A parametric study of Proton Electrolyte Membrane (PEM) fuel cell performances

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A PARAMETRIC STUDY OF PROTON ELECTROLYTE MEMBRANE (PEM) FUEL CELL PERFORMANCES

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Abstract

A two-dimensional, steady-state and isothermal model of the proton electrolyte membrane (PEM) fuel cell has been developed numerically, using a commercial package COMSOL. The single channel cell, which consists of seven regions, is used as the computational domain. The governing equations for mass, momentum, mass transport and charge equations are coupled and solved to produce the polarization curves for the fuel cell performance. The resultant polarization curves obtained from the numerical simulation are validated by comparing with the experimental results under normal operating conditions. Further, the benchmarked numerical model is used to investigate the effect of the temperature, concentration of hydrogen, concentration of oxygen, operating pressure, stoichiometric flow ratio, channel height, gas diffusion layer (GDL) thickness, membrane thickness and GDL porosity on the performance of the PEM fuel cell.

The modeling results agree reasonably well with the experimental polarization curves within allowable numerical scatter, except the mass transport region. As the fuel cell and the gas humidification temperature increases, the current density and maximum power density both increase. This trend is also observed in the concentration of hydrogen and the concentration of oxygen in air. As the concentration increases, the improvement of the fuel cell performance becomes negligible. The increase in operating pressure in both flow channels also increases both the current density and maximum power density. Between the two flow channel's operating pressure, the cathode flow channel's operating pressure plays a predominant role in affecting the performance of the fuel cell. As the stoichiometric flow ratio of hydrogen and air are increased at both flow channel inlets, the current density, the limiting current density and maximum power density increase. For the stoichiometric flow ratio of 5.0 and above, the improvement in the fuel cell performance is negligible. Further investigation shows that, the air stoichiometric flow ratio has a predominant effect in improving the performance of the fuel cell while the hydrogen stoichiometric flow ratio does not have any effect, based on the present simulation. As the channel height increases, the current density and the maximum power density increases. Above a particular height, *i.e.* 1mm, the improvement in the performance of the fuel

cell is negligible. The increase in thickness of both GDL, reduces the current density and maximum power density. The GDL thickness of cathode and anode have almost equal contribution towards the performance of the fuel cell. As the thickness of the membrane increases, the current density and the maximum power density reduces. By increasing the GDL porosity of both anode and cathode, the current density and the maximum power density will be increased. For the porosity of 0.5 and above, the improvement of current density and maximum power density are negligible. Further investigation on the effect of individual GDL porosity shows that the cathode GDL porosity has predominant effect in improving the performance of the fuel cell while the anode GDL porosity does not have any effect on the performance of the fuel cell.

A sensitivity analysis has been conducted on the fuel cell operation, using analysis of variance (ANOVA), which is a statistical tool, used to determine how sensitive the parameters are. The factors are separated into two categories. For the operating parameters, the more sensitive factors that affects the fuel cell's current density are the temperature of the fuel cell and the humidification of both hydrogen and air, the operating pressure of the cathode flow channel and the concentration of oxygen in air supplied to the cathode flow channel. While for the maximum power density, the more sensitive factors are the operating pressure of the cathode flow channel and the concentration of oxygen in air supplied to the cathode flow channel. The most sensitive factors among the design parameters in affecting the fuel cell's current density and maximum power density are the membrane thickness, cathode GDL thickness and anode GDL thickness.

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Chapter 1

Introduction

1.1 Background

As the world's population increases, and the development of the industry sectors, power consumption and energy requirement increases as well. Majority of the power generators depend on the combustion of the fossil fuel. However, the consumption of fossil fuel is not environmental friendly. It creates air pollution from combustion of fuel and spill in seas from tankers or pipe leaks. Furthermore, the supply of fossil fuel is finite. It is estimated that oil, gas and coal will be depleted in 35, 37 and 107 years respectively [1]. Therefore, there is a need to develop a new energy source and reduce the reliance on fossil fuel.

Among the energy alternatives, fuel cell has been widely recognized as the most promising candidate. The efficiency of fuel cell is higher than internal combustion engine, which makes it a good energy alternative for the automobile applications. Fuel cell's efficiency is higher than conventional power plant's. This makes it suitable as a power generator. There is a prospect of micro scaling the fuel cell, to as thin as $200\mu\text{m}$ [2], which attracts portable electronic device manufacturers to use fuel cell as an energy source. Fuel cell is environmental friendly, and generates little emission. For most fuel cells, their by-product are water. For those using alcohol, they emit carbon monoxide, but much less than those conventional energy conversion device. This also makes fuel cell suitable for indoor and underwater transportation. Fuel cell is made from a simple structure, and for

more power, it can combine many individual cell to form a stack. This repetitive nature of stack fuel cell makes it possible to lower the cost of manufacturing those components. Regardless of the benefits, it remains unchanged that even though it has been 160 years since the chemical energy was successfully converted into electrical energy in a fuel cell, it is still difficult to commercialize the usage of the fuel cell. This is due to the high cost per unit electricity output and its low durability, which can be attributed to the lack of cheaper materials and manufacturing methods that is currently available. Therefore, a lot of studies are to increase the performance of the fuel cell and finding cheaper alternatives for the currently expensive components.

Among the fuel cells, proton electrolyte membrane (PEM) fuel cell is suitable for portable devices and transportation, due to its high efficiency, fast start up time and low operating temperature. One of the key issues of the PEM fuel cell is water management. Sufficient water is needed in the membrane to maintain its high ionic conductivity. The water molecules transport through the membrane, electro-osmotic drag, water diffusion and fluid convection, which makes retaining high water content in the membrane difficult. Therefore, the gases are humidified at the inlet, to supply water to the membrane, especially at the start up when the membrane is still dry. But then, water is generated at the cathode side from the electrochemistry reaction, at the interface between the membrane and the catalyst layer. Usually, it's the pressure from the cathode gas flow that help remove this water from the gas diffusion layer (GDL) and catalyst layer, but if the water is not removed at an appropriate rate, then flooding will occur. Flooding will cause pores blockages at the GDL, which hinders the oxygen gas transport, thus result to poor performance. On the other hand, if the membrane is dry or not fully hydrated, its ionic conductivity will be too low which reduces the performance of the fuel cell. Therefore proper water management is essential to balance the two-phase flow.

This two-phase transport phenomena cannot be observed directly, as a result, mathematical modeling is a critical tool to understand the phenomena. Researchers have developed models to describe the operation of the PEM fuel cells with the assumption of its single-phase flow [3–12]. To understand the phenomena of water transport and distribution in

PEM fuel cell, researchers have developed two-phase flow models [13–18]. Even so, more studies are required to develop a more comprehensive two-phase flow model to simulate extreme operating conditions, e.g. operating a PEM fuel cell at room temperature, where the formation of liquid water occurs even at low current density, operating with dry gases, etc. In a nutshell, a two-phase flow model is essential to study the liquid water and gas transport phenomena and subsequently, to plan a mitigation of water management strategy. The current study validates the single phase isothermal model to benchmark the experimental results. Further, it will be extended to investigate a more comprehensive two-phase flow transport, non-isothermal model of PEM fuel cell to simulate the flow of liquid water under normal operating conditions. The effect of the process parameters will also be a further point of interest in this study. Furthermore, a sensitivity analysis is conducted to determine which parameter has the most effect on the fuel cell. This can serve as a guideline when designing and fabricating fuel cells.

1.2 Objectives

The objectives of this research are

- To develop a two-dimensional, single-phase, isothermal model for PEM fuel cell performance studies.
- To investigate the effect of various parameters, which includes the concentration of oxygen, back pressure of the gas channels, air inlet velocity channel height, GDL thickness, membrane thickness and GDL porosity, on the performance of the PEM fuel cell.
- To investigate which parameters are the most sensitive in affecting the fuel cell's performance.

1.3 Outline of Report

1. A comprehensive and extensive literature search and review is given in Chapter 2 to provide a better understanding of the available models.
2. Chapter 3 gives details and the methodology of developing a two-dimensional, single-phase, isothermal PEM fuel cell model.
3. The model was created and a validation is made by comparing the simulated result with the performance of an experimental result available in the literature. The model is further investigated by parametric study by investigating the effect oxygen etc. which is described in Chapter 4.
4. Chapter 5 describes the methodology and the result of the sensitive analysis of the fuel cell model.
5. The final remarks on the conclusion and recommendations are given in Chapter 6.

Chapter 2

Literature Review

2.1 Overview of PEM Fuel Cell

Polymer electrolyte membrane (PEM) fuel cell, is a fuel cell that operates at low temperature ($60^{\circ}\text{C} \sim 90^{\circ}\text{C}$). Its difference from most other type of fuel cells is its electrolyte, which is made of polymer membrane which conducts protons. It's because of the membrane electrolyte, it is able to operate at a low temperature compared to other fuel cells. The benefits of a PEM fuel cell includes low operating temperature, simple design, high energy efficiency, fast start up, high power density. As a result, it is suitable for stationary and portable applications, especially in transportation, as most car manufacturer has demonstrated at least one prototype vehicle. But its material and manufacturing cost is high, especially with the use of platinum catalyst, polymer membrane and other expensive components, is its downside. It also has poor tolerance with carbon monoxide and sulphur and in need of active water management. These limitations have spur researchers to investigate ways to improve the cell performance and to find alternative materials which eventually leads to the reduction of the cost. Ultimately, the final goal will be to make fuel cell affordable and reliable to people to use it as an alternative energy source to the finite fossil fuel.

Figure 2.1: An illustration of a PEM fuel cell. [19]

2.2 Working Principle of PEM Fuel Cell

Generally, PEM fuel cell consists of three main parts, anode, cathode and electrolyte which is made of membrane. Anode is where the fuel reacts, cathode is where the air / oxygen react and the electrolyte separates both anode and cathode and only allows hydrogen ions travel through. This is illustrated in Figure 2.2.

Figure 2.2: The working principle of PEM fuel cell. [20]

On the anode side, at the catalyst layer where the reaction take place, the hydrogen molecule from the hydrogen gas is oxidized into hydrogen ion and electron. Hydrogen

ion travels through the electrolyte to cathode and electron travels through the external circuit.

On the cathode side, the oxygen molecule from air, combine with the hydrogen ion from the electrolyte and electron from the external circuit, produces water.

The electrons that travel through the external circuit produce electricity.

Therefore, by putting in hydrogen gas as fuel, and air, it produces electricity and water as by product.

