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Experimental and numerical study of feeding channel in Proton Exchange Membrane Fuel Cell

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EXPERIMENTAL AND NUMERICAL STUDY
OF FEEDING CHANNEL IN PROTON
EXCHANGE MEMBRANE FUEL CELL

A Thesis
Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
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in

The Department of Mechanical Engineering

by
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ABSTRACT

The performance of a Proton Exchange Membrane Fuel Cell (PEMFC) using different feeding configurations has been studied, with a focus on the water flooding due to electrochemical reaction. Feeding channel or Bipolar plate in Proton Exchange Fuel Cell is a dominating part. As feeding channel keeps direct contact with the gas diffusion layer, it helps efficiently supplying fuel and air into the gas diffusion layer for efficient production of electricity. Experimental data have been taken at hydrogen flow rates of 20, 40, 60, 80, 100 sccm for various bipolar plate arrangements. Three bipolar plates, namely serpentine, straight channel and interdigitated designs, were arranged in different combinations for the PEMFC anode and cathode sides. Nine combinations in total were tested under different flow rates, working temperatures and loadings. The cell voltage versus current density and the cell power density versus current density curves were obtained. Experimental results showed that for different feeding configurations, interdigitated bipolar plate in anode side and serpentine bipolar plate in cathode side had the best performance in terms of cell voltage-current density curve, power density output rate, percentage of flooded area in the feeding channels, the pattern of water flooding and the fuel utilization rate. It is found that the water patterns had a most dominating role for the cell performance. Naturally water forms due to the chemical reaction. The water could accumulate in the cell and lead to a lower cell performance. After operating the PEMFC under high current densities, the cell was split and the water flooding pattern in the feeding channels was visually inspected. Detailed studies of cell performance using a single channel bipolar plate have been performed. Experimental data for one channel were taken under a variety of flow rates. Computational simulations have been conducted for this one channel ‘cell’ and the simulation results were compared with the experimental results. Comparison shows very little difference between the experimental and the simulation work. It is expected that the outcomes of this study could help the future design of Proton Exchange Fuel Cell.
CHAPTER 1

INTRODUCTION

Fuel cell is a promising source for future electricity generation. It is an electrochemical energy conversion device, which converts hydrogen and oxygen into water, producing electricity and heat by this process. It is very much like a battery that can be recharged while drawing power from it. Instead of recharging using electricity, a fuel cell uses hydrogen and oxygen. Fuel cells may operate at higher efficiencies than conventional internal combustion engines as the fuel is converted chemically to electricity. The efficiency of a fuel cell is not constrained by the Carnot efficiency, which limits the maximum efficiency that an internal combustion engine may achieve. Fuel cell is particularly important because they convert primary energy into electricity and heat at efficiencies between 60% and 65%, which are considerably higher than in conventional power systems. The environmental impact is one to two orders of magnitude lower than those in conventional systems because of their very low level of pollutant emissions due to the relatively low operating temperature.

1.1 History of Fuel Cell

Swiss scientist Christian Friedrich Schönbein discovered the principle of fuel cell in 1838 and published in the January 1839 edition of the "Philosophical Magazine". The first fuel cell was developed by Welsh scientist Sir William Grove based on this work. A sketch of fuel cell was published in 1843. In 1932 British engineer Francis Thomas Bacon developed successful fuel cell devices. Bacon and his colleagues demonstrated a practical five-kilowatt unit capable of powering a welding machine twenty-seven years later in 1959. Pratt and Whitney from the U.S. licensed Bacon's patents. In the 1960s where the concepts were used in the U.S. space program to supply electricity. Further technological advances in the 1980s and 1990s. One of that is using of Nafion as the electrolyte, and reductions in the quantity of expensive platinum catalyst required, have made the prospect of fuel cells in consumer applications such as automobiles more realistic.
1.2 Chemistry in Fuel Cell and Combustion Theory

The fuel cell works by injecting hydrogen (H\textsubscript{2}) molecules into the anode gas diffusion layer. The hydrogen molecules react with the catalyst, which is usually a thin coat of powdered platinum on carbon paper. This breaks up the hydrogen into proton and electron. The proton goes across the electrolyte (electrolyte permits only protons to pass through it) while the electron goes through the circuit and the result is output power. Upon finishing their job, the electrons return to the cell through the cathode. There, the catalyst assists the oxygen molecules, the hydrogen protons and the hydrogen electrons in making water. The chemical reactions involving all these steps are the following:

Anode side:
\[ 2\text{H}_2 \rightarrow 4\text{H}^+ + 4e^- \]

Cathode side:
\[ \text{O}_2 + 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2\text{O} \]

The combined reaction is:
\[ 2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} \]

This reaction only creates about 0.7 volts after the considering all the losses in the cell. Because of this, there several cells have to build into a stack. This multiplies the voltage up to useable levels.

1.3 Measurement of Energy and Power Production

One of most important parameter in fuel cell is the cell potential, which is a measure of the maximum amount of energy per unit charge. This maximum work is equal to the change in Gibbs free energy, \( \Delta G \), in the reaction. These relationships can be expressed as:

\[ \text{Maximum work} = \Delta G = -nFE^{\circ}_{\text{cell}} \]

Where, \( n \) is the number of electrons transferred per mole of fuel used and \( F \) is Faraday constant and \( E^{\circ}_{\text{cell}} \) is the cell potential.

This change of Gibbs free energy is the indication of energy of the cell and Power production is related to that cell potential. Current generation by this cell and cell potential indicate power production by the cell.

1.4 Types of Fuel Cell

There are several types of fuel-cell technologies being developed for possible commercial uses:

1.4.1 Solid Oxide Fuel Cell (SOFC)

These fuel cells are best suited for large-scale stationary power generators that could provide electricity for factories or towns. It operates at very high temperatures (around 1,832 F/1,000 C). High temperature makes reliability a problem, but it also has an advantage: the steam produced by the fuel cell can be channeled into turbines to generate more electricity. This improves the overall
efficiency of the system. Due to its solid electrolyte, it is known as solid oxide fuel cell. Due to the high operating temperature of SOFC’s, they have no need for expensive catalyst. Solid oxide fuel cells have so far been operated on methane, propane, butane, fermentation gas, gasified biomass and paint fumes. Unlike most other types of fuel cells, SOFC's can have multiple geometries. The planar geometry is the typical sandwich type geometry employed by most of fuel cells where electrolyte is sandwiched in between the electrodes. SOFC’s can also be made in tubular geometries where either air or fuel is passed through the inside of the tube and the other gas is passed along the outside of the tube. The tubular design is advantageous because it is much easier to seal and separate the fuel from the air compared to the planar design. The performance of the planar design is currently better than the performance of the tubular design because the planar design has a lower resistance comparing to the tubular design. Since SOFC are made of ceramic materials, they tend to be brittle; they are therefore unsuited as drive trains in mobile applications. Furthermore, thermal expansion demands a uniform and slow heating process at startup that will cause very long startup times: typically, 8 hours or more although micro-tubular geometries promise much faster start up times. Ongoing research focuses on the lower-temperature SOFC (600ºC) in order to decrease the materials cost, which will enable the use of metallic materials with better mechanical properties and thermal conductivity. Research is also going on reducing start-up time for mobile applications.

1.4.1.1 Working Principle of Fuel Cell

The diagram represents a functioning Fuel cell. It consists of three components - a cathode, an anode, and an electrolyte sandwiched between the two. Oxygen from the air flows through the cathode, and a fuel gas containing hydrogen flows past the anode. Negatively charged oxygen ions migrate through the electrolyte and react with the hydrogen to form water, which reacts with the methane fuel to form carbon dioxide and hydrogen. This electrochemical reaction generates electrons, which flow from anode to an external load and back to cathode, a final step that both completes the circuit and supplies electric power. In electrochemistry (galvanic cell) anode is where oxidation occurs and cathode is where reduction occurs, so in electrochemistry anode is negatively charged electrode and cathode is positively charged electrode, which is opposite of electrolytic cell. An electrolytic cell is powered by electricity to produce a change in the chemicals in the cell.
A proton Exchange Fuel Cell, Fig.1.3, works in a similar way like other fuel cells except that Hydrogen ion passes through the membrane and interacts with the oxygen ion to form water and electricity. Here Water forms on the cathode side, which is opposite to other cells.

