. It is designed for two or more immiscible fluids where the position of the interface between the fluids of interest. The Eulerian model is the most complex of the multiphase models in FLUENT. Two-phase flow analysis with this model take more computational time than the other models and streamwise periodic flow with specified mass flow rate cannot be modeled when the Eulerian model is used. The mixture model is designed for two or more phases. As in the Eulerian model, the phases are treated as interpenetrating continua. The mixture model solves for the mixture momentum equation and prescribes relative velocities to describe the dispersed phases. This model can be used for bubbly flows. It can also be used without relative velocities for the dispersed phases to model homogeneous multiphase flow.

For the current model analysis, mixture model theory is used. The new design is run only for hydrodynamic analysis. It is not solved for the energy equation. The new governing equations for continuity and momentum equations are

\[
\frac{\partial}{\partial t} (\rho_m) + \nabla \cdot (\rho_m \vec{\mathbf{v}}_m) = 0
\]  

(Eq. 5.1)
\[
\frac{\partial}{\partial t}(\rho_m \bar{\varvec{u}}_m) + \nabla \cdot (\rho_m \bar{\varvec{u}}_m \bar{\varvec{u}}_m) = -\nabla p + \nabla \cdot \left[ \mu_m \left( \nabla \bar{\varvec{u}}_m + \nabla \bar{\varvec{u}}_m^T \right) \right] + \rho_m \bar{\varvec{g}} + \bar{\varvec{F}}
+ \nabla \cdot \left( \sum_{k=1}^{n} \alpha_k \rho_k \bar{\varvec{u}}_{dr,k} \bar{\varvec{u}}_{dr,k} \right)
\]

(Eq. 5.2)

where \( \bar{\varvec{u}}_m \) is the mass-averaged velocity, \( \rho_m \) is the mixture density, \( \alpha_k \) is the volume fraction of phase \( k \), \( n \) is the number of phases, \( \bar{\varvec{F}} \) is a body force, \( \mu_m \) is the viscosity of the mixture and \( \bar{\varvec{u}}_{dr,k} \) is the drift velocity for secondary phase \( k \).

5.3 Model Set-up

Since the new geometry selected is symmetrical along the x-axis, only half of the geometry is used for analysis to reduce the computational time. The half geometry taken for analysis is shown in Fig 5.1

Fig 5.1 Half section of the new bipolar plate CAD model with four inlets
The operating conditions are the same as considered for the flow and temperature distribution analysis in the previous chapter. In the boundary conditions, since the energy equation is not solved, heat flux is not defined at the bottom walls of the channels. Since the number of inlets is reduced to 2, the mass flow rate is also halved (0.15 lpm). In this experiment, water is split to hydroxide ions and hydrogen ions inside the channels as mentioned earlier. But, since the chemical reaction is not considered in this part of the analysis, it is assumed that oxygen is supplied from the bottom of the channels, where earlier, the heat flux was defined. The mass flow rate of the oxygen supplied is given as 0.012 g/s. This value is given by Proton Energy Systems.

5.4 Results and Parametric Study

5.4.1 Case-1

This case is run with the operating conditions and the boundary conditions mentioned in the previous section. After simulation, the velocity profile of the water inside the channels is plotted and is shown in Fig 5.2. The slice taken at the same location as discussed in the previous chapters.

From the plot shown below, it can be found that even for two phase flow analysis, the bipolar plate designed gives uniform flow distribution. Thus it can be accepted as an optimized design of the bipolar plate for the PEM electrolysis cell. But, before that parametric study is carried out by varying the mass flow rate of the oxygen and water supplied. The results of these cases are shown in the following sections as different cases.
Operating Conditions:

\[ \text{Re} = 172 \]

Volumetric flow rate of \( \text{H}_2\text{O} = 0.3 \ \text{lpm} \)

Mass flow rate of \( \text{O}_2 = 0.012 \ \text{g/s} \)

5.4.2 Case-2

In this case the volumetric flow rate of the water is unchanged but the mass flow rate of the oxygen is reduced to 0.01 g/s. All other operating conditions and boundary conditions are unchanged. The model is then run and the velocity profile of water inside the channels is plotted. The velocity profile is shown in Fig 5.3. When the velocity profile of Case-2 is compared with that of Case-1, not much difference is observed. The velocity profile is still uniform inside the channels.
Operating Conditions:

Re = 172

Volumetric flow rate of H₂O = 0.3 lpm

Mass flow rate of O₂ = 0.01 g/s

5.4.3 Case-3

In this case, the volumetric flow rate of the water is increased to 1.5 lpm so as to observe the behavior of water for high flow rates. The mass flow rate of the oxygen is assumed to be increased linearly and increased to 0.06 g/s. The velocity profile of this case is shown in Fig 5.4
Operating Conditions:

$Re = 859$

Volumetric flow rate of $H_2O = 1.5$ lpm

Mass flow rate of $O_2 = 0.06$ g/s

Fig 5.4 Velocity profile for 1.5 lpm of water and 0.06 g/s oxygen

As the volumetric flow rate of the water increased from 0.3 lpm to 1.5 lpm, it is found that there is a small non homogeneity in the flow distribution inside the channels. But, the percentage error in the uniformity is not very high (5%) and this can be still accepted as an optimized design.