2.3 PEM Fuel Cell Components

Membrane As the name suggest, PEM fuel cell's electrolyte is made from proton conducting polymer electrolyte membrane. More specifically, the membrane is made of perfluorinated sulfonic acid ionomers, and the most commonly known material is Nafion™ by Dupont as shown in Figure 2.3. The functions of a membrane are to allow the proton to move through it while separating the gases. Therefore, the characteristics of a good fuel cell membrane are high proton conductivity, low permeability of the gases and chemically and mechanically stable under fuel cell operating environment [21, 22].

Figure 2.3: Chemical structure of Nafion™. [23].

NafionTM is used because it meets most of the requirement of a good membrane, like, high proton conductivity and good mechanical strength [24]. From the structure, the sulphonic acid end (SO^{3-} ion and H^+ ion) is ionically bonded and therefore has high tendency to cluster within the whole membrane structure. Although the backbone is hydrophobic, the sulphonic acid end is highly hydrophilic. This creates a highly hydrophilic region around the cluster of sulphonic acid ends, which makes it able to absorb large amount of water. As H^+ ions move well in these hydrated regions, it makes the membrane proton conductive [21].

Gas Diffusion Layer The membrane is sandwiched in between two gas diffusion layer (GDL) (also known as porous backing layer or current collector). The GDL is used to diffuse gas from the channel to the electrodes, provide mechanical support to the membrane electrode assembly (MEA), connect electrically between the electrode and bipolar plate, remove heat from the electrode to the bipolar plate (as the electrochemical process is exothermic) and remove water from the electrodes [22, 21]. Therefore, an ideal GDL should have high electrical and thermal conductivity, high gas permeability, high water removal rate and good mechanical properties [24]. The GDL is usually made of carbon paper or carbon cloth. Both of them exhibit excellent stability, good corrosion resistance and good mechanical properties [24].

It is treated with hydrophobic material to prevent water from blocking the pores in order to let the gases to pass through freely towards the electrode. Polytetrafluoroethylene (PTFE) is commonly used as the hydrophobic material.

It is a common practice to add an intermediate layer, known as micro porous layer (MPL), between the GDL and electrode, to improve the interface between them. It consists of sub-micron sized graphite particles and polymeric binder, and applied on the GDL. The MPL helps in the transition of the GDL's large porosity to the electrodes fine porosity. It also helps in the removing of water from the electrode and decrease in electrical contact resistance between the GDL and electrode. Qi et al. [25] concluded that MPL help eliminates the effect of performance variation from different carbon papers. They also

found out that the MPL enhanced the water management in the GDL and it reduces the penetration of the catalyst when it is applied on the GDL, which increases the active area of the catalyst. According to Atiyeh et al. [26], applying MPL on either side of the electrodes or both sides, improves the performance and durability of the fuel cells compare to those without MPL.

Electrode (Catalyst Layer) For electrode, it consists of a thin layer of catalyst integrated together with the binder, which is sandwich in between the membrane (both side) and the gas diffusion layer. Electrode is where the electrochemical reactions take place. More precisely, the reactions take place at the three-phase boundary, the membrane, the catalyst layer and the gas diffusion layer. The membrane is where the protons travel, the electrons travel through the catalyst and the gas travel through the porous gas diffusion layer. Therefore, it's the catalyst surface area that determines the performance of the fuel cell, the more three-phase boundary exist, the more reaction take place, the higher the performance. The common catalyst used for both the oxygen reduction and hydrogen oxidation reactions is platinum. Due to the high cost of platinum, efforts have been put in to minimize the use of platinum. It is reported, the activity per unit mass platinum is near optimal when the particle size of platinum is about $3.5nm$, and is disperse on the catalyst support, typically carbon or graphite [22]. This is because the small particle size increases the platinum's surface area and increases the utilization of the platinum.

Bipolar Plate Bipolar plate is the housing for the PEM fuel cell. Usually consist of two plates, directly covering the GDL. Its functions include provide structural support for the cell, housing the flow field channels, conducts heat generated from the reaction to the air and corrosion resistance under the fuel cell operating conditions (pH 2 to 3 and temperature $60^{\circ}C$ to $80^{\circ}C$ [21]. The bipolar plates need to be electrically conductive, impermeable to gases, high strength yet lightweight and thermally conductive. Graphite is commonly used as the bipolar plates, due to its chemically inertness under the fuel cell operating environment. But it's not easy to machine and its brittle. Metallic plates are used too as bipolar plates. They are high strength in nature, and easier to be machine

(stamping, embossing) but corrosive in the fuel cell operating environment. Therefore, they needed to be coated with a thin layer of noncorrosive and electrically conductive material at their surface. Another option is graphite composite plates. They are made using thermoplastic or thermoset resin with fillers and possible fiber reinforcement. The advantage is they are chemically stable under fuel cell operating environment and can be manufacture by moulding at high speed, which can reduce cost. But they are brittle and their electric conductivity is much lower than those made of metallic.

2.4 Modeling

Modeling and simulation have been used to investigate the performance of the PEM fuel cells in recent years. Modeling helps investigate complex geometries and different situations using less time and effort compared to experimental investigations. Plus, laboratory experiments and tests are also a financial burden. Using experimental measurements to obtain relevant information are exceedingly difficult due to its small dimensions and electrochemically active environment of fuel cells, the complexity of the couplings, and the transient nature of the processes. Furthermore, experiments is limited to design which already exist, thus it does not facilitate innovative design. Theoretical studies is not only useful in test scenarios but they also provide fundamental insight of the fuel cell, quantities which are difficult to obtained through experiments, such as potential , temperature, reactant and current distributions of individual components. Thus, mathematical models can be used to provide details on the physical processes occurring within the fuel cell during operation; thus providing greater insight on the internal workings of a fuel cell.

A few researchers had done some reviews on PEM fuel cell. Wang [27] reviewed on the fundamental of modeling based on the different aspect of modeling. The review is categorized in the transports of water, heat, electron, liquid water and the experimental diagnostics. Shah et al. [28] reviewed on the trends and development in PEM fuel cell modeling. They categorize theirs into macroscopic approach, performance models, degradation models and small scale modeling. Siegal [29] reviewed on the heat and mass

transfer modeling. He categorized them into the number of dimensions, the approaches and the numerical procedures. Cheddier and Munroe [30] reviewed and compared the approaches used in the PEM fuel cell modeling. They reviewed the types of models, modeling considerations and compared the unified approach and the multi-domain approach. Haraldsson and Wipke [31] evaluated on the available PEM fuel cell system models. They reviewed on the single cell models and the fuel cell systems models. Bıyıkoglu [32] reviewed on the PEM fuel cell models. He reviewed on the modeling of each component of the fuel cell, and the diagnostics of the fuel cell available.

One of the earliest produced models were Bernardi and Verbrugge [9, 10] and Springer et al. [7, 8]. They analyzed species transport, water addition and removal, cathode flooding and the effect of gas humidification. Bernardi and Verbrugge’s model used a one dimensional approach for mass transport at the MEA and gas channels, assumed to operate under steady state and isothermal conditions. The Stefan Maxwell equations were used for gas phase diffusion in the electrode regions. For the catalyst layers, the model considered it to have finite thickness and composed of porous mixture of carbon/platinum catalyst and polymer electrolyte. For the dissolved species fluxes in electrolyte and catalyst layers, they used Nerst-Planck equation to describe it, Butler Volmer equation for the electrode kinetic rate and Schogl equation for the water transport. The membrane electrolyte is assumed to be fully hydrated at all times and constant throughout. However, water content in the electrolyte affects the ionic conductivity, with a high water content increases the ionic transport. Water is produced on the cathode side during operation, where the electro-osmosis drag encourages water migration from anode side to the cathode side. Therefore, water content is not constant in the MEA. On the other hand, Springer et al.’s [7] model addressed this issue. Their model was also one dimension, steady state and isothermal. Their model treated the catalyst layer as a surface. The electrolyte transport model allowed water content gradient. The molar flux of water in the electrolyte was expressed as a function of current density, water content gradient and pressure gradient. Hydrogen ion migration is described using Ohm’s law, where the ionic conductivity is a function of water content. They use the model to predict the net water

per hydrogen flux ratio and discussed the model behavior. Although these models were just one dimensional models, they provided the framework to build multidimensional, multiphysics models that follows.

Later on, Fuller and Newman [5], Nguyen and White [6] and Yi and Nguyen [33, 12], developed pseudo-two-dimensional models, accounting for compositional changes along the flow path. Fuller and Newman's [5] model used concentrated solution theory to account for diffusive transport through the membrane. It showed that adequate heat removal is important in order to prevent dehydration of the membrane and also to maintain high performance. They also studied the effects of dry gas feeds. Nguyen and White's [6] model treated the catalyst layer as an interface. The concentration along the electrodes used algebraic expressions and liner assumptions. They reported the relationship between the transport number and electro-osmotic drag coefficient. Yi and Nguyen [33, 12] analyzed flow-field design and temperature distribution, and liquid water effects at different operating conditions. They also examined cooling strategies. These pseudo-two-dimensional models further showed the essential roles played by water and heat management in maintaining high performance of the cells. Gurau et al. [11] presented a two-dimensional, non-isothermal, along-the-channel model of transport phenomena in PEM fuel cell. They analyzed the transport of water through the membrane but not the liquid phase water within the GDL. This model illustrated the utility of a multidimensional model in the understanding of the internal conditions of a fuel cell, such as the reactant and water distribution. This model is based on multi-domain approach, gas flow channels / GDL, catalyst layers and membranes. The single-domain approach is used at the gas flow channels and GDL, which is combining both the regions as one domain since the governing differential equations in both regions are similar. The only difference is the material properties and source terms, gas flow channels and GDL.

The concept of modeling a PEM fuel cell within the computational fluid dynamics (CFD) framework was proposed by Um et al. [34], Um et al. [35] and Dutta et al. [36, 37]. Um et al. [34] developed a two-dimensional model, which simulated coupled electrochemical and transport equations using CFD code. The three-dimensional versions were also developed

by Um et al. [35, 38]. Independently, Dutta et al. [36] developed a model using Fluent, a commercial to simulate it. Later on, Dutta et al. [37] and Lee et al. [39] presented their models, where the MEA is not included in the computational domain but just as an interface, where the water transport and ohmic potential drop across the membrane is assumed to be linear.