1.4.2 Proton Exchange Membrane Fuel Cell (PEM)

Among various types of fuel cells, proton exchange membrane fuel cell (PEMFC) is regarded as the type most likely to reach the full-scale commercialization. Proton exchange membrane (PEM) fuel cells work with a polymer electrolyte in the form of a thin, permeable sheet. Its name came as membrane helps here in exchanging or transferring protons. The PEMFC was invented in 1950’s. An ion exchange resin (a solid polymer membrane) was used as the electrolyte for such fuel cell. PEMFC have a low operating temperature (about 80 °C) and they are compact. For each cell, an anode layer and a cathode layer are situated on either side of the electrolyte layer. The oldest and most commonly used membrane is Nafion by Dupont. This membrane is thin and light, and it works at low temperatures (about 80 °C/175 °F). To speed the reaction a platinum-based catalyst is used on both sides of the membrane. Hydrogen atoms are stripped of their electrons, or "ionized," at the anode, and the positively charged protons diffuse through the membrane and migrate toward the cathode. The electrons pass from the anode to the cathode...
through an exterior circuit and provide electric power along the way. At the cathode, the electrons, hydrogen protons and oxygen from the air combine to form water. So water forms in the cathode side of PEM which is dissimilar to other cells. Efficiency for a PEM cell reaches about 40 to 50 percent. The PEMFC is a prime candidate for vehicle and other mobile applications of all sizes down to mobile phones, because of its compactness.

1.4.3 Alkaline Fuel Cell (AFC)

This is one of the oldest designs. It has been used in the U.S. space program since the 1960s. The AFC is very susceptible to contamination, so it requires pure hydrogen and oxygen. It is also very expensive, so this type of fuel cell is unlikely to be commercialized.

![Figure 1.5: Working stage of an AFC](image)

NASA has used alkaline fuel cells since the mid-1960s, in Apollo-series missions and on the Space Shuttle. AFCs consume hydrogen and pure oxygen producing potable water, heat, and electricity. They are among the most efficient fuel cells, having the potential to reach 70%. The two electrodes are separated by a porous matrix saturated with an aqueous alkaline solution, such as potassium hydroxide (KOH). Aqueous alkaline solutions do not reject carbon dioxide (CO₂) so the fuel cell is easily poisoned. Because of this, the fuel cell requires pure oxygen, or at least purified air. On the other hand, the catalyst required for the electrodes can be a chemical that is relatively inexpensive compared to the PEMFC.

1.4.4 Phosphoric-Acid Fuel Cell (PAFC)

The phosphoric-acid fuel cell has potential for use in small stationary power-generation systems. It operates at a higher temperature than PEM fuel cells, so it has a longer warm-up time. This makes it unsuitable for use in cars. Phosphoric-Acid fuel cells (PAFC) are a mature technology that is commercially available. Unfortunately, the phosphoric acid solidifies under 40°C, making startup very difficult.
1.4.5 Molten Carbonate Fuel Cell (MCFC)

These fuel cells are also best suited for large stationary power generators. They operate at 1,112 F (600 C), so they also generate steam that can generate more power. They have a lower operating temperature than the SOFC, which means they do not need such exotic materials. This makes the design a little less expensive.

1.4.6 Direct Methanol Fuel Cell (DMFC)

A subcategory of Proton-exchange fuel cells is the DMFC, or direct-methanol fuel cell; here, the methanol is not reformed, but fed directly to the fuel cell. One does not need complicated catalytic reforming, and storage of methanol is much easier than that of hydrogen because it does not need to be done at high pressures. The energy density of methanol (the amount of hydrogen in a given volume) is orders of magnitude greater than even highly compressed hydrogen. However, efficiency is low, due to the high permeation of methanol through the membrane, and the dynamic behavior is sluggish. Methanol is also extremely poisonous. Because of these strengths and problems, DMFCs are limited in the power they can produce, but can still store a lot of energy in a small space. This means they can produce a small amount of power over a long period of time, which makes them well suited to power consumer electronics such as cell phones and laptops but rules them out of automotive applications.
1.4.7 Biological Fuel Cell

A biological fuel cell is a type of fuel cell that uses bacteria to reform glucose into hydrogen, or directly extract energy from the glucose. Where a microbial fuel cell exploits electrical currents generated by bacteria.

The main concepts of fuel cell are a product of the twentieth century [5]. Detailed description of the development of fuel cells different parts can be found [6]. One individual PEMFC only produces limited voltage and power, thus hundreds or thousands of cells need to be connected together, using bipolar plates, in order to form a practical fuel cell stack. The major functions of bipolar plates include the distribution of fuel and air uniformly over the entire active areas; the heat removal from the stack; the conduction of current density from cell to cell; and the prevention of leakage. Typically, a PEMFC involves complex species transport, chemical reactions, thermal and electrochemical processes. Transport resistances of the gaseous species in the feeding channels and the porous electrodes lead to the so-called concentration overpotential [7, 8]. The local concentration of fuel and oxidant is affected by the mixing of multiple gases in the feeding channels; the mass transfer inside the porous anode/cathode; the reaction of fuel and oxygen and the transportation of fuel and electrochemical products, mainly water, near the three-phase boundary. It is well known that the mass transfer processes could limit the cell power density. In order to achieve good PEMFC performance, high membrane conductivity is one of the key parameters. The proton conductivity of Nafion (DuPont) membrane, a most commonly used exchange membrane, increases with the water content [9]. To maintain high membrane water content along the channel, the reactant gases have to be humidified. However, more water is to be generated at cathode due to the electrochemical reactions. This may result in saturated liquid water. When the pores of the porous cathode are filled with excess liquid water, the diffusion of reactant gas through the cathode becomes difficult, thus the PEMFC cannot work efficiently. Another reason for PEMFC not to work efficiently is that the liquid water may block the oxygen form direct contact with catalyst. For a PEMFC, a delicate balance between adequate humidification and not to flood the cathode has to be carefully controlled. PEMFC flow channel design is a key factor for its normal operation. For a high performance PEMFC, choosing the best feeding configuration is one of the possible ways to mitigate the water-flooding problem. Li et al.[10] has shown the enhanced mass transfer in terms of different bipolar plate designs. Goodman et al.[11] has designed various channels and tried to find out the best performance in terms of minimum flow rate, temperature distribution, heat flux distribution, output power and cooling in bipolar plate. Lim et al. [12] used hydrophobic polymer content in the Gas Diffusion Layer (GDL) to deal with water flooding and found an enhanced performance of cell. However, very few works have been done systematically to demonstrate that how the feeding configurations could affect the PEMFC performance.

The prediction of fuel cell performance is one of the most challenging problems in fuel cell research. To simulate the transport phenomena using software is a powerful way to understand the fundamental physical and chemical processes of a fuel cell. In this study, the performance of a PEMFC was simulated using a partial-differential equation solver, FEMLAB. The results of the simulation study using FEMLAB will be beneficial for further and more complete analyses of the performance of fuel cells.

The objective of this study is to find the best performance cell using a combination of three basic feeding bipolar plate designs: Straight Channel, Serpentine channel and Interdigitated Channel. Performance data are examined in terms of percentage water in the gas-feeding channel,
water flooding pattern, fuel utilization rate, different reacting fluid flow rates and the cell voltage versus current density curve. It has been found that a cell with interdigitated bipolar plate at anode side and Serpentine bipolar plate at cathode side gives the best performance.

1.5 Fuel Cell Simulation Software

There have a number of software available in the market now a days to simulate fuel cells. The well-known ones are Femlab, Fluent, and Star-CD etc. These software packages may programmed to compute complicated 3-D partial differential equations involved in Fuel cell. A combination of modeling and experiments could lower costs and accelerate the pace of building prototypes and understanding these new systems. A number of models, with different focus and degree of complexity, have been presented in the literature [13-16].

When creating a model in FEMLAB, the typical modeling steps include:

1. Creating or importing the geometry using drawing tool bars
2. Meshing the geometry using Meshing tool bar
3. Defining the physics on the domains and at the boundaries
4. Solving the model using proper solver from list of solvers: Stationary Liner, Stationary Nonlinear, Time Dependant solver, Eigenvalue solver, Parametric linear and Parametric Nonlinear
5. postprocessing the solution to see scenario inside the cell
6. Performing parametric studies
CHAPTER 2

EXPERIMENTAL DESCRIPTION

Figure 2.1: (a) Interdigitated (b) Serpentine (c) Straight bipolar plate
Three designs of bipolar plates, Serpentine Channel, Straight Channel and Interdigitated channel [17-19], are shown in Fig.2.1. Straight and Interdigitated bipolar plates can be conveniently produced by modifying the channels of a Serpentine type bipolar plate. Afterwords the single channel bipolar plate test model was made by blocking all channels of a straight channel bipolar plate except one single channel. For this study, a commercially available fuel cell with a five layer Membrane-Electrode Assembly (MEA) was used.