5.5 Validation

The basic bipolar plate and the new bipolar plate designed were simulated numerically and by plotting the results it was found that the new bipolar plate design
gives us uniform flow and temperature distribution inside the channels. Before accepting these numerical results, it should be validated that the results obtained from the numerical analysis are reasonable with the analytical calculations. For this, back-of-the-envelope calculations are to be done and compared with the numerical results.

In this experiment, to validate the results obtained, the volume fraction of the oxygen is calculated at the outlet and then it is compared with the numerical results. If the calculated value is comparable with the results obtained by the numerical analysis, then the experiment is said to be validated and the model can be used. The percentage of volume fraction of oxygen is calculated by

\[ VOF = \frac{Q_{\text{oxygen}}}{Q_{\text{oxygen}} + Q_{\text{water}}} \times 100 \]

where \( Q_{\text{oxygen}} \) is the volumetric flow rate of oxygen and the \( Q_{\text{water}} \) is the volumetric flow rate of the water at the respective inlets.

From the results obtained from the numerical analysis, the VOF of oxygen at the outlet is plot for all the three cases and are shown in Figs 5.5, 5.6 and 5.7, respectively. And the comparisons between numerical and analytical values are shown in Table 5.5-1.
Fig 5.5 VOF of oxygen at outlet in case-1

Fig 5.6 VOF of oxygen at outlet in case-2
Table 5.5-1 Comparison between numerical and analytical results

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Description</th>
<th>Numerical Result (%)</th>
<th>Analytical Results (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Mass flow rate of oxygen = 0.012 g/s; Volumetric flow rate of water = 0.3 lpm</td>
<td>62.8 – 69.6</td>
<td>64.8</td>
</tr>
<tr>
<td>2</td>
<td>Mass flow rate of oxygen = 0.010 g/s; Volumetric flow rate of water = 0.3 lpm</td>
<td>59 – 65.4</td>
<td>60.6</td>
</tr>
<tr>
<td>3</td>
<td>Mass flow rate of oxygen = 0.06 g/s; Volumetric flow rate of water = 1.5 lpm</td>
<td>64 – 65.7</td>
<td>64.8</td>
</tr>
</tbody>
</table>

Fig 5.7 VOF of oxygen at outlet in case-3
From the above table, it can be found that the values obtained by the numerical analysis are close to the analytical values. The percentage error between both the values is not more than 5%. Hence, the values obtained from the numerical analysis are acceptable.
CHAPTER 6

CONCLUSIONS AND FUTURE WORK RECOMMENDATIONS

6.1 Conclusions

Numerical modeling has been performed to study the flow and temperature distribution inside the bipolar plate of PEM electrolysis cell in this thesis. The conclusions pertaining to this research work are summarized as follows

- The basic bipolar plate design which was given by Proton Energy Systems USA, was simulated and was found that the flow distribution inside the channels in not uniform. This is because; the flow of the water inside the header, after exiting the inlet duct channels is almost in the perpendicular direction to the channels. Thus the flow through the end channels is more when compared with the middle channels.

- This problem is solved by designing new bipolar plates to which the inlet and outlet ducts are connected in such a way that the flow direction of the water which enters the header from the ducts is almost parallel to the channels. With this kind of design, uniform flow and temperature distributions are achieved inside the bipolar plate.

- The new bipolar plate design was then simulated for two-phase hydrodynamic flow analysis. The results gave little non-uniformity for higher mass flow rates of
water and oxygen. But, since the percentage of non-uniformity is significantly less, it can be accepted as the good design of the bipolar plate.

6.2 Future Recommendations

The current experiment resulted in the design of a new bipolar plate which gives uniform flow and temperature distributions. But, there were several assumptions made to achieve these approximate results. To achieve better results and to study the design of the bipolar plate more accurately, few modifications have to be made in the simulations and few other simulations must also be performed which might give better results. Some of them are mentioned below

- In two-phase flow analysis, the model was simulated only for continuity and momentum equations. It should be simulated for the energy equation also.

- In a bipolar plate of the PEM electrolysis, the water is split into hydrogen ions and hydroxide ions and later the hydroxide ions give oxygen gas and water due to reduction reaction. In current two phase flow analysis, it was assumed that the oxygen is supplied from the bottom walls of the channels. Numerical analysis with a chemical reaction defined at the surface will give much realistic solutions.

- It was also assumed that the oxygen is supplied uniformly along those bottom surfaces where as in reality; the oxygen generation might not be uniform along the surface. So, the two phase flow analysis must be done with a user defined function to define the generation of oxygen inside the plate.

- In the current numerical experiment, the escape of the hydrogen ions from the bipolar plate into the gas diffusion layer was not studied. So, simulation of the
complete PEM assembly must be carried out to see the actual behavior of water, oxygen and hydrogen ions inside the bipolar plate.

- No experimental work has been done on the current PEM electrolysis cell. The experimental results will help in validating the results obtained from the numerical simulations performed, more accurately. So, a real time experiment must be carried out to know the exact behavior of each component in the cell.
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