Few three-dimensional models for general purpose were developed. Zhou and Liu [40] used an in-house CFD code, Berning et al. [41] used CFX, a commercial package, and Mazumder and Cole [15] used CFD-ACE+, another commercial package. Recently, STAR-CD and Fluent packages have been used in large scale fuel cell modeling, through their own user-coding feature [42].

There are two ways to treat the liquid water formation in PEM fuel cell. The single phase model, which is the easier approach among the two, where the gas and liquid are considered as a single fluid mixture, therefore, it share the same velocity field. In addition, the inter-facial tension effect is ignored. The amount of water can therefore be obtained by solving a single equation. With the water concentration field obtained, the water concentration can be allowed to go beyond saturation level, assuming supersaturation in gas phase [7, 34, 38]. On the other hand, the water concentration can be truncated at the gas saturation level and account for the extra water in the form of liquid water in post processing. The more difficult approach is the two-phase model, in which two phases travel at different velocities. It also takes into account the inter-facial tension effect and GDL wettability, which are essential for successful PEM fuel cell operation. Efforts were been made to model the two-phase flow and transport in PEM fuel cell, a more realistic but difficult modeling of the water transport.

2.4.1 Single Phase

As stated earlier, single-phase model considers the total amount of water without distinguishing liquid phase from vapor phase. This is valid under the condition that liquid saturation within the GDL is low or liquid droplets are small and disperse in gas flow to form a mist flow, which means, it is well suited for fuel cell simulations under low

humidity operations.

The model considers the anode feed consisting of hydrogen, water and nitrogen or just hydrogen and water, while the cathode feed consist of humidified air, which are oxygen, water and nitrogen. The chemical reactions of hydrogen oxidation and oxygen reduction are assumed to occur only within the catalyst layers.

The fundamental PEM fuel cell model consists of five principles of conservation, mass, momentum, species, charge and energy. This set of equations is to be used in all regions of the whole fuel cell. Since the pressure gradient and Reynolds number are small, the flow is assumed to be laminar and incompressible. The mixture gas is assumed ideal as well.

For the mass and momentum equations at gas channels and GDL, superficial velocity is used to ensure mass flux continuity at the interface of the two regions. The fluid velocity at the membrane is set as zero since the membrane's permeability is assumed to be very small, about 10^{-30}m^2 . For flow through medium, the source term for the momentum equation, is Darcy's drag. The momentum equation is now reduced to Navier-Stokes equation in gas channels, Darcy's law in GDL and catalyst layers.

$$\frac{1}{\epsilon} \left[\frac{\partial \rho \vec{U}}{\partial t} + \frac{1}{\epsilon} \nabla (\rho \vec{U} \vec{U}) \right] = -\nabla p + \nabla \tau + S_u \quad (2.3)$$

$$S_u = -\frac{\mu}{K} \vec{U} \quad \text{in GDL \& catalyst layers}$$

$$\vec{U} = 0 \quad \text{in membrane}$$

where ϵ is the porosity, ρ is the gas density, $\vec{U}$ is the velocity field, p is the pressure, τ is the stress tensor, μ is the gas viscosity, K is the permeability.

There is a nonzero mass source in the mass equation at the catalyst layers, which arose from the summation of the species equations.

$$\frac{\partial (\epsilon \rho)}{\partial t} + \nabla (\rho \vec{U}) = S_m \quad (2.4)$$

$$S_m = \begin{cases} -M_{H_2} \frac{j}{2F} + M_{H_2O} [\nabla (D_{w,m} \nabla C_{H_2O}) - \nabla (n_d \frac{i_e}{F})] & \text{in anode catalyst layer} \\ M_{O_2} \frac{j}{4F} - M_{H_2O} \frac{j}{2F} + M_{H_2O} [\nabla (D_{w,m} \nabla C_{H_2O}) - \nabla (n_d \frac{i_e}{F})] & \text{in cathode catalyst layer} \\ 0 & \text{in membrane \& GDL} \end{cases}$$

where M_i molecular weight of species i , j is the local current density, F is the Faraday constant, C_{H_2O} is the local water concentration, i_e is the current density, n_d is the electro osmotic drag coefficient. The $D_{w,m}$ is the diffusion coefficient of water through membrane only. The water fluxes through the membrane, by electro-osmotic drag and molecular diffusion, are part of the source / sink term for the gas mixture mass in both the anode and cathode catalyst layers.

The species equation, applies to species H_2 , O_2 and H_2O , while N_2 is the remaining species of the gas mixture. As the mole fraction of the mixture is unity, the concentration of N_2 can be easily calculated. Fick's law is used to modeled the species diffusion, which is exact for binary gases but for the multicomponent gases, its a close approximation. The electro-osmotic drag coefficient, n_d is only relevant for water molecule, therefore its zero for the other species.

$$\frac{\partial (\epsilon C_k)}{\partial t} + \nabla (\vec{U} C_k) = \nabla (D_k^{eff} \nabla C_k) + S_k \quad (2.5)$$

$$S_k = \begin{cases} -\nabla (n_d \frac{i_e}{F}) - \frac{s_k j}{nF} & \text{in catalyst layer} \\ -\nabla (n_d \frac{i_e}{F}) & \text{in membrane} \\ 0 & \text{in GDL} \end{cases}$$

where C_k is the mass fraction of species k , D_k^{eff} is the diffusion coefficient of species k , s_k is the stoichiometry coefficient of species k .

Gas density is needed in the above conservative equations. Ideal gas law is used to find the gas density.

$$\rho = \sum M_k C_k \quad (2.6)$$

The molar concentration for N_2 can be calculated by

$$C_{N_2} = \frac{p}{RT} - C_{H_2O} - C_{O_2}$$

This is for cathode gas mixture. C_{O_2} can be replaced with C_{H_2} for anode gas mixture. For the case where the anode gas mixture consist of H_2 and H_2O ,

$$C_{H_2} = \frac{p}{RT} - C_{H_2O}$$

The charge equation is as follow

$$\nabla \left(\kappa^{eff} \nabla \Phi_e \right) + S_\Phi = 0$$

$$\nabla \left(\sigma^{eff} \nabla \Phi_s \right) - S_\Phi = 0 \quad (2.7)$$

$$S_\Phi = \begin{cases} j & \text{in catalyst layer} \\ 0 & \text{in membrane \& GDL} \end{cases}$$

where κ^{eff} , σ^{eff} are the electronic conductivities of the membrane and electrode and Φ_e , Φ_s electric potential for the membrane and electrode.

Those equations include the electrochemical kinetics for anode and cathode catalyst layers. Assuming that infinite large electric conductivity of the electronic phase, the electrode becomes an equipotential line,

$$\Phi_s = 0 \quad \text{in anode}$$

$$\Phi_s = V_{cell} \quad \text{in cathode}$$

The source term describe the transfer current between the electronic and electrolyte phases of each catalyst layer. The local transfer current densities are

$$j = ai_{0,a}^{ref} \left(\frac{C_{H_2}}{C_{H_2,ref}} \right)^{\frac{1}{2}} \left(\frac{\alpha_a + \alpha_c}{RT} F \eta \right) \quad \text{in anode}$$

$$j = -ai_{0,c}^{ref} \left(\frac{C_{O_2}}{C_{O_2,ref}} \right) \exp \left(-\frac{\alpha_c}{RT} F \eta \right) \quad \text{in cathode}$$

where a is the active specific surface area, i_0^{ref} is the reference exchange current densities, C_{H_2} is the local H_2 concentration, C_{O_2} is the local O_2 concentration, $C_{H_2,ref}$ is the reference H_2 concentration, $C_{O_2,ref}$ is the reference O_2 concentration, α_a is the charge transfer coefficient (anode side), α_c is the charge transfer coefficient (cathode side), R is the universal gas constant, T is the gas temperature, η is the activation overvoltage.

These represent the hydrogen oxidation reaction (HOR) in the anode catalyst layer and oxygen reduction reaction (ORR) in the cathode catalyst layer. These are simplified from the Butler-Volmer equation.

$$j = ai_0 \left[\exp \left(\frac{\alpha_a F}{RT} \eta \right) - \exp \left(-\frac{\alpha_c F}{RT} \eta \right) \right]$$

The anode expression is a linearized version of the Butler-Volmer equation, taking the assumption that HOR reaction is simple and fast, therefore the surface potential is small. The ORR reaction is slow and sluggish, which cause high over-potential. Therefore, the cathode expression neglects the anodic term for the Butler-Volmer equation. The value $(\alpha_a + \alpha_c)$ in the anode expression should be equal 2. While, α_c in the cathode expression is equal to 1, to corresponds to a Tafel slope approximately $60mV/decade$.

The equilibrium open-circuit potential for a H_2 /air fuel cell can be express as

$$U_0 = 1.23 - 0.9 \times 10^{-3} (T - 298.15) + \frac{RT}{2F} \left(\ln p_{H_2} + \frac{1}{2} \ln p_{O_2} \right)$$

It is calculated from thermodynamic data of the reaction enthalpy and entropy changes. The energy equation takes into account the heat generation caused by irreversible heat of the electrochemical reaction, reversible or entropic heat and Joule heating [43].

$$\frac{\partial [(\rho c_p)_m T]}{\partial t} + \nabla (\rho c_p \vec{U} T) = \nabla (k^{eff} \nabla T) + S_T$$

$$S_T = \begin{cases} 0 & \text{in GDL} \\ j \left(\eta + T \frac{dU_0}{dT} \right) + \frac{i_e^2}{\kappa^{eff}} & \text{in catalyst layers} \\ \frac{i_e^2}{\kappa^{eff}} & \text{in membrane} \end{cases}$$

where c_p is the specific heat capacity, k^{eff} is the thermal conductivity.

2.4.2 Water Transport

Water management is one of the most important issues in PEM fuel cell. It requires to balance between a well hydrated membrane and the avoidance of flooding, which are two conflicting phenomena.

Early modeling studies [7, 9, 5, 6, 11, 34, 36, 44, 45] used the fully humidified fuel / air streams, to ensure a fully hydrated membrane, and thus providing a constant proton conductivity. But under fully humidified conditions, the gas inside the fuel cell will become over-saturated and condensation of water at the cathode side may happen even at low operating current densities. This flooding of cathode causes the blockage of oxygen, preventing it to flow into the catalyst layer, which results in significant concentration polarization. Furthermore, humidifying the gas and air externally requires additional parasitic volume and power. Therefore, recent trend is to operate the PEM fuel cell at low humidity conditions, while maintaining the membrane at adequate hydration. This strategy reduces the flooding at cathode but it depends on the understanding of water

generation, transport and distribution in the fuel cell.