The test cell has a MEA area of 5.05 cm by 4.95 cm. Hydrogen and oxygen flows over anode and cathode in a co-flow manner i.e. both flow are parallel and in the same direction. Laboratory temperature was air-conditioned at 21°C. The pressure of oxygen and hydrogen in the cell was close to ambient pressure.

Figure 2.2 describes the test rig. Waste oxygen was released at the cathode side outlet port. No suction device was used. For the hydrogen side, the outlet hydrogen port was connected via a long tube to a laboratory suction blower for rapid dispersion of unused hydrogen gas out of the building thus no hydrogen gas could accumulate in the lab.

The bipolar plate block has an outer dimension of 7.65cm by 7.65cm, and has a thickness of 1.3cm. The feeding channels have a width of 1mm and a depth of 1mm. The fuel cell was connected to variable load resistors to observe the variation of cell performance with loads. Twelve resistors: four 0.68 ohm, two 0.56 ohm, two 0.39 ohm and four 0.27 ohm, were used to form the loading bank. By connecting some or all of these resistors in parallel, different loadings were achieved for the experiments. Flow rate of hydrogen was varied in the tests to observe the cell performance dependence. However, the oxygen flow rate was maintained constant at 46 sccm for all the tests. The fuel cell output voltage was monitored using a multi-meter. The cell output current density is obtained by dividing the measured voltage by the relevant resistance and the cell power density is obtained by multiplying the current density and the voltage. The testing cell is instrumented with two cartridge heaters for maintaining an elevated operating temperature. To avoid the overheating of the cell, thermocouple readings could be taken from the testing cell when these heaters were used.
Oxygen flowmeter used in the tests has a scale from unit zero to 65 marked on the tube. Calibration curve for this flowmeter was made using sccm unit. In the experiments, the flowrate of oxygen was measured by converting this scaled unit to sccm unit. Figure 2.2 shows this calibration curve for oxygen flowmeter reading.

![Figure 2.3: Oxygen Flowmeter calibration curve](image)
CHAPTER-3

EXPERIMENTAL RESULT

Power density-current density relations at 21°C operating temperature using Serpentine bipolar plate at anode side and Serpentine plate at cathode side is shown in Fig. 3.1 for various flow rates of hydrogen. As the local current density is a function of hydrogen and oxygen partial pressure, increasing the fuel flow rate will increase the partial pressure at the later portion of fuel feeding channels and this ultimately could enhance the performance of the cell.

Figure 3.1: Power Density versus current Density curve for Serpentine (Anode)-Serpentine (Cathode) feeding configuration under different hydrogen flow rates at 21°C

Figure 3.2: Voltage versus current density curve for Serpentine (Anode)-Serpentine (Cathode) feeding configuration under different hydrogen flow rates at 21°C
Figure 3.3: V-I curve at 20 sccm H₂ flow rate using different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St” – Straight channel, “I” - Interdigitated channel.

Voltage-Current density relations at 20 sccm flow rate and 21°C operating temperature for various arrangements of bipolar plates are shown in Fig.3.3. Data were taken for nine combinations of bipolar plates. For Straight channel bipolar plate, once the gases enter the bipolar plate, they will try to find the shortest way out so flow distribution in straight channel bipolar plate is unlikely to be uniform. For Serpentine channel bipolar plate, gases have to follow the direction of the serpentine channel. However, it is also possible that some of the gases could pass through
the porous gas diffusion layers. Due to the relatively clearly defined flow path, a long travel distance and thus high-pressure losses are expected for the serpentine design. Interdigitated bipolar plate forced the fluid to go inside the porous gas diffusion layer towards the membrane thus high fuel/oxygen partial pressure at the three-phase reaction boundary is expected and the fuel might be better efficiently used. It is found that voltage and current density relation of interdigitated bipolar plate in anode side and Serpentine bipolar plate in cathode side shows the best performance in comparison to other bipolar plate configurations.

Voltage-Current density curves under 40, 60, 80 and 100 sccm hydrogen flow rates and at 20°C operating temperature for various arrangements of bipolar plates are shown in Fig.3.4, 3.5, 3.6 and 3.7 respectively. Again, it is found that overall performance of Interdigitated bipolar plate in anode side and Serpentine bipolar plate in cathode side has the best performance in comparison to other bipolar plate configurations. Same reasons are applicable for these cases. It is found that the Interdigitated in Anode side and Serpentine in Cathode side always has a superior performance, regardless of the hydrogen flow rates.

Figure 3.5: V-I curve under 60 sccm H₂ flow rate for different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St” – Straight channel, “I” - Interdigitated channel.

Table 3.1 shows velocity, Reynolds number and total pressure loss data for various reactant fluids and bipolar plates. It is shown that for Serpentine and Interdigitated bipolar plate's pressure loss is higher compared to that of straight channel bipolar plates. Reynolds number of all the flow indicates flows are laminar flows. Serpentine channel shows higher-pressure drop than straight channel, resulting depleted reactant through the length of the channel.Velocity is measured from flow rate of a particular flow and area of the channel cross section. Reynolds number is calculated by using this velocity value. Total pressure loss for serpentine channel is calculated by using the same equation for channel flow and minor losses due to bending (90° bend formula was used). The parallel channel is simulated as a single short channel, whose cross section area is 30 times the serpentine plus two 90-degree bends. Total pressure loss for Interdigitated channel is calculated by using the same equation for channel flow in all the gas flow path and minor losses is considered in porous region of gas diffusion layer[Appendix-I]
Figure 3.6: V-I curve under 80 sccm H₂ flow rate for different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St” – Straight channel, “I” - Interdigitated channel.

Figure 3.7: V-I curve under 100 sccm H₂ flow rate for different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St” – Straight channel, “I” - Interdigitated channel.
Experimented data were analyzed in terms of transient and steady data. The meaning of transient and steady is not similar to the conventional engineering terms of transient and steady. Transient is defined in this study as that water generation did not occur and the data were taken quickly when the voltage reading was showing steady values after starting the experiment. In contrast, the steady data are taken when water flooding occurred in the cell. Variation of steady and transient data for different bipolar plate configurations is a good measure of the cell performance. If steady data vary in large amount comparing to the transient data, the implication is that there exists a serious water-flooding problem. From table 3.1, interdigitated bipolar plate in anode side and Serpentine bipolar plate in cathode side has very small variation between the steady and transient measurements, which means a minor water-flooding problem. This is mainly due to the high oxygen velocity and high pressure drops through the cathode side, which can blow the water droplets out of the cell.

Table 3.1: Velocity, Reynolds number and total pressure loss data for various reactants and bipolar Plates

<table>
<thead>
<tr>
<th>Reactant fluid</th>
<th>Velocity (m/s)</th>
<th>Reynolds Number (Re)</th>
<th>Total pressure loss (KPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpentine Oxygen</td>
<td>0.767</td>
<td>79.6</td>
<td>1.5567</td>
</tr>
<tr>
<td>Straight Oxygen</td>
<td>0.02556</td>
<td>5.147</td>
<td>0.000202</td>
</tr>
<tr>
<td>Interdigitated Oxygen</td>
<td>0.010223</td>
<td>2.0585</td>
<td>0.0019689</td>
</tr>
<tr>
<td>Serpentine Hydrogen</td>
<td>0.333</td>
<td>20.2</td>
<td>0.32</td>
</tr>
<tr>
<td>Straight Hydrogen</td>
<td>0.01111</td>
<td>1.3055</td>
<td>0.00004189</td>
</tr>
<tr>
<td>Interdigitated Hydrogen</td>
<td>0.004444</td>
<td>0.522</td>
<td>0.00039823</td>
</tr>
</tbody>
</table>

Hydrogen utilization of a cell is also a key fuel cell performance parameter. As hydrogen utilization is the ratio of the theoretical flow rate of hydrogen over experimental flow rate of hydrogen into the cell. In equation form, this becomes:-

\[
\text{Hydrogen Utilization Ratio} = \frac{\text{Theoretical flow rate of Hydrogen}}{\text{Experimental flow rate of Hydrogen}}
\]

From this equation, experimental flow rate of hydrogen is obtained from the flow rate reading from the flowmeter and theoretical flow rate of hydrogen is obtained from the measured H₂ usage (shown in Appendix-I). Therefore, a high hydrogen utilization ratio value means small fuel wastage. After all, high hydrogen utilization ratio indicates a better performance. From figure 3.8, for different feeding configurations, the cell hydrogen (and thus oxygen) utilization rates can be found. Curves indicate that for all the configurations hydrogen utilization ratio show near to
similar trend. This near to similar trend indicates near to same way utilization of hydrogen utilization.