Water is produced in the cathode catalyst layer from the ORR or can be brought in from external humidification. Through the membrane, the water can transport through electro-osmotic drag effect and the back diffusion which is driven by concentration gradient. The water flux from the electro-osmotic drag effect is directly proportional to the protonic flux ($\frac{I_{cell}}{F}$). The water's diffusion flux in the membrane depends on the water diffusion coefficient and the gradient in molar concentration of water.

Efforts haven been made to simulate water management in PEM fuel cell. According to Wang [27], these studies can be categorized into three groups. The first group, generally focused on the physics of water transport, specially water transport through the membrane [7, 5, 6, 46–49]. They tried to determine the membrane water content at the interface by the activity of water vapor, assuming equilibrium between the gas phase and membrane phase of water in the membrane. Although this group of models gives a deeper understanding of the water distribution through the membrane, it still fail to obtain some of the detail features of water transport at low humidity.

The second group, used CFD approach to model the water transport throughout the whole fuel cell [41, 15]. These models do not properly model water transport through the membrane. This group of models is unable to describe water transport phenomena through the membrane.

The third group [34, 36–38], united different modes of water transport in various parts of the PEM fuel cell and develop a comprehensive water transport, that describe water transport through membrane by diffusion and electro-osmotic drag, and easy to implement using the CFD approach. It is able to simulate water management under low humidity conditions.

A unified water transport model, is developed by Wang et al. [34, 35, 38]. It can be applied throughout the PEM fuel cell, and thus, a comprehensive CFD simulation can be carried out. The model recognizes the different phases of water in the PEM fuel cell, i.e., water in gas phase and in membrane. Hence, the unified water transport model considered phase equilibrium and incorporated diffusion, convection and electro-osmotic

drag of the water molecule. The development of the unified water transport equation in a single domain CFD framework, is with the aid of the equilibrium uptake curve in the membrane phase.

2.4.3 Heat Transport

PEM fuel cell produces heat waste as much as its electric power output (energy conversion efficiency about 50%). The heat generation arises from entropic heat of reactions(55%), the irreversibility of the electrochemical reactions (35%) and ohmic resistance or Joule heating (10%) [43]. Hydration of membranes strongly depends on the temperature because water vapor saturation pressure is an exponential function of temperature. Therefore, thermal management is as important as water management, with these two factors combine to achieve good performance of the PEM fuel cell.

Nguyen and White [6] incorporated a one-dimensional heat transfer along the flow direction in a two-dimensional PEM fuel cell model. It considered the phase change of water in the flow channel as the only heat source, allowing convective heat transfer between gas and solid phase. Fuller and Newman [5] incorporated a one-dimensional heat transfer in the flow direction, one-dimensional mass transfer in the through-membrane direction, into a pseudo two-dimensional PEM fuel cell model. It is able to calculate the temperature rise of the gas streams, with other external heat transfer coefficients. These models do not differentiate the temperatures of the membrane and the electrodes, even though the temperature variation is significant at those regions, in the through membrane and flow directions. Besides, the entropic and irreversible reaction heat sources were not included. Yi and Nguyen [12] further developed Nguyen and White's [6] model, and included the entropic and irreversible reaction heat along the phase change heat. But it only allowed temperature variation of the solid phase in the flow direction, and assuming uniform temperature in the through-membrane direction.

Wöhr et al. [50] incorporated the heat and mass transfer in the through-plane direction into a one-dimensional model, especially for PEM fuel cell stacks, and the model accounted the entropic and irreversible reaction heats. It is able to provide the tem-

perature profile in the through-plane direction and predict the maximum temperature for a given number of cells in the stack. Rowe and Li [51] developed a one-dimensional model in the through-membrane direction, similar as the previous model. Apart from taking into account of the entropic, irreversible and phase change heats, it also included the Joule heating in the membrane and catalyst layers. This model able to predict the temperature variation in the through-membrane direction for a given current density and electrode thermal conductivity. One of the shortcomings of this model is, it assume the cathode catalyst layer to be fully hydrated and the water content in the membrane is linearly interpolated, which implies that it is unable to simulate low humidity condition. For multidimensional thermal models, Maggio et al. [52] developed a pseudo three-dimensional model neglecting the temperature gradient in the flow direction. They consider the overall heat source term as $(U_o - V_{cell}) I$. Shimpalee and Dutta [53] and Costamagna [54] developed three dimensional models, which treated the heat source terms globally, and not location specific. Berning et al. [41] developed a three-dimensional model, which included the irreversible and entropic heat terms in the catalyst layers, Joule heating in the membrane. But due to its fully humidified membrane assumption, it can't simulate low humidity condition.

In order to accurately model the temperature distribution for a PEM fuel cell, the accurate heat source, thermal properties of the material of the components and thermal boundary conditions are needed. In addition, the experimental temperature distribution is needed for validation purposes. The main heat removal mechanism of the catalyst layer is through lateral heat conduction along the in-plane direction to the current collector plate. Heat removed by gas convection, through the channels, is about 5% under normal operating conditions. Solving the energy equation provides the temperature distribution of the fuel cell, and the temperature effects on the performance of the PEM fuel cell. An example of the temperature distribution is shown in Figure 2.4.

Figure 2.4: Temperature distribution at the cathode side catalyst layer for two different GDL thicknesses: (a) 0.2 mm and (b) 0.3 mm. [55]

2.4.4 Electron Transport

GDL provides lateral conduction to electron, serve as a bridge in between the catalyst layer and the current collector plate. Most PEM fuel cell models published, ignored the electron transport in the catalyst layer, GDL and current collecting plate, with the assumption that the electric conductivity is large enough and the electronic phase potential is uniform in these materials. The graphite plate has an electric conductivity of $2 \times 10^4 \text{S/m}$, but the effective electric conductivity of the catalyst layers and GDL are only $300 - 500 \text{S/m}$. The current distribution could be significantly changed due to this electronic resistance. Solving the electron transport equation provides

- the contact resistance at interfaces between two mating components
- the implementation of the total current as a boundary condition instead of cell voltage
- the modeling of stack fuel cell in series

Solving equation 2.7, the electron-transport through the GDL can flow plate can be calculated. The equation accounts for ohmic loss at the flow plates with limited conductivity and small thickness when applied to it.

A three dimensional study of the effects of electron transport through GDL was conducted by Meng and Wang [42]. Figure 2.5 shows a current distribution on the middle of the membrane.

Figure 2.5: Ionic current distributions (A/m²) in the middle of membrane under different electronic conductivities in GDL ~at 0.65 V. [42]

Without accounting for the lateral electron transport, the current density is the highest in the middle of the channel, due to easiest access to the oxygen. This is shown on the right hand side of Figure 2.5, where $\sigma_s^{\text{eff}} = \infty$, correspond to 0 electronic resistant of GDL in the in plane direction. Once this electronic resistant is considered, the maximum current density is now located under the edges between the gas channel and the current collecting rib. This is due to the best combination of easy access of oxygen and a short path for electron transport onto the rib. This is shown clearly in the left hand side of Figure 2.5. From these finding, it can be concluded that the lateral electron transport in GDL is essential in determining the current distribution locally between flow channel and current collecting rib, and need to be included in future models.

2.4.5 Transient Phenomena

For automotive application, dynamic characteristic of a fuel cell engine is essential. There are three processes that govern the time response of a PEM fuel cell,

- electrochemical double layer discharging
- gas transport through flow channel and GDL
- membrane hydration and dehydration

For the double layer discharging process, the time constant is about micro and milliseconds, which is short enough to be ignored. For the gas transport flow, the time constant can be estimated using its diffusion time, i.e., $\frac{\delta_{GDL}^2}{D_g}$. Among the three, the slowest is the membrane hydration process, which the time constant can be estimated by

$$\frac{\left(\frac{\rho\delta_m\Delta\lambda}{EW}\right)}{\left(\frac{I}{2F}\right)}$$

It is assumed that the dry membrane is hydrated by the water produced at the current density, I . For the case of Nafion 112 at $1\text{A}/\text{cm}^2$, the time constant is about 25s. Therefore for low humidity condition, the water accumulation term is important for transient analysis.

Um et al. [34] studied the transient response of a PEM fuel cell to a voltage step change. The model assumed the gas feed on both side are fully humidified, which results to the membrane hydration no longer a contribution to the cell transients, therefore, the gas transport transient is included under the fully humidified conditions. Wang and Wang [56] further extended Um et al.'s work [34], by including membrane hydration transient process for low humidity conditions.

Figure 2.6: Dynamic responses of average current density to the step change of cell voltages from 0.6 to 0.7V, under $RHa/c = 100/100\%$ and $100/0\%$. [56]

Figure 2.6 shows a time response of a current density to a step change in cell potential. It can be observed that the current density does not follow the smooth variation as the steady states of 0.6V to 0.7V. There are undershooting and overshooting due to the transient phenomena of gas transport and membrane hydration. For the dry air feed case, the current density drop instantaneously once the cell potential is increase from 0.6V to 0.7V, due to the negligibly small time constant of the electrochemical double layer effect. The undershoot in the current density is due to the oxygen concentration at the cathode catalyst layer is still low after the large consumption rate at 0.6V. As the oxygen concentration recovers, the current density increases. The time for the current to rise correspond with the characteristic time of gas phase transport. The overshoot appears due to the membrane still maintains a higher water content which corresponds to 0.6V. It then takes approximately 15s for the membrane to adjust its water content to the one which corresponds to the steady state 0.7V's water content. This shows that the membrane hydration and dehydration plays an essential role in the transient dynamics of PEM fuel cell.

2.4.6 Liquid Water Transport

At high current density, PEM fuel cell's performance is limited by the transport of reactants and products. Furthermore, liquid water is generated and condenses, filling the pores of the GDL and electrodes, blocking the reactant from flowing to the catalyst site. This is known as 'flooding', and is an important limiting factor of the PEM fuel cell's performance. Flooding is usually linked with high current density operation, which has higher water production rate. Flooding can also occur at low current densities conditions, e.g. at low temperatures and low gas flow rates, which is caused by faster saturation of gas phase by water vapor. In automotive fuel cells, cell start up is usually performed at conditions lower than desired operating temperature, known as 'cold start'. The saturation pressure of water at this temperature is very low, results in saturation of gas phase with water vapor, and hence flooding may occur at low current densities, which affects the start-up and transient dynamics of the cell. Therefore, the study and understanding of the two-phase transport in the PEM fuel cell is important in order to increase the performance of the cell.