Table 3.2: Transient and Steady data at high loading for various feeding configurations. Here the left notation indicates anode and right notation indicates Cathode. “S”-Serpentine channel, “St” – Straight channel, “I” - Interdigitated channel.

<table>
<thead>
<tr>
<th>Feeding</th>
<th>Steady data</th>
<th>Transient data</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current density (A/m²)</td>
<td>Voltage (V)</td>
<td>Current density (A/m²)</td>
</tr>
<tr>
<td>S S</td>
<td>5030</td>
<td>0.43</td>
<td>5880</td>
</tr>
<tr>
<td>St S</td>
<td>4900</td>
<td>0.42</td>
<td>5688</td>
</tr>
<tr>
<td>S St</td>
<td>4960</td>
<td>0.42</td>
<td>5384</td>
</tr>
<tr>
<td>I I</td>
<td>3150</td>
<td>0.27</td>
<td>5188</td>
</tr>
<tr>
<td>I S</td>
<td>5560</td>
<td>0.47</td>
<td>5616</td>
</tr>
<tr>
<td>S I</td>
<td>4470</td>
<td>0.38</td>
<td>6372</td>
</tr>
<tr>
<td>I St</td>
<td>5290</td>
<td>0.45</td>
<td>6500</td>
</tr>
<tr>
<td>St I</td>
<td>3710</td>
<td>0.32</td>
<td>6732</td>
</tr>
<tr>
<td>St St</td>
<td>4780</td>
<td>0.41</td>
<td>6488</td>
</tr>
</tbody>
</table>

After running the fuel cell at high current density for a long time, the cell was opened up and the water flooding in the cathode side gas distribution channels were visualized. In table 3.3, the area percentage covered by water in the flow channel is shown for different combination arrangement of bipolar plates. All of the cells have water-flooding problem, which is generated due to the reaction of hydrogen and oxygen and electro-osmotic drag of water particles from anode towards cathodes. To operate the PEMFC properly, the membrane has to be humidified. In the tests, the anode side hydrogen was passed through a humidifier to pick up water vapor. After observing this table it is found that for all arrangements, the water flooding in the flow channel is nearly 25%. The main flooding problem, which seriously damages the cell performance, occurs in the porous gas diffusion layers close to the three-phase boundary. The water accumulations in the feeding channels can only be used as an indicator for potential water flooding in the gas diffusion
layers with the help of flow knowledge for the gases in both the flow channels and in the porous layers.

![Graph showing hydrogen utilization ratio vs. load curve for 60-sccm H₂ flow rate for different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St”- Straight channel, “I”- Interdigitated channel.]

**Figure 3.8**: Hydrogen utilization ratio vs. load curve for 60-sccm H₂ flow rate for different feeding configurations. Here the left notation indicates anode and right notation indicates cathode. “S”-Serpentine channel, “St”- Straight channel, “I”- Interdigitated channel.

**Table 3.3**: Water flooding in the cathode side feeding channels for various feeding configurations. Here the left notation indicates anode and right notation indicates Cathode. “S”-Serpentine channel, “St”- Straight channel, “I”- Interdigitated channel.

<table>
<thead>
<tr>
<th>Feeding Configuration</th>
<th>% Water in the channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>St I</td>
<td>17.23%</td>
</tr>
<tr>
<td>S St</td>
<td>22.19%</td>
</tr>
<tr>
<td>S S</td>
<td>23.10%</td>
</tr>
<tr>
<td>St St</td>
<td>25%</td>
</tr>
<tr>
<td>I S</td>
<td>25.42%</td>
</tr>
<tr>
<td>S I</td>
<td>25.88%</td>
</tr>
<tr>
<td>I St</td>
<td>26.97%</td>
</tr>
<tr>
<td>St S</td>
<td>33.81%</td>
</tr>
<tr>
<td>I I</td>
<td>37.48%</td>
</tr>
</tbody>
</table>
Experiments were also conducted to get the difference of data with the use of humidifier and without humidifier. Figures 3.8 & 3.9 show this difference of data. It is observed that experimented humidifier wet the membrane more so more water is found in the bipolar plate cathode side due to transport of water by electro-osmotic drag. Figures 3.8 & 3.9 show the results without using humidifier. The performance was found to be better for higher loads as for higher loads indicate more water generates and stronger transportation of water from anode to cathodes due to the electro-osmotic drag.

![Power Density vs. Current Density curve at 20sccm showing humidifier effect](image1)

Figure 3.9: Power Density vs. Current Density curve at 20sccm showing humidifier effect

![Voltage vs. Current Density curve at 20sccm showing humidifier effect](image2)

Figure 3.10: Voltage vs. Current Density curve at 20sccm showing humidifier effect

Water pattern in cathode side bipolar plate gives reasonable indication of performance of cell. A uniform water generation in the middle of the cell feeding channels could wet the membrane uniformly for its proper functioning and has shown good cell performance. By reading the performance curves and the water patterns in the bipolar plate feeding channels, non-harmful and detrimental water patterns could be identified for further investigation. Figure 3.11(a) shows the water flooding in the channels near the inlet port. As cathode side is Interdigitated one, water in those places introduces hindrance to the flow. The oxygen flow rate is not large enough to blow them through the channels. In addition, the result is a bad cell performance. Figure 3.11(b) is a very bad water pattern which is almost everywhere in the bipolar plate. For this case, because the
anode side is Straight channel, hydrogen will try to take the shortest distance to find the exit port situated at the bottom straight channels, the result is more water generation in the upper side, water will flow from upper side to the bottom, and water jamming occurred in the lower side. Figure 3.11(c) shows a water pattern more at inlet and outlet and very few water flooding in the middle. It appears there is an uneven distribution of oxygen at cathode side. Close to the cathode near side and far side, oxygen flow rate in the interdigitated bipolar plate is not high enough to remove water from the porous diffusion layer. In the region close to the bottom half of bipolar plate, the far side, due to the high losses, after the generation of water, the channels might be blocked permanently. Most oxygen found a flow path through the middle of the bipolar plate. Figure 3.11(d) shows small patches localized flooding pattern in the flow channels. For this case, at cathode side, straight bipolar plate was used. Result of the cell performance shows this configuration is good under high loading. The Interdigitated channels at anode distribute hydrogen relatively uniformly over the anode side, which is another reason for good cell performance.
As water flooding is an important phenomenon in a Proton Exchange Membrane Fuel Cell, work has been conducted on water management. It is predicted that if water flooding could be predicted along one channel accurately then the multiple channel prediction will be found. The reason for not simulating the completely bipolar flow channel is the unprecedented number of grids required for the narrow but long flow channels, which is well beyond the current computing power in the lab. After the 29 channels of the used bipolar plate were blocked, more tests were performed using the single channel test cell. Flow rates were maintained for the similar 20, 40, 60, 80 and 100sccm and Power density vs. Current Density and Voltage vs. Current Density curves were measured. Figures 3.12 & 3.13 indicate these flow rates for one channel are too high so all the curves show similar result. In addition, current density is higher compared to thirty-channel current density. This is reasonable, as same flow rates for a narrow region like one channel will have higher current density due to smaller area compare to area in thirty channels. However, these measurements provide valuable data for the simulation software validation.

Figure 3.12: Experimental result for power density vs. Current Density Curve for various flow rates for the single channel test cell

Figure 3.13: Experimental result for Voltage vs. Current Density curve for various flow rates for the single channel test cell
After considering various issues such as the water filled area percentage in the bipolar plate, fuel utilization rate, variation of steady and unsteady data, different arrangements of bipolar plates, and flow rates of hydrogen, it is found that Interdigitated bipolar plate in anode side and Serpentine bipolar plate in cathode side is the best combination for a high performance fuel cell.
CHAPTER 4

NUMERICAL MODELING

To perform a parametrical optimization for the flow field design and to understand the experimental data, multiphysics-based numerical simulations using FEMLAB were performed. It offers detailed flow field, pressure field and concentration distribution along the feeding channels. FEMLAB is a commercial Partial Differential Equation (PDE) solver, which can solve coupled multi-physical problems.

Partial differential equations are the governing equations for most physical phenomena and provide the foundation for modeling a wide range of scientific and engineering problems. There are three ways of describing PDEs in FEMLAB, coefficient form, general form and the weak form. The coefficient form is suitable for linear or nearly linear models and the rest two are suitable for nonlinear models. The weak form was used in the simulation. FEMLAB runs finite element analysis to solve the PDEs, together with adaptive meshing and error controls. To overcome the memory and speed limitation facing a three dimensional multiphysics calculation, source terms in the simulation works were multiplied by a factor and increased this factor value from 0.001 values to the value 1 was developed.