There are several studies investigating the two-phase transport in the PEM fuel cell [7, 8, 57, 58, 14, 59], but most didn't consider the effect of GDL hydrophobicity. Some studied to predict the cell's performance at a given flooding level without analyzing the transport of liquid water. He et al. [57] presented a two dimensional two-phase model, using the interdigitated flow field, and included the capillary transport of liquid water in a hydrophilic GDL. Wang et al. [13] developed a two-phase PEM fuel cell which also utilize a hydrophilic GDL, based on Wang et al.'s [60] multiphase mixture model formulation (M^2). You et al. [14] investigated the effects of several operating parameters on two-phase transport. Mazumder and Cole [15] presented a model also based on Wang et al.'s [60] M^2 formulation, but it is only valid in the two-phase regime where liquid water exist. Berning and Djilali [16] published a two-phase model, which ignored the water transport through MEA.

Nam and Kaviani [17] developed a one-dimensional model which includes the liquid water transport through hydrophobic GDL. In this study, it was assumed that the gas-phase

pressure is uniform, which results in the liquid phase transport depending on the gradient in capillary pressure. This study was used to investigate the effects of GDL fiber diameter, porosity and capillary pressure on liquid water distribution. Pasaogullari and Wang [18] in their work proposed a theory for liquid water transport through hydrophobic GDL. The condensation of liquid water forms a tree-like percolation network in the GDL. As the liquid water reaches the interface between the GDL and the flow channel, it forms liquid droplets. The liquid water is being driven by capillary action in the GDL. For the case of hydrophobic GDL, the capillary pressure is negative, which results in the liquid pressure higher than gas phase pressure, while the gas phase pressure is higher than the liquid phase pressure for the case of hydrophilic GDL. The liquid pressure gradient is formed from higher to lower liquid saturation regions due to the pressure increases with the liquid saturation. Therefore, the liquid water flow is mainly driven by the pressure gradient. For PEM fuel cell, the catalyst layer's liquid saturation is higher than the interface between GDL and flow channel, because of the water generation and electro osmotic drag at the catalyst layer.

Both Nam and Kaviani [17] and Pasaogullari and Wang's [18] theories of transport of liquid water through hydrophobic GDL, require the liquid saturation's boundary value at the interface between the GDL and flow channel. This inter-facial saturation should not be the immobile saturation, but depends on the liquid droplets' break-off diameter and population density, both which are functions of contact angle at the GDL surface and the gas velocity in the flow channel.

In order to properly simulate the liquid water transport in PEM fuel cell, and investigate the effect of flooding on the cell performance, according to Wang [27], these four sub-models must be considered.

- A model where in the catalyst layer, the catalytic surface is covered by liquid water.
- A model of the transport of liquid water through the hydrophobic MPL and GDL.
- A model of GDL surface's inter-facial droplet.
- A model of two-phase flow in the gas channel.

Pasaogullari and Wang [61] developed a three dimensional, isothermal model, which integrated the theory of transport of liquid water in the hydrophobic GDL. A comparison is made between a single-phase and two-phase model, by comparing the current density along the flow channel of a two channel serpentine fuel cell.

Figure 2.7: Comparison of local current density distributions in a two-channel serpentine PEFC at $V_{cell} = 0.4V$. [27]

From Figure 2.7, the current density near the inlet is higher for the single-phase model compare to the two-phase model. Liquid water that caused the flooding limits oxygen from traveling into the catalyst layer, which results in lower performance. The flooding also limit the performance as it goes downstream, which results in a more uniform performance as predicted in the two-phase model compare to the single-phase model. At the downstream, there is more oxygen available, therefore, the current density is higher compare to the single-phase model. At the U-turn of the flow channel, it can be observed that there is a higher performance in current density. This is caused by the mixing effect and secondary flow around the U-turn, which enhance the oxygen convective transport into the catalyst layer.

Figure 2.8: Local current density profiles along the channel direction for different humidification levels at $V_{cell} = 0.65V$. Anode and cathode stoichiometries are 1.4 at $1.0A/cm^2$. [27]

A two dimensional model is made to investigate the influence of some operating parameters to the PEM fuel cell performance, namely, humidity of both anode and cathode [61]. In Figure 2.8, it shows the current densities of the fuel cell with respect to the distance from the cathode inlet. For the fully humidified case, the current density decreases along the flow channel from the inlet, which is caused by the depletion of oxygen and flooding. For the relative humidity of 70% anode and 20% cathode case, the membrane is dry and cause the ionic resistance limitation behavior. The current density increases along the flow channel from the inlet, due to the increase of water content in the membrane from the ORR. For the fully humidified anode and 20% relative humidity cathode case, and fully humidified anode and 40% relative humidity cathode case, it can be observed that three different regime existed,

1. the dry membrane that caused the ionic resistant limitation behavior
2. the middle section where the membrane fully humidified, and the performance is the highest

3. the limited mass transfer of oxygen due to flooding or oxygen depletion

In the last two cases, the membrane near the anode inlet is dry, because of the electro osmotic effect drag of water molecule from anode to cathode. In addition, the cathode side near the inlet has low concentration of water content, which fails to compensate the water content at the anode side through the back diffusion of water molecule from cathode to anode, and therefore leads to the membrane at the anode side near the inlet dry out.

Figure 2.9: Liquid saturation profiles at cathode GDL catalyst layer interface along the channel direction for different humidification levels at $V_{cell} = 0.65V$. Anode and cathode stoichiometries are 1.4 at $1.0A/cm^2$. [27]

Figure 2.9 shows the liquid saturation along the flow direction at different relative humidity of cathode feed. For the fully humidified cathode case, at the inlet, the maximum liquid saturation level is about 0.1, decreases along the flow direction because of the cathode catalyst layer's decreasing reaction rate. For the low cathode humidity cases, liquid water is not produced immediately. It is when the the water vapor concentration reaches the saturation value, that the condensation starts, and being driven downstream, where its location is related to the relative humidity of cathode.

Figure 2.10: Local current density profiles along the channel direction of single-channel PEFC for different inlet stoichiometric ratios at $V_{cell} = 0.65V$ at the inlet relative humidity: 20% cathode and 100% anode at 80°C. [27]

Figure 4.15 shows the current densities along the flow direction for different stoichiometry. As the distance along the flow direction increases, the current density increases due to the hydration of the membrane. After the GDL gets saturated with water vapor, liquid water starts to condense, and flooding occur, this explains the current density peak, then drop after the flooding started. Membrane is hydrated faster at lower flow rates, which results in the performance peak earlier for the lower stoichiometric case.

As the phase change for the two-phase transport, the latent heat involved plays a big part in the temperature distribution of the fuel cell, and therefore must be included in the non-isothermal, two-phase flow model. The resulting temperature non-uniformity will affect the saturation pressure, condensation and evaporation rate and hence the liquid water distribution.

All the models that describe the liquid water transport through GDL can be categorize into

- M^2 model

- unsaturated flow theory (UFT)

The gas phase pressure is assumed constant for UFT, which makes decoupling the liquid water transport and gas flow effective. Nguyen et al. [57, 58], Berning and Djilali [16], Nam and Kavinay [17] and Pasaogullari and Wang's [61] models belong to this category. On the other hand, M^2 model accounted the liquid and gas phases. Wang et al. [13], You and Liu [14], Mazumder and Cole's [15] model belong in this category.

2.5 Sensitivity Analysis

Several researches start to appreciate the importance of the sensitive analysis on the fuel cell. There were several papers published regarding this issue. Stockie et al. [62] conducted sensitivity study and concluded that some geometrical and operational parameters are essential to fuel cell performance. Grujicic et al. [63] conducted a sensitivity analysis using ANOVA method on the thickness of the active layer, empirical value, molar diffusion volume of oxygen, molar diffusion volume of water, molar diffusion volume of nitrogen and porosity of cathode to determine their effects on the PEM fuel cell performance. They concluded that these parameters have a major effect on the performance, but their optimally designed that fuel cell is not affected by the variation of those parameters value. Correa et al. [64] and Srinivasulu et al. [65] both conducted sensitivity analysis on a PEM fuel cell stack. Using multi-parametric sensitivity analysis (MPSA), the parameters were classified into insensitive, sensitive and very sensitive. Tao et al. [66] and Min et al. [67] conducted a parametric sensitivity analysis on a PEM fuel cell, to determine the influence of eleven parameters on the performance of the fuel cell. The parameters were classified into insensitive, sensitive and highly sensitive. Kulkarni and Wang [68] conducted a sensitivity analysis on a PEM fuel cell using ANOVA on seven important GDL properties. They concluded that the porosity has the most influence on the fuel cell performance, followed by through-plane permeability. Thermal and electrical conductivities do not have any significant influence on the performance.

Chapter 3

Two Dimensional Model

3.1 Modeling Domain

The model that is presented in this study is a two dimensional and along the channel model. It consists of seven regions,

- Anode flow channel
- Anode GDL
- Anode catalyst layer
- Membrane
- Cathode catalyst layer
- Cathode GDL
- Cathode flow channel

The model and all seven regions are illustrated in Figure 3.1.

3.2 Assumptions of The Model

Due to the complex nature of the fuel cell, which involves microscale and macroscale geometric features, some simplifying assumptions are needed to reduce the complicated

Figure 3.1: The 2D model used in this study.

fuel cell system to a numerically tractable two-dimensional model. The assumptions below are used in this model.

- The fuel cell operates under steady state condition.
- The single-phase water transport is used in the flow channels, GDLs and catalyst layers, where water in vapor phase is the only product.
- The ideal gas law is assumed for all gases.
- The gases are assumed to be fully humidified.
- The gas is assumed to be well mixed, sharing the same feature, e.g. velocity, pressure.
- The channels' flow is assumed to be laminar flow.
- The membrane is assumed to be fully hydrated, therefore the ionic conductivity is constant.
- The membrane is assumed to be impermeable, therefore no crossover is permitted.
- The bipolar plate's potential drop is assumed negligible, due to the high conductivity of graphite.
- The GDL and catalyst layer are assumed to be homogeneous and isotropic.
- The density of the gases in both anode and cathode channels is assumed to have constant density.
- The model is operating at constant temperature (isothermal).