For the simulated model, problems with high reaction rates (high $R_i$), or more generally, large source terms in FEMLAB, resulted in convergence problems and error message "NaN repeatedly found in solution", or "Damping factor too small" was shown. This problem was solved using reduced source terms, and then gradually increases, using the previous solution when solving, until reaching the solution to original problem. Reaction terms were handled by multiplication of the reaction (source) term ($R_i$) by a multiplication factor variable, "$k$". The List of Parameter Values in the Solver Parameter were specified to be a range of increasing values, starting at a low value and increasing to unity, for example "1e-3 1e-2 1e-1 1" and was started to Solve button helped to get the solution. FEMLAB started to solve the problem using the first multiplication factor (0.001). Then, if that worked, FEMLAB used the solution as initial guess for the next parameter value, and solved until it reacheded the last parameter value. Because specification of the last parameter value to be unity leaded to the last solution corresponded to the original problem solution.

The simulated geometry was very thin in width and height direction comparing to its length. Since the FEMLAB mesh generator creates tetrahedra that are isotropic in size, a large number of elements may create in the thin layer. In addition, large differences in scale may cause the mesh generator to fail in creating the mesh. So, width and height of the simulated cell is scaled during the meshing process to reduce the number of elements created before meshing and then scaled the mesh back so that it fits the original geometry. The mesh was scaled by a factor of five without losing too much accuracy because a scale factor of 3-5 or 5-10 in one direction can sometimes be acceptable.

The simulation domains were the three dimensional Electrolyte and Electrodes on both two sides of this electrolyte. The simulation includes the multi species transportation in the porous electrodes and the coupled electrical current and potential distributions. Stefan-Maxwell diffusion equations were applied to a mixture of $O_2$ and $H_2O$ in the cathode side. As the anode, side gas is not
a two or more gas mixture so Stefan- Maxwell diffusion equations were not applied in the gas diffusion layer. Only Darcy’s porous gas law was applied in anode side gas diffusion layer. At the same time for the flow goes through the porous electrodes, the Darcy’s law was employed. In the electrolyte membrane, the ionic balance was calculated.

4.1 Darcy’s Law in Porous Media Flow [27]

In porous structure of anode and cathode, the global transport of momentum by shear stresses in the fluid is negligible as the pore walls impede momentum transport to the fluid outside the individual pores. Since a detailed description down to the resolution of every pore is not practical in the simulated model, homogenization of the porous and fluid media into one single medium was a common approach. Darcy’s Law is used in that domain as it is based upon this approach and describes flow in porous media where pressure gradient is the only driving force.

Darcy’s Law stated in the gas domain is the pressure gradient, the fluid viscosity and the structure of the porous media determine that velocity vector.

\[
\vec{u} = -\frac{\kappa}{\mu} \nabla p
\]

Where, \( \vec{u} \) = velocity vector
\( \kappa \) = permeability
\( \mu \) = viscosity
\( \nabla p \) = pressure gradient

The Darcy’s law application mode in the Chemical Engineering module of FEMLAB combines Darcy’s Law with the continuity equation. So that equation becomes:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
\]

\[
=> \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \frac{\rho}{\mu} \nabla p \right) = 0
\]

Where, \( \rho \) is the density of the fluid

Gas density in the simulated model depended on pressure that, for an ideal gas, was described by the ideal gas law:

\[
\rho = \frac{PM}{RT}
\]

Where, \( M \)=molar weight of the gas, R is Universal gas constant and T is temperature.

For the simulated model, impervious or symmetric boundary condition is defined as:

\[
-\frac{\kappa}{\mu} \nabla p \cdot \vec{n} = 0
\]

Impervious or symmetric boundary condition actually resides in the surface between the electrolyte and electrode surface.
4.2 Maxwell-Stefan Diffusion and Convection [27]

For the mixture of $O_2$ and $H_2O$ in the cathode electrode Maxwell-Stefan diffusion and convection module was used. Fick’s law of diffusion is based upon the assumption that species dissolved in a solution interact with the solvent only and independent of concentration. In concentrated solutions, the solvent is affected by the solute species, and they interact with each other. Their diffusion coefficients are concentration dependent. The Maxwell-Stefan Diffusion and convection application mode makes it possible to treat convection and diffusion problems where there is full interaction between the species dissolved in a solution. In these solutions, the diffusion coefficients corresponding to the Fickian diffusion coefficients are highly dependent on the composition of the solution [20].

\[
\frac{\partial \rho \omega_i}{\partial t} + \nabla \cdot \left[ -\rho \omega_i \sum_{j=1}^{N} D_{ij} \left\{ \frac{M}{M_j} \left( \nabla \omega_j + \frac{\nabla M}{M} \right) + (x_j - \omega_j) \frac{\nabla p}{p} \right\} + \omega_i \rho \frac{\partial u}{\partial t} + D_i \frac{\partial T}{\partial t} \right] = R_i
\]

Where, $M$ denotes Molar mass of the mixture, $M_j$ is the molar mass of species $j$, $x_j$ is the mole fraction of component $j$, $\omega_j$ is the mass fraction of component $j$, $R_i$ is the reaction rate of species $i$, $D^T$ is the thermal diffusivity, $D_{ij}$ is the binary diffusivities.

Mass fractions are related to:

\[
\sum_i \omega_i = 1
\]

In addition, molar mass fraction is related to:

\[
x_i = \frac{\omega_i}{M_i \sum_k \frac{\omega_k}{M_k}}
\]

4.3 Conductive Media DC [27]

In the simulated model this module is used for the electrodes and electrolyte because its relation with these conductive media. Generally, electrolysis involves a medium with conductivity and a steady current. When handling conductive media considering equation of continuity works well. In a stationary coordinate system, the point form of Ohm’s law states that:

\[
\bar{J} = \sigma \bar{E} + \bar{J}^e
\]

Where, $\bar{J}$ is current density, $\sigma$ is conductivity, $\bar{E}$ is electric field intensity and $\bar{J}^e$ is externally generated current density. The static form of the equation of continuity then gives:

\[
\nabla \cdot \bar{J} = -\nabla \cdot \left( \sigma \nabla V - \bar{J}^e \right) = 0
\]

To handle current sources, generalizing the equation to:

\[
-\nabla \cdot \left( \sigma \nabla V - \bar{J}^e \right) = \bar{Q}_j
\]

Where, $\bar{Q}_j$ is the current source.

This generalized equation was used in the electrodes and electrolyte.

4.4 Governing Equations and Source Terms of the Model [27]

In the simulated model, multiphysics modeling of a proton exchange membrane fuel cell was applied. The model uses current balances, mass balance (Maxwell-Stefan diffusion for reactant and water) and momentum balances (gas flow) to simulate the PEM fuel cell behavior.
The modeled section of the fuel cell consists of three domains: an anode, a proton exchange membrane and a cathode. Each of the porous electrodes has an inlet channel, a current collector and outlet. An agglomerate model will here describe the electrode reactions in the active catalyst layers. The agglomerates consist of catalyst and carbon particles embedded in polymer electrolyte. The equations for the agglomerate model originate from the analytical solution of a diffusion-reaction problem in a spherical porous particle [21, 22]. At the anodic active catalyst layer, hydrogen is the diffusing and reacting species in the agglomerates, while oxygen is the diffusion and reacting species in the agglomerates at the cathode. An agglomerate model of the cathodic active catalyst layer of a PEM fuel cell has been presented by Broka et al [23].

The potential distribution is modeled using the application mode conductive media DC in the three subdomains, and is given by the following equations:

\[
\nabla \cdot (\kappa^{s,\text{eff}} \nabla \phi_s) = 0 \quad \text{in anode subdomain}
\]

\[
\nabla \cdot (\kappa^{m,\text{eff}} \nabla \phi_m) = 0 \quad \text{in membrane subdomain}
\]

\[
\nabla \cdot (\kappa^{c,\text{eff}} \nabla \phi_c) = 0 \quad \text{in cathode subdomain}
\]

Where, \( \kappa^{\text{eff}} \) is the effective conductivity. The potentials in the electrode are denoted by \( \phi_s \), while in the membrane it is denoted as \( \phi_m \).

The gas flows in the gas backings is modeled using the Darcy’s law application mode. The velocity of the gas is given by the continuity equation, according to:

\[
\nabla \cdot (c^g \vec{u}) = 0 \quad \text{in anode and cathode subdomain}
\]

Here, \( c^g \) is total molar concentration of the gas phase and \( \vec{u} \) denotes velocity of the gas.

Darcy’s law for porous media states that the gradient of pressure, the viscosity of the fluid, and the structure of the porous media determines the velocity vector:

\[
\vec{u} = -\frac{\kappa_p \nabla p}{\mu}
\]

Here, \( \kappa_p \) denotes the permeability of the electrode, \( \mu \) viscosity of the gas and \( p \) is pressure.

The ideal gas law gives the total molar concentration of the gas phase:

\[
c^g = \frac{p}{RT}
\]

Where, \( R \) denotes gas constant and \( T \) is the temperature.

The model takes into account two species at the cathode (\( \text{O}_2 \) and \( \text{H}_2\text{O} \)). Maxwell-Stefan diffusion and convection application mode is used for cathode side electrode in the model.

At the electrode-membrane interface, the gas velocity boundary condition in the Darcy’s law application mode is calculated from the total mass flux, according to:

\[
\vec{u} = \frac{n_{\text{total}}}{\rho}
\]

Where, \( n_{\text{total}} \) is given by the local current density and molar masses of the reacting species.

The boundary condition for the current density at the interface between the anode and the membrane, normal to the anode domain, can be written as:

\[
(\kappa^{s,\text{eff}} \nabla \phi_s) \cdot \vec{n} = i_a
\]

This term act as source term for that region. Where,
In addition:

\[ K_1 = \frac{6\delta (1 - \varepsilon) F D_{agg}^{agg}}{(R_{agg}^{agg})^2} \]

\[ K_2 = \frac{2F}{RT} \]

\[ K_3 = \frac{i_{o,d}S}{\sqrt{2F^2D_H^{agg}R_{agg}^{agg}}} \]

In these expressions, \( c_{agg}^{agg} \) denotes dissolved gas concentration at the surface of the agglomerates, \( c_{ref}^{agg} \) denotes dissolved gas concentration at a reference state, and \( \Delta \phi_{eq} \) is potential difference between the electrode and membrane at equilibrium conditions. Active layer thickness of the electrode is denoted by \( \delta \), while dry porosity of the electrode is denoted by \( \varepsilon \). \( F \) denotes as Farady’s constant, \( D_{agg}^{agg} \) diffusion coefficient of the dissolved gas inside the agglomerate, \( R_{agg}^{agg} \) the agglomerate radius, \( i_o \) the exchange current density and \( S \) the specific surface area of the electrode.

For the interface between the membrane and the cathode, the corresponding boundary condition, normal to the cathode domain, becomes:

\[-K_{c,eff} \nabla \phi_{eq} \cdot \vec{n} = i_c \]

This term also act as source term for this region.

Where,

\[ i_c = K_4 c_{o,ref}^{agg} (1 - \sqrt{K_5 \exp(-K_6 (\phi_s - \phi_m - \phi_{eq}^c))}) \coth \sqrt{K_5 \exp(-K_6 (\phi_s - \phi_m - \phi_{eq}^c))} \]

And, \( K_4 = \frac{12\delta (1 - \varepsilon) F D_o^{agg}}{(R_{agg}^{agg})^2} \]

\[ K_5 = \frac{i_{o,d}S(R_{agg}^{agg})^2}{4F^2C_o^{ref}D_o^{agg}} \]

\[ K_6 = \frac{0.5F}{RT} \]

The dissolved hydrogen and oxygen concentrations at the surface of the agglomerates are related to the molar fraction of the respective species in the gas phase through Henry’s law:

\[ c_H^{agg} = \frac{P_H y_H}{H_H} \]

\[ c_o^{agg} = \frac{P_o y_o}{H_o} \]

Here, \( H \) is the Henry’s constant.

It was chosen the anodic and cathodic reference states to be equal to the molar fraction at the inlet channels of the anode and cathode respectively, at 1 atm. The dissolved gas concentration at the reference state is related to the molar fraction by the above-described Henry’s law.
The current densities at the interfaces between the electrodes and the membrane, and normal to the membrane domain, are given by:

\[ (-\kappa_{m,\text{eff}} \nabla \phi_m) \cdot \vec{n} = -i_a \quad \text{at the interface of anode and membrane subdomain} \]

\[ (-\kappa_{m,\text{eff}} \nabla \phi_m) \cdot \vec{n} = -i_c \quad \text{at the interface of cathode and membrane subdomain} \]

These two terms also act as source terms for those specified regions.

Clearly, what goes out from the anode goes into the membrane while the opposite is valid for the cathode.

The potential difference between the cathode and anode current collectors corresponding to the total cell voltage. The potential at the anode current collector is arbitrarily chosen to be zero, while the total cell voltage is used as boundary condition at the cathode current collector. For the rest of the boundaries we have either insulation or symmetry conditions:

\[ \phi_s = 0 \quad \text{at the outer boundary of anode} \]

\[ \phi_s = V_{\text{cell}} \quad \text{at the outer boundary of cathode} \]

The pressure at the gas inlets and outlets are set to:

\[ p = p_{a,\text{in}} \quad \text{at anode side inlet} \]

\[ p = p_{\text{ref}} \quad \text{at anode side outlet} \]

\[ p = p_{c,\text{in}} \quad \text{at cathode side inlet} \]

\[ p = p_{\text{ref}} \quad \text{at cathode side outlet} \]

Hydrogen is consumed in the active catalyst layer at the anode while oxygen is consumed at the cathodic active layer. The mass transfer of species across the anodic and cathodic active layers is related to the local current density according to:

\[ -\vec{n} \cdot \vec{n}_{H_2} = -\frac{i_a}{2F} \quad \text{at anode subdomain} \]

\[ -\vec{n} \cdot \vec{n}_{O_2} = \frac{i_c}{4F} \quad \text{at cathode subdomain} \]

These two terms also act as source terms in that region.

At the remaining boundaries, either insulation or symmetry conditions were used.

**4.5 Finite Element Method [27]**

Finite element method is a computational method that subdivides an object into very small finite-size elements. FEMLAB generally uses finite element in the mathematical sense. Finite element in mathematical sense is a mesh element together with a set of shape functions and corresponding degrees of freedom. The linear combinations of the shape functions form a space of functions called the finite element space. In the traditional FEA sense, the concept of a finite element also includes the discretized form of the PDEs that govern the physics. A computer-based analysis method for field problems using the finite element method is known as finite element analysis (FEA).

The number of degrees of freedom (DOFs) in FEA is the physics of one element which can be approximately described by a finite. Each element is assigned a set of characteristic equations (describing physical properties, boundary conditions, and imposed forces), which are then solved as a set of simultaneous equations to predict the object’s behavior.

In simulated work Non-linear solver was used which follows Newton step in the solution of a nonlinear PDE problem. Each nonlinear iteration involves the solution of a linear system of
equations. The nonlinear solver uses an affine invariant form of the damped Newton method as described in [24].

FEMLAB internally needs an accurate Jacobian matrix to establish convergence of a solution for nonlinear models. A model described with weak form modes produces an exact Jacobian whereas the other modes generally do not. By selecting the solution form weak for a model, FEMLAB automatically generates the weak form of the equation, but the original application mode is still available. A partial differential equation in the weak form is a more general formulation than the strong form. It is produced by multiplying the strong form PDE with an arbitrary function called the test function and integrating over the computational domain.
CHAPTER 5

NUMERICAL SIMULATION RESULTS

The basic calculation model has an electrolyte in the middle and two gas diffusion layers on either side of the electrolyte. Catalyst for this fuel cell resides on the surface of the electrolyte indicates the most important part for a fuel cell. So, more gridding was used around the electrolyte/electrode interfaces. Extremely fine elements were used for meshing the model. Figure 5.1 shows the mesh of the model.

Figure 5.1: Meshing of the single channel model

Parametric Nonlinear solver was used in FEMLAB software to solve all the PDE equations. Parameter Nonlinear solver is similar to Nonlinear Solver; extra feature is iteration is done with varying one variable. Source terms in every boundary were increased in a systematic way from a very smaller value to the value of one. Convergence of this model is hindered by source terms. Therefore, this type of systematically increasing of source terms could accelerate the convergence of the calculation.
Similar to experimental work, flow rates of hydrogen was varied 20, 40, 60, 80, 100 sccm in the simulation works. However, the oxygen flow rate was maintained constant at 46 sccm for all the simulation models. Figures show mass fraction of water patterns variation and partial pressure of Hydrogen variation with variation of hydrogen flow rates but for fixed oxygen flow rate. Simulation results of water patterns are shown in the following figures.