3.3 Modeling Equations

Gas Channel

In the gas channel, the gas flow field is obtained by the Navier-Stokes equations.

- Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.1)$$

where ρ is the density of the gas mixture, $\mathbf{u}$ is the velocity vector of the gas mixture.

- Momentum equation

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \mu \nabla^2 \mathbf{u} \quad (3.2)$$

where P is the pressure, μ is the viscosity of the gas mixture.

The mass balance can be described with the divergence of mass flux, through diffusion and convection. This model takes into account H_2 and H_2O species in the anode, while O_2 , H_2O and N_2 species in the cathode. Maxwell-Stefan multi-component diffusion is used to describe the diffusion phenomena. The mass transport equation for species p can be written as,

$$\nabla \cdot \left(-\rho \omega_p \sum_q D_{pq} \left\{ \nabla x_q + \left[(x_q - \omega_q) \frac{\nabla P}{P} \right] \right\} \right) + \nabla \cdot (\rho \mathbf{u} \omega_p) = 0 \quad (3.3)$$

where ω_p , ω_q are the mass fractions for species p and q , D_{pq} is the binary diffusion coefficient for two species, p and q , x_q is the molar fraction for species q . Subscript p denotes O_2 at the cathode side, H_2 at the anode side, q is H_2O in both sides.

The binary diffusion coefficient, D_{pq} can be calculated using the following equation based on kinetic theory of gases [69].

$$P \cdot D_{pq} = a \left(\frac{T}{\sqrt{T_{cp} T_{cq}}} \right)^b (P_{cp} P_{cq})^{\frac{1}{3}} (T_{cp} T_{cq})^{\frac{5}{12}} \left(\frac{1}{M_p} + \frac{1}{M_q} \right)^{\frac{1}{2}} \quad (3.4)$$

where T is temperature, M_p , M_q are the molecular weights of species p and q , and T_{cp} , T_{cq} , P_{cp} , P_{cq} are critical temperatures and pressures of species p and q . Table 3.1 summarizes M , T_c and P_c values for the gases used in the simulation. For the remaining parameters in Equation 3.4, $a = 2.745 \times 10^{-4}$ and $b = 1.823$ for species H_2 , O_2 and N_2 and $a = 3.640 \times 10^{-4}$ and $b = 2.334$ for species H_2O .

Table 3.1: Critical properties of gases.

Species	Molecular Weight	T_c (K)	P_c (atm)
H_2	2.016	33.3	12.80
N_2	28.013	126.2	33.5
O_2	31.999	154.4	49.7
H_2O	18.015	647.3	217.5

Gas Diffusion Layer (GDL)

For GDL, transport of gas mixture needed to be modeled as a transport in the porous media.

- Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.5)$$

- Momentum equation

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \mu \nabla^2 \mathbf{u} - \frac{\epsilon_g \mu}{\kappa_g} \mathbf{u} \quad (3.6)$$

where ϵ_g and κ_g are the porosity and hydraulic permeability of the GDL.

The mass transport is similar to the one in the flow channel, except the diffusion coefficient need to be corrected for porous media. Therefore, mass transport equation is

$$\nabla \cdot \left(-\rho \omega_p \sum_q D_{pq} \left\{ \nabla x_q + \left[(x_q - \omega_q) \frac{\nabla P}{P} \right] \right\} \right) + \nabla \cdot (\rho \mathbf{u} \omega_p) = 0 \quad (3.7)$$

The diffusion coefficient D_{pq}^{eff} needs to be corrected for porous media, using the Bruggemann correction [70],

$$D_{pq}^{eff} = D_{pq} \times \epsilon_g^{1.5} \quad (3.8)$$

Catalyst Layer

The catalyst layer is also modeled as a porous media, therefore it is similar to the GDL with different porosity, ϵ , and hydraulic permeability, K .

- Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.9)$$

- Momentum equation

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \mu \nabla^2 \mathbf{u} - \frac{\epsilon_{cl} \mu}{\kappa_{cl}} \mathbf{u} \quad (3.10)$$

where ϵ_{cl} and κ_{cl} are the porosity and hydraulic permeability of the catalyst layer.

The mass transport equation in porous media is as follows

$$\nabla \cdot \left(-\rho \omega_p \sum_q D_{pq}^{eff} \left\{ \nabla x_q + \left[(x_q - \omega_q) \frac{\nabla P}{P} \right] \right\} \right) + \nabla \cdot (\rho \mathbf{u} \omega_p) = \begin{cases} -\frac{j_a}{2F} & \text{in anode} \\ -\frac{j_c}{4F} + \frac{j_c}{2F} & \text{in cathode} \end{cases} \quad (3.11)$$

where j_a, j_c are the local current densities of anode and cathode, which are obtained from Equations 3.14 and 3.15 and F is the Faraday constant. The diffusion coefficient, D_{pq}^{eff} needed to be corrected for porous media, similar to Equation 3.8

$$D_{pq}^{eff} = D_{pq} \times \epsilon_{cl}^{1.5} \quad (3.12)$$

The charge balance equation is used to define the potential distribution

$$\nabla \cdot (-\sigma_{cl} \nabla \phi_{cl}) = j \quad (3.13)$$

where σ_{cl}, ϕ_{cl} are the electronic conductivity and electric potential for the catalyst layer, j is the local current density, depending whether its in anode, j_a , or in cathode, j_c .

$$j_a = a i_{0,a}^{ref} \left(\frac{C_{H_2}}{C_{H_2,ref}} \right)^{\frac{1}{2}} \left[\exp \left(\frac{\alpha_a}{RT} F \eta_{act,a} \right) - \exp \left(-\frac{\alpha_c}{RT} F \eta_{act,a} \right) \right] \quad \text{in anode} \quad (3.14)$$

$$j_c = -a i_{0,c}^{ref} \left(\frac{C_{O_2}}{C_{O_2,ref}} \right) \left[\exp \left(\frac{\alpha_a}{RT} F \eta_{act,c} \right) - \exp \left(-\frac{\alpha_c}{RT} F \eta_{act,c} \right) \right] \quad \text{in cathode} \quad (3.15)$$

where a is the active specific surface area, i_0^{ref} is the reference exchange current densities, C_{H_2} is the local H_2 concentration, C_{O_2} is the local O_2 concentration, $C_{H_2,ref}$ is the reference H_2 concentration, $C_{O_2,ref}$ is the reference O_2 concentration, α_a is the charge transfer coefficient (anode side), α_c is the charge transfer coefficient (cathode side), R is the universal gas constant, T is the gas temperature, η_{act} is the activation overvoltage. The activation overvoltage is the voltage loss while driving the electron transfer reaction.

Membrane

The charge balance equation is

$$\nabla \cdot (-\sigma_m \nabla \phi_m) = j \quad (3.16)$$

where σ_m , ϕ_m are the electronic conductivity and electric potential for the membrane and j is the local current density, depending whether its in anode, j_a (Equation 3.14), or in cathode, j_c (Equation 3.15).

Equations Coupling

Figure 3.2 shows the coupling between the equations for this model. For a given voltage, initially, the mass and momentum equations are solved using the initial values of velocity field, pressure and mass fraction of all the species. S_u is the general source term for the momentum equation. For the GDL, the source term is $-\frac{\epsilon_g \mu}{\kappa_g} \mathbf{u}$. While for the catalyst layer, the source term is $-\frac{\epsilon_{cl} \mu}{\kappa_{cl}} \mathbf{u}$. The gas channel's source term is 0. Solving these equations will give the velocity field, $\mathbf{u}$ and pressure, P . Then the species transport equations are solved using updated value of velocity field and pressure and initial values of mass fraction of all species and local current density. S_ω is the general source term for the species transport equation. At the catalyst layer, $-\frac{j_a}{2F}$ is the source term at the anode, while $-\frac{j_c}{4F} + \frac{j_c}{2F}$ is the source term at the cathode. For the gas channel and GDL, the source terms are 0. Solving these equations will give the mass fraction of all the species, ω_i . Lastly, the charge equation is solved with the updated mass fractions to

Figure 3.2: Equation coupling for PEM fuel cell in this study.

get the local current density, j . These steps are repeated till the values are converge. After the convergence criterion is fulfilled, the final current density can be calculated by integrating the current density of the anode catalyst layer.

3.4 Boundary Conditions

For the momentum transport of both anode and cathode, the gas mixture's velocities are set at the inlets, and pressure is set at the outlets of the flow channel. The pressure set at the outlets also applies to the whole cell, which is constant. The no slip boundary condition is applied to both sides of the walls of the channels. For the mass transport and diffusion phenomena, the mass fractions of the gas mixtures are set at the inlets. For the current density, the driving force is the electric potential difference between the anode and cathode catalyst layers. The anode voltage is set to be zero, while the cathode voltage is set at the cell operating voltage. The polarization curve is produced by setting some cell voltage, solving the model, and then integrate the local current density of the catalyst layer. Usually, the cell voltage is set at open cell voltage (OCV), then reduce 0.05V continuously, till 0.3V. At each reduction, the current density is calculated.

3.5 Modeling Parameters

The following parameters were used as the base case for the model.