Figure 5.2: Simulation of (a) water pattern and (b) $P_{H_2}$ for 20sccm Hydrogen flow rate at 0.5V

Figure 5.3: Simulation of (a) water pattern and (b) $P_{H_2}$ for 20sccm Hydrogen flow rate at 0.6V
Figure 5.4: Simulation of (a) water pattern (b) $P_{H_2}$ for 20sccm Hydrogen flow rate at 0.7V

Figure 5.5: Simulation of (a) water pattern (b) $P_{H_2}$ for 20sccm Hydrogen flow rate at 0.8V
Figure 5.6: Simulation of (a) water pattern (b) $P_{H_2}$ for 20sccm Hydrogen flow rate at 0.9V

Figure 5.7: Simulation of (a) water pattern (b) $P_{H_2}$ for 40sccm Hydrogen flow rate at 0.5V
Figure 5.8: Simulation of (a) water pattern (b) $P_{H_2}$ for 40sccm Hydrogen flow rate at 0.6V

Figure 5.9: Simulation of (a) water pattern (b) $P_{H_2}$ for 40sccm Hydrogen flow rate at 0.7V
Figure 5.10: Simulation of (a) water pattern (b) $P_{H_2}$ for 40sccm Hydrogen flow rate at 0.8V

Figure 5.11: Simulation of (a) water pattern (b) $P_{H_2}$ for 40sccm Hydrogen flow rate at 0.9V
Figure 5.12: Simulation of (a) water pattern (b) P$_{\text{H}_2}$ for 60sccm Hydrogen flow rate at 0.5V

Figure 5.13: Simulation of (a) water pattern (b) P$_{\text{H}_2}$ for 60sccm Hydrogen flow rate at 0.6V
Figure 5.14: Simulation of (a) water pattern (b) $P_{H_2}$ for 60sccm Hydrogen flow rate at 0.7V

Figure 5.15: Simulation of (a) water pattern (b) $P_{H_2}$ for 60sccm Hydrogen flow rate at 0.8V
Figure 5.16: Simulation of (a) water pattern (b) P_{H2} for 60sccm Hydrogen flow rate at 0.9V

Figure 5.17: Simulation of (a) water pattern (b) P_{H2} for 80sccm Hydrogen flow rate at 0.5V
Figure 5.18: Simulation of (a) water pattern (b) $P_{H_2}$ for 80sccm Hydrogen flow rate at 0.6V

Figure 5.19: Simulation of (a) water pattern (b) $P_{H_2}$ for 80sccm Hydrogen flow rate at 0.7V
Figure 5.20: Simulation of (a) water pattern (b) $P_{112}$ for 80sccm Hydrogen flow rate at 0.8V

Figure 5.21: Simulation of (a) water pattern (b) $P_{112}$ for 80sccm Hydrogen flow rate at 0.9V
Figure 5.22: Simulation of (a) water pattern (b) $P_{H_2}$ for 100sccm Hydrogen flow rate at 0.5V

Figure 5.23: Simulation of (a) water pattern (b) $P_{H_2}$ for 100sccm Hydrogen flow rate at 0.6V
Figure 5.24: Simulation of (a) water pattern (b) P_{112} for 100sccm Hydrogen flow rate at 0.7V

Figure 5.25: Simulation of (a) water pattern (b) P_{112} for 100sccm Hydrogen flow rate at 0.8V
Figure 5.26: Simulation of (a) water pattern (b) \( P_{H_2} \) for 100sccm Hydrogen flow rate at 0.9V

Figure 5.27: Simulation of (a) water pattern (b) \( P_{H_2} \) for 1sccm Hydrogen flow rate at 0.7V
Figure 5.28: Simulation of (a) water pattern (b) $P_{H_2}$ for 1sccm Hydrogen flow rate at 0.8V

Figure 5.29: Simulation of (a) water pattern (b) $P_{H_2}$ for 1sccm Hydrogen flow rate at 0.9V
Simulations are shown for various flow rate and various loads. Red color indicates higher and blue color indicates lower value. Every of the flow rate simulation result shows reasonable result. For low load, less water is formed and for high load, more water is formed. Also as the hydrogen and oxygen flow directions are from left to right so simulation result are also showing water formation more in the outlet side of oxygen flow and less in the entrance. Partial pressure of hydrogen is also reasonably varying from high to low from the entrance to the exit of the channel. In addition, for lower loads, less fuel is utilizing and for higher loads, fuel utilization is high.

Figure 5.30 shows water mass fraction variation along the channel for 40sccm Hydrogen flow rate for various voltage readings. This figure shows reasonable indications of water particle generation from the entrance to the exit of the channel. Water content is less in the entrance and more in the exit.

![Figure 5.30: Water mass fraction along the channel](image)

Table 5.1: Water Vapor Saturation region from the entrance

<table>
<thead>
<tr>
<th>Voltage (Volt)</th>
<th>The distance for cathode flow to reach saturation from entrance (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>4.5</td>
</tr>
<tr>
<td>0.8</td>
<td>0.2852</td>
</tr>
<tr>
<td>0.7</td>
<td>0.095</td>
</tr>
<tr>
<td>0.6</td>
<td>0.0495</td>
</tr>
<tr>
<td>0.5</td>
<td>0.03095</td>
</tr>
</tbody>
</table>

From [25] table- 4.1 at nearly 20 C, Saturated Vapor Pressure is 2.338 KPa. After a certain distance from the entrance of the channel water vapor will turn to liquid droplet due to partial pressure of water will be greater than the saturation of pressure of water vapor. Table 5.1 shows the location of that region from the entrance of the channel for various loads. Table 5.1 shows reasonable data as with increasing of loads, the unsaturated region getting smaller due to rapid electrochemical reaction from the entrance. After that distance, partial pressure of water is greater than saturated pressure of water vapor. So some of the water vapor start turning into liquid. From
the entrance of cathode side to that particular region, water vapor pressure is lower than saturation vapor pressure. Therefore, in that region, water will be in vapor form.

In addition, 2D numerical simulation has also been conducted. Compare to 3D model, 2D model is done without considering thickness of the channel. For 3D model, we had length of the channel, width of the channel and thickness of the channel but for 2D simulation length of the channel and width of the channel is considered. Figure 5.31 shows a 2D model with grids. Three layers are made for this 2D model. Middle layer is the electrolyte and gas diffusion layers are surrounding the two sides of this electrolyte. Catalyst is residing in the junction of gas diffusion layer and electrolyte. More gridding is used in both two sides of electrolyte, because of its importance in current generation.

![Figure 5.31: Grid of 2D model](image)

It is found that all simulations for 2D models show same shape of water patterns like 3D model. All the simulations show that with increasing loads water generation increases and with decreasing load water generation decreases. Figure 5.32 shows 2D numerical simulation of water pattern for 20sccm Hydrogen flow rate at a cell voltage of 0.7 volt with contour lines showing variation of water generation. Figure 5.33 shows 2D numerical simulation of partial pressure of Hydrogen for the same condition. Pressure decreases along the anode gas diffusion layer.

![Figure 5.32: 2D numerical Simulation of water pattern for 20sccm Hydrogen flow rate at 0.7V with contour lines](image)
After conducting 2D numerical simulations, results are compared with 3D numerical simulations. Simulation results for 2D and 3D are compared and shown in figures 5.34 & 5.35. It is found that difference is very little between these two sets of data. For 2D simulation, reactants passing along the channel are considered but as thickness is not considered, so electrochemical reaction across the channel is not considering in those 2D simulation. In 3D numerical simulations as reactants are getting more space to react with the surface due to the thickness resulting more efficiency of the cell.

Figure 5.34: Power density vs. Current Density curve for 2D and 3D simulation result for a 20sccm flow rate of Hydrogen.
Simulation of 1 channel for various flow rates of hydrogen is shown in figures 5.36 and 5.37. Simulation result shows that 20 and 40 sccm. Hydrogen flow rate shows similar trend in the curve and matches well. It is due to those flow rates are more than enough for a single channel fuel cell. Simulation result is also shown for 1sccm. Under a small feeding rate, lower performance curve was found.
Figure 5.37: Simulation of Voltage vs. Current Density curve for various hydrogen flow rates
Figure 6.1 and 6.2 show the comparison of experimental and simulation result for one channel. These results show good agreement between experimental and simulation results. There have very little variation between these two types of data. Very little deviation of experimental data is due to factors involved in uncertainty in getting proper data. Uncertainty calculation is shown in Appendix-II.

Figure 6.1: Comparison of Experimental and Simulation result of Power density vs. Current Density data for 20sccm Hydrogen flow rate for one channel.