Table 3.2: Fuel cell dimensions for base case

Parameter	Symbol	Value	Unit
Channel length	L	0.02	m
Channel width	W	1×10^{-3}	m
GDL thickness	δ_{GDL}	3×10^{-4}	m
Catalyst layer thickness	δ_{CL}	1.29×10^{-5}	m
Membrane thickness	δ_{mem}	1.08×10^{-4}	m

Table 3.3: Operating conditions for base case

Parameter	Symbol	Value	Unit
Anode pressure	P_a	3	atm
Cathode pressure	P_c	3	atm
Anode gas velocity	v_a	0.05	ms^{-1}
Cathode gas velocity	v_c	0.15	ms^{-1}
Anode inlet temperature	T_a	353.15	K
Cathode inlet temperature	T_c	353.15	K

Table 3.4: Electrode and membrane properties at base case conditions

Parameter	Symbol	Value	Unit
GDL porosity	ϵ_g	0.4	-
Catalyst layer porosity	ϵ_{cl}	0.3	-
GDL permeability	κ_g	1.76×10^{-11}	m ²
Catalyst layer permeability	κ_{cl}	3.52×10^{-12}	m ²
Catalyst layer electronic conductivity	σ_{cl}	180	S/m
Membrane electronic conductivity	σ_m	19	S/m
Anode reference exchange current density	$i_{o,a}^{ref}$	1×10^5	A/m ²
Cathode reference exchange current density	$i_{o,c}^{ref}$	1	A/m ²
Anodic charge transfer coefficient at anode	α_a^a	0.5	—
Cathodic charge transfer coefficient at anode	α_c^a	0.5	—
Anode charge transfer coefficient at cathode	α_a^c	3	—
Cathode charge transfer coefficient at cathode	α_c^c	1.5	—
Reference H_2 concentration	$C_{H_2,ref}$	3.39	mol/m ³
Reference O_2 concentration	$C_{O_2,ref}$	546.5	mol/m ³
Active specific surface area	a	1×10^4	m ² /m ³

Chapter 4

Parametric Studies: Result and Discussion

4.1 Parametric Studies

For the first stage of the study, in order to confirm the credibility of the model, a validation is conducted with an experiment result which was conducted in Wang et al.'s study [71]. For the second stage, parametric studies were being conducted using this model. Parameters are categorized into

- Operating parameters
- Design parameters
- Physical parameters

4.1.1 Operating Parameters

Operating parameters are parameters which the values can be change during the fuel cell operation to achieve the desired output. The concentration of oxygen, pressures of channels, air and hydrogen inlet velocities, stoichiometries for both inlet gases, temperature of the gases, humidity of air, etc. are under operating parameters. In this study, the effect of

the fuel cell temperature, concentration of hydrogen, concentration of oxygen, pressures of the channels, stoichiometry ratios for both channels on the fuel cell's performance are investigated.

Temperature

For the investigation of the effect of temperature on the fuel cell's performance, different temperatures of the fuel cell and the humidification temperature of both flow channel's inlet gas were set at 50°C, 60°C, 70°C and 80°C, while the other parameters were fixed as the same as the base case condition. The polarization curves and the power density curves of the respecting oxygen concentration were compared.

Concentration of Hydrogen

For the investigation of the concentration of hydrogen on the fuel cell's performance, different concentration of hydrogen on the anode flow channel inlet were set at 10%, 30%, 50%, 70% and 90%, while the other parameters were fixed as the same as the base case condition. The polarization curves and the power density curves of the respecting oxygen concentration were compared.

Concentration of Oxygen

For the investigation of the concentration of oxygen on the fuel cell's performance, different concentration of oxygen in the air supplied into the cathode flow channel inlet were set at 5%, 10%, 15%, 20%, 25% and 30%, while the other parameters were fixed as the same as the base case condition. The polarization curves and the power density curves of the respecting oxygen concentration were compared.

Operating Pressure

The effect of the operating pressure on the fuel cell's performance is investigated by setting the back pressure of both flow channel at 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar, 3.5bar

and 4.0bar, with the other parameters fixed as the same as the base case condition. The polarization curves and power density curves of the respecting pressures were compared. Then to investigate further the effect of individual flow channel's operating pressure, the cathode flow channel's back pressure were set at 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar, 3.5bar and 4.0bar, fixing the anode flow channel's back pressure at 1.0bar. This is followed by setting anode flow channel's back pressure at 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar, 3.5bar and 4.0bar while fixing the cathode flow channel's back pressure at 1.0bar. The polarization curves and power density curves of the respecting pressures were compared, and the effect between the cathode flow channel pressure and the anode flow channel pressure is compared.

Stoichiometric Flow Ratio of Air

Lastly, the effect of the stoichiometric flow ratio of the gases supplied on the fuel cell's performance is investigated. The stoichiometry ratios of both flow channels are set at 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0, with the other parameters fixed as the same as the base case condition, and the polarization curves and power density curves are compared. Further investigation was done to determine the effect of individual flow channel's supplied gas stoichiometry ratio. First, the cathode flow channel's stoichiometry is fixed at 1.0, while the anode flow channel's stoichiometry is set at 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0. Then the anode flow channel's stoichiometry is fixed at 1.0, while the cathode channel's flow stoichiometry is set at 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0. The polarization curves and power density curves are compared.

4.1.2 Design Parameters

Design parameters are parameters used during the design phase before the fabrication of the fuel cell. It is also known as geometrical parameters. These include the channel height, the GDL thickness, the catalyst layer thickness and membrane thickness. In this study, all the four parameters mentioned above were investigated.

Channel Height

The investigation of the effect of the channel height on the performance of the fuel cell is done so by setting the heights at 0.4mm, 0.6mm, 0.8mm, 1.0mm, 1.2mm, 1.4mm and 1.6mm, with other parameters fixed as the same as base case. The polarization curves and the power density curves of the different heights were then compared.

GDL Thickness

The study of the effect of GDL thickness on the performance of the fuel cell is done by setting the thickness at 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm, with the other parameters fixed as the same as the base case. The polarization curves and the power density curves were then compared. Further investigation is done to study the effect of the individual side GDL thickness. This was done by fixing the cathode GDL at 0.3mm and setting the anode GDL at 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm. Then, the anode GDL is fixed at 0.3mm and the cathode GDL is set at 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm. The polarization curves and the power density curves were compared.

Membrane Thickness

Then the effect of the membrane thickness on the fuel cell's performance is studied, by setting the thickness at 10 μ m, 50 μ m, 108 μ m, 150 μ m, 200 μ m, 250 μ m and 300 μ m, with the other parameters fixed as the same as the base case. The polarization curves and the power density curves were compared.

4.1.3 Physical Parameters

Physical parameters includes porosities of both GDL and catalyst layer and permeabilities of both GDL and catalyst layer. The effect of the GDL porosity on the fuel cell's performance is investigated for this study. It was done by using different porosity for the

GDL, with the other parameters fixed as the same as the base case condition and the polarization curves and the power density curves are compared. The porosities of the GDLs are set as 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6. Then the cathode GDL porosity is fixed at 0.4, while the anode porosity is changed among 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6. This is followed by fixing anode porosity at 0.4, and change cathode porosity among 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6. The polarization curves and the power density curves were compared to investigate the effect of individual GDL porosity on the fuel cell performance.

4.2 Validation of Model

Figure 4.1: Comparison of polarization curve between simulation model and experiment.

Figure 4.1 shows the comparison of the polarization curve of the model with the experimental data obtained from Wang et al. [71]. The model shows a good agreement with

Wang et al.'s experimental data for the activation region (the first downward slope) and the ohmic region (the straight line thereafter), but not the mass transport region (the ending downward slope of the experiment data). The mass transport region is dominated by the concentration losses which is caused by poor mass transport due to reactant depletion or product clogging, especially the clogging of liquid water. Since the model assume to be single-phase transport and it is also assumed to have constant supply of reactant, the polarization curve of the model doesn't show the losses due to concentration losses. Instead, it continues to be the ohmic losses at the mass transport region, which is the straight line shown in Figure 4.1.

Figure 4.2: Velocity profile of the gases at each channel of the model.

Figure 4.2 shows the velocity profile of the model, which is consistent to the 1 : 3 ratio of the given velocity at the inlet. The velocity exhibits a parabolic profile, with the maximum velocity at the center of the channel and reduces to zero as it goes nearer to the channel wall and the GDL-channel interface.

Figure 4.3: The hydrogen gas mole fraction in the anode flow channel.

Figure 4.3 shows the mole fraction of the hydrogen gas at the anode flow channel and GDL. The hydrogen gas is being consumed for the electrochemical reaction, which results in the reduction of hydrogen gas from the inlet to the outlet.

Figure 4.4: The oxygen gas mole fraction in the cathode flow channel.

Figure 4.5: The water vapor mole fraction in the cathode flow channel.

Figure 4.4 and 4.5 shows the mole fraction of the oxygen gas at the cathode flow channel and GDL. The oxygen mole fraction reduces along the cathode flow channel, as it is consumed for electrochemical reaction. On the other hand, the water vapor mole fraction increases along the cathode channel because water is the by-product of the electrochemical reaction.

4.3 Operating Parameters

4.3.1 The Effect of Temperature on Cell Performance

The temperatures were set at 50°C, 60°C, 70°C and 80°C. This includes the cell's temperature and the humidification temperature for both inlet gases. The results are shown in Figure 4.6.

Figure 4.6: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different temperatures.

From Figure 4.6, it shows that as the temperature increases from 50°C to 80°C, the current density at 0.51V increases from 1.40A/cm² to 1.85A/cm², the maximum power density increases from 0.755W/cm² to 1.029W/cm². The performance of the fuel cell increases as the temperature increases, because as the humidification temperature increases, the concentration of water increases, and that increases the number of water molecule in the membrane which improves the ionic conductivity of the membrane. Apart from that, higher cell temperature improves the mass transport of the gases, increases the diffusivity of the gas mixture and increases the exchange current density. But since the water reaches boiling point at 100°C, the membrane will be depleted of water molecule, therefore the fuel cell can't be operated at 100°C or above.

4.3.2 The Effect of Concentration of Hydrogen on Cell Performance

The hydrogen concentrations at the anode flow channel's inlet were 10%, 30%, 50%, 70% and 90%. The results are shown in Figure 4.7.

Figure 4.7: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different concentration of H_2 .

Figure 4.7 shows that as the concentration of hydrogen increases from 10% to 90%, the current density at 0.51V increases from 1.74A/cm^2 to 1.88A/cm^2 , the maximum power density increases from 0.971W/cm^2 to 1.044W/cm^2 . When the concentration of the hydrogen increases, more hydrogen is supplied for the reaction, therefore there are more electrons produced, that results in better fuel cell performance. As the concentration of hydrogen increases, the improvement of the fuel cell becomes negligible.

4.3.3 The Effect of Concentration of Oxygen on Cell Performance

The air's oxygen concentrations at the cathode flow channel's inlet were 5%, 10%, 15%, 20%, 25% and 30%. The results are shown in Figure 4.8.

Figure 4.8: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different concentration of O_2 .

From Figure 4.8, as the concentration of oxygen increases from 5% to 30%, the current density at 0.61V increases from $0.87\text{A}/\text{cm}^2$ to $1.24\text{A}/\text{cm}^2$, the maximum power density increases from $0.545\text{W}/\text{cm}^2$ to $1.072\text{W}/\text{cm}^2$. With the sluggish ORR, the cathode reactant is the bottleneck for the whole fuel cell performance. As the concentration increases, there are more reactant for the reaction and increases the number of electron which results in better performance. It is also observed that for concentration 25% and above

the improvement of the cell's current density diminishes. This means that at a certain concentration or above, the improvement is negligible.

Figure 4.9: The mole fraction of the oxygen at the cathode flow channel and GDL for each concentration of oxygen. From left to right are 5%, 10% at 0.61V.

Figure 4.10: The mole fraction of the oxygen at the cathode flow channel and GDL for each concentration of oxygen. From left to right are 15%, 20% at 0.61V.

Figure 4.11: The mole fraction of the oxygen at the cathode flow channel and GDL for each concentration of oxygen. From left to right are 25%, 30% at 0.61V.

Figures 4.9 to 4.11 illustrate the mole fraction of oxygen on the cathode side. By taking the difference between the estimation average inlet mole fraction and the outlet one, 0.02 for 5%, 0.0344 for 10%, 0.0367 for 15%, 0.0389 for 20%, 0.0411 for 25%, 0.0433 for 30%, it can be seen that the consumption of oxygen increases as the concentration increases. This contributes to the increase in performance for the fuel cell.

4.3.4 The Effect of Operating Pressure on Cell Performance

The operating pressures used were 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar, 3.5bar and 4.0bar. The result is shown in Figure 4.12.

Figure 4.12: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different pressures.

It can be observed from Figure 4.12 that as the pressure increases from 1.0bar to 4.0bar, the current density at 0.51V increases from 1.53A/cm² to 1.94A/cm² and the maximum power density increases from 0.803W/cm² to 1.077W/cm². This can be attributed to the mass fraction of the reactants. As the pressure increases, the mass fraction of the reactants increases as well, this increases the concentration and allow more reactant for the electrochemical reaction. This gives the same effect as the effect of the concentration of hydrogen and effect of the oxygen on the fuel cell performance. Secondly, the diffusion coefficient is affected by pressure, which results in increase in diffusivity when the pressure increases. This trend is consistent with the findings of Tohidi et al. [72].

Further analysis is done to investigate the effect of the individual flow channel operating pressure. First, the cathode's pressures were set at 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar,

3.5bar and 4.0bar, while setting the anode's pressure constant at 1.0bar, to observe the effect from the cathode flow channel pressure. The results are shown in Figure 4.13.

Figure 4.13: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different cathode pressures.

Then the anode's pressure is set at 1.0bar, 1.5bar, 2.0bar, 2.5bar, 3.0bar, 3.5bar, and 4.0bar, while fixing the cathode's pressure at 1.0bar. The result is shown in Figure 4.14.

Figure 4.14: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different anode pressures.

From Figure 4.13, it can be observed that as the pressure at the cathode channel increase from 1.0bar to 4.0bar, the current density at 0.51V increase from 1.53A/cm² to 1.77A/cm², while the maximum power density increases from 0.803W/cm² to 0.996W/cm². On the other hand, from Figure 4.14 as the pressure at the anode channel increase from 1.0bar to 4.0bar, the current density at 0.51V increases from 1.53A/cm² to 1.64A/cm², while the maximum power density increases from 0.803W/cm² to 0.847W/cm². The current density increases by 16% at the cathode flow channel and 7% for the anode flow channel when the pressure is increase from 1.0bar to 4.0bar, while the maximum power density increases by 24% at the cathode flow channel and 5% at the anode flow channel. This shows that the pressure at the cathode channel is more dominant in increasing the performance of the fuel cell compare to the anode side when the pressure increases. This

is due to the sluggishness of the transport of air. With the high efficiency of transport of hydrogen gas, increasing the pressure only improves its transport minimally, while for the sluggish air, the increase of pressure improves its transportation a lot more.

4.3.5 The Effect of Stoichiometric Flow Ratio on Cell Performance

The stoichiometries for both hydrogen and air both were varied between 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0. The results are shown in Figure 4.15.

Figure 4.15: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different stoichiometric flow ratio of both hydrogen and air.

From Figure 4.15, as the stoichiometric flow ratio increases from 1.0 to 9.0, the current density at 0.62V increases from 0.98 A/cm^2 to 1.19 A/cm^2 . The limit current density

increases from $1.00\text{A}/\text{cm}^2$ for stoichiometric flow ratio of 1.0 to $3.11\text{A}/\text{cm}^2$ for stoichiometric flow ratio of 5.0. The maximum power density also increases from $0.609\text{W}/\text{cm}^2$ to $1.041\text{W}/\text{cm}^2$, where at stoichiometric flow ratio of 5.0 and above, the improvement of maximum power density is negligible. The limit current density and the current density's improvement is negligible for stoichiometric flow ratio of 5.0 and above. This shows that at lower stoichiometric flow ratio, the amount of gases in both inlets is only sufficient to achieve $1.00\text{A}/\text{cm}^2$, when the stoichiometric flow ratio increases, more gases are supplied, and therefore the cell able to achieve a higher current density and higher power density. For stoichiometric flow ratio of 6.0 and above, the reaction has reach its limit, therefore, even by increasing the stoichiometric flow ratio, the improvement of the cell performance is negligible.

With the air stoichiometric flow ratio fixed at 1.0, and the hydrogen stoichiometric flow ratio is varied among 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0. The results are shown in Figure 4.16.

Figure 4.16: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different stoichiometric flow ratio of hydrogen.

Figure 4.16 shows that as the hydrogen stoichiometric flow ratio increases from 1.0 to 9.0, the performance remains unchanged, the current density at 0.62V is 0.98 A/cm^2 and the maximum power density is 0.609 W/cm^2 .

Then the hydrogen stoichiometric flow ratio fixed at 1.0, and the air stoichiometric flow ratio is varied among 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0. The results are shown in Figure 4.17.

Figure 4.17: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different stoichiometric flow ratio of air.

Figure 4.17 shows that as the air stoichiometric flow ratio increases from 1.0 to 9.0, the current density at 0.62V increases from 0.98A/cm² to 1.18A/cm², the maximum power density increases from 0.609W/cm² to 1.031W/cm². This shows that the air stoichiometric flow ratio has a predominant effect on the performance of the fuel cell, while the hydrogen stoichiometric flow ratio does not have any effect on the performance of the fuel cell.

4.4 Design Parameters

4.4.1 The Effect of Channel Height on Cell Performance

The channel heights used were 0.4mm, 0.6mm, 0.8mm, 1.0mm, 1.2mm, 1.4mm and 1.6mm. The results are shown in Figure 4.18.

Figure 4.18: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different channel height.

It can be observed from Figure 4.18 that as the channel height increases from 0.4mm to 1.6mm, the current density at 0.51V increases from $1.78\text{A}/\text{cm}^2$ to $1.86\text{A}/\text{cm}^2$ and the maximum power density increases from $0.939\text{W}/\text{cm}^2$ to $1.036\text{W}/\text{cm}^2$. The bigger the channel, there are more gas being supplied to reaction site. For the heights above 1.0mm, the improvement of the performance of the fuel cell diminishes, no longer improve much, which suggest that even with more gas in the channel, not all can be transport to the

reaction site.

4.4.2 The Effect of GDL Thickness on Cell Performance

The GDL thicknesses used were 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm. The results are shown in Figure 4.19.

Figure 4.19: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different GDL thickness of both sides.

It can be observed that from Figure 4.19, as the thickness of the GDL increases from 0.1mm to 1.0mm, the current density at 0.51V reduces from 2.22A/cm^2 to 1.20A/cm^2 and the maximum power density reduces from 1.257W/cm^2 to 0.641W/cm^2 . As the GDL is thicker, it increases the resistance for the gases to transport from the channel to the catalyst layer. Therefore, at 1.0mm, the cell performance is the poorest among the other

thickness. Although for better performance, the thinner the GDL the better, but due to the fragility of the GDL, it will be a challenge to fabricate a fuel cell with that thin GDL. Further investigation is done to investigate the contribution of each GDL thickness on the total effect on the cell performance. For the anode side, the thicknesses were 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm, while the cathode GDL fixed at 0.3mm. The results are shown in Figure 4.20.

Figure 4.20: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different anode GDL thickness.

From Figure 4.20, the current density at 0.51V reduces from 2.00A/cm² to 1.49A/cm² as the thickness of the anode GDL increases from 0.1mm to 1.0mm, while the maximum power density reduces from 1.111W/cm² to 0.819W/cm².

For the cathode side, the thickness used were 0.1mm, 0.2mm, 0.3mm, 0.4mm, 0.5mm, 0.6mm, 0.7mm, 0.8mm, 0.9mm and 1.0mm, while the anode GDL fixed at 0.3mm. The

results are shown in Figure 4.21.

Figure 4.21: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different cathode GDL thickness.

As the thickness of the cathode GDL increases from 0.1mm to 1.0mm, the current density at 0.51V reduces from 2.04A/cm² to 1.40A/cm², which is illustrated in Figure 4.21, and the maximum power density reduces from 1.147W/cm² to 0.738W/cm².

For the anode side, the current density reduces by 25% and the maximum power density reduces by 26%, while for the cathode side, the current density reduces by 31% and the maximum power density reduces by 36%, as the GDL thickness increases from 0.1mm to 1.0mm. It can be concluded that both side's GDL thickness have almost equal contribution towards the effect of on the performances of the fuel cell, with the cathode side having considerably more effect on the cell performance than the anode side. Therefore, performance of the fuel cell can be improved by reducing the thickness of both the GDLs.

As mentioned above, due to the nature of the graphite sheet, it will be a challenge to fabricate a fuel cell using very thin layer of graphite sheet as GDL without damaging it.

4.4.3 The Effect of Membrane Thickness on Cell Performance

The membrane thicknesses used were $10\mu\text{m}$, $50\mu\text{m}$, $108\mu\text{m}$, $150\mu\text{m}$, $200\mu\text{m}$, $250\mu\text{m}$ and $300\mu\text{m}$. The results are shown in Figure 4.22.

Figure 4.22: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different membrane thickness.

It can be observed from Figure 4.22, that as the thickness of the membrane thickness increases from $10\mu\text{m}$ to $300\mu\text{m}$, the current density at 0.51V reduces from $2.80\text{A}/\text{cm}^2$ to $1.15\text{A}/\text{cm}^2$ and the maximum power density reduces from $1.515\text{W}/\text{cm}^2$ to $0.623\text{W}/\text{cm}^2$. This shows that as the membrane thickness increases, the protons need to travel longer distance. That increases the ionic resistance and membrane loss. This leads to loss in

voltage output. Although thinner membrane is recommended in order to improve the performance of the fuel cell, however, it would be a challenge to assemble the fuel cell with a thin membrane without damaging it, which might