Figure 6.2: Comparison of Experimental and Simulation result of Voltage vs. Current Density data for 20 sccm Hydrogen flow rate for one channel.
CHAPTER 7

CONCLUSION

Performance of PEM fuel cell is presented for different designs of bipolar plates. Performance is quantified in terms of polarization curve, percentage water in the feeding channels, water flooding pattern, fuel utilization rate, different reacting fluid flow rates and different combinations of cathode and anode bipolar plate arrangement. The study of nine bipolar plate combinations identified that an interdigitated anode bipolar plate with a Serpentine cathode bipolar plate gave the best result. For this arrangement, the hydrogen is forced to flow inside the anode porous gas diffusion layer towards the reaction sites. The water flooding is partially eliminated by the using of serpentine bipolar plate in cathode side, due to the high flow speed and thus the capability of blowing the water droplets out of the cell. The study of one channel simulation identified water patterns for various flow rates and load conditions to predict patterns of water generation inside the channel. It is expected that this arrangement of bipolar plates could significantly help the operation of PEMFC in practical applications.
CHAPTER 8

FUTURE WORKS

Performance prediction is done by comparing polarization curves, Power density vs. Current density curves, fuel utilization rate, Transient and Steady state data, water patterns in bipolar plate. More factors involving performance prediction will be valuable.

It is assumed that water patterns that will generate eventually from this three layers simulation will come to the bipolar plate. A comparative study on water pattern in the bipolar plate for this simulation work will be valuable.
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**APPENDIX-I**

**CALCULATION**

**O₂ Usage**
Charge = \(4 \times F \times \text{Amount of O}_2\)

So, Amount of O₂ = \(\frac{\text{Charge}}{4 \times F}\)

= \(\frac{I}{4 \times F}\) moles/s

Now, Power, \(P = V \times I\)

So, \(I = \frac{P}{V}\)

So, Amount of O₂ = \(\frac{P}{4 \times F \times V}\) moles/s

= \(\frac{32 \times 10^{-3} \times P}{4 \times F \times V}\) kg/s

= \(\frac{32 \times 10^{-3} \times P}{4 \times 96485 \times V}\) kg/s

= \(\frac{8.29 \times 10^{-3} \times P}{V}\) kg/s

Now, Density of oxygen = 1.429 kg/m³

So, Volume flow rate of O₂ = \(\frac{8.29 \times 10^{-3} \times P}{V \times 1.429}\) m³/sec

= \(\frac{5.8013 \times 10^{-3} \times P}{V}\) m³/sec

= \(\frac{5.8013 \times 10^{-3} \times 60 \times P}{V}\) m³/min

= \(\frac{3.48078 \times P}{V}\) cm³/min

Plug in proper values of \(P\) and \(V\) or \(I\), can give O₂ flow rate by the cell. To ensure enough O₂ in the gas diffusion layer O₂ flow rate maintained in the experiments was a little bit higher than theoretical calculated value.

**H₂ Usage**

\(H₂\) usage = \(\frac{I}{2 \times F}\) moles/sec
\[
\frac{P}{2 \times F \times V} \text{ moles/sec} = \frac{2.02 \times 10^{-3} \times P}{2 \times 96485 \times V} \text{ kg/sec}
\]

So, \( \text{H}_2 \) mass flowrate = \( \frac{1.05 \times 10^{-3} \times P}{V} \) kg/sec

Now, Density of \( \text{H}_2 \) = 0.0899 kg/m\(^3\)

So, volume flowrate of \( \text{H}_2 \) = \( \frac{1.05 \times 10^{-3} \times P}{0.0899 \times V} \) m\(^3\)/sec

= \( \frac{1.168 \times 10^{-7} \times P}{V} \) m\(^3\)/sec

= \( \frac{1.168 \times 10^{-7} \times 10^6 \times 60 \times P}{V} \) cm\(^3\)/min

So, Volume flowrate of \( \text{H}_2 \) = \( \frac{7.008 \times P}{V} \) cm\(^3\)/min

Plug in proper values of \( P \) and \( V \) or \( I \), can give \( \text{H}_2 \) flow rate by the cell. To ensure enough \( \text{H}_2 \) in the gas diffusion layer \( \text{H}_2 \) flow rate maintained in the experiments a little bit higher than theoretical calculated value.

**Water Generation after the Electrochemical Reaction**

Water is generated at the rate of one mole for every two electrons.

So, Water generation = \( \frac{P}{2 \times V \times F} \) moles/s

= \( \frac{P \times 18.02 \times 10^{-3}}{2 \times V \times 96485} \) kg/s

= \( \frac{9.34 \times 10^{-3} \times P}{V} \) kg/s

Plug in proper values of \( P \) and \( V \) or \( I \), can give \( \text{H}_2 \text{O} \) generation after the electrochemical reaction by the cell. It is reasonable that experimental water generation is little bit higher than theoretical calculated value.

**Calculation of Time Taken by \( \text{H}_2 \) to Go Inside the Gas Diffusion Layer**

Let, porosity of gas diffusion layer = 30\% = 0.3

Volume of gas diffusion layer = \( 0.0505 \times 0.0495 \times 50 \times 10^{-6} \) = \( 1.2499 \times 10^{-7} \) m\(^3\)

Now, 20 sccm = \( 20 \times \frac{10^{-6}}{60} \) m\(^3\)/s
=3.333×10^{-7}\ m^3/s
So, Porous gas diffusion layer volume= 1.2499×10^{-7}×0.3
=3.7497×10^{-8}\ m^3

Time takes to go inside hydrogen into the gas diffusion layer:
For, 20 sccm flow rate of H_2=\frac{3.7497×10^{-3}}{3.333×10^{-7}}
=0.1125\ sec.
For, 40 sccm flow rate of H_2=\frac{0.1125}{2}
=0.05625\ sec.
For, 60 sccm flow rate of H_2=\frac{0.1125}{3}
=0.0375\ sec.
For, 80 sccm flow rate of H_2=\frac{0.1125}{4}
=0.028125\ sec.
For, 100 sccm flow rate of H_2=\frac{0.1125}{5}
=0.0225\ sec.

The above calculation of time taken by H_2 to fill the gas diffusion layer indicates a very short time (fraction of a second) needed for H_2 to fill the gas diffusion layer.

**Minor Loss in Interdigitated Bipolar Plates**

Pressure loss through the porous backing layer can be estimated by Darcy’s Law according to Vafai and Hadim(2001) et al. [26]:

\[ \Delta P_{\text{backing}} = \frac{V\mu\Delta S}{\kappa} \]

Where, V is the velocity of the fluid through the porous medium, \( \Delta S \) is the porous medium thickness in the direction of flow, \( \kappa \) is the permeability of the backing layer. \( \mu \) is the viscosity of fluid.

The backing layer permeability is a non-linear function of porosity and can be shown by the Kozeny-Carmen relation according to Vafai and Hadim(2001) et al. [26]:

\[ \kappa = \frac{\varepsilon^3 d_s^2}{180(1 - \varepsilon)^2} \]

Where, \( \varepsilon \) is the porosity of the backing layer and \( d_s \) is the diameter of the theoretical spherical particles the medium is modeled to consist of.

\[ \varepsilon = 0.3 \text{[assumed 30% porosity]} \]
\[ d_w \text{ 1 mm} = 0.001 m \]

So, \[ \kappa = \frac{0.3^3 \times 0.001^2}{180(1-0.3)^2} \]

\[ = 3.0612 \times 10^{-10} \]

Now, \[ \Delta P_{\text{backing}} = \frac{0.010227 \times 1.862 \times 10^{-5} \times 31 \times 10^{-4}}{3.0612 \times 10^{-10}} \quad \text{[For, cathode side interdigitated channel]} \]

\[ = 1.9284 \text{ Pa} \]

\[ = 0.0019284 \text{ KPa} \]
APPENDIX - II
UNCERTAINTY ANALYSIS

In every experimental result, experimental uncertainty is an important parameter and must be discussed and quantified. Student’s t-distribution is commonly regarded as the standard method for determining experimental uncertainty. The average experimental uncertainties of all the data for this study can be determined by this Student’s t-distribution if uncertainty in any of the variable can be obtained. For fifteen sets of voltage data under different times at 0.106-ohm load, uncertainty in experimental data are as follows:

Mean values of these data, $\bar{X}_n = 0.3034$

Standard deviation of these data, $S_n = 0.001164965$

With the 95% confidence limit

$A = 1.753$ (value taken from [27])

No. of samples, $n = 15$

Now, $\bar{X}_n \pm A \times \frac{S_n}{\sqrt{n}}$

$= 0.3034 \pm 1.753 \times \frac{0.001164965}{\sqrt{15}}$

$= 0.30392729$ and $0.30287271$

Therefore, we can determine that at 95% confidence, we have a true mean value of voltage lying between: $[0.30287271, 0.30392729]$
VITA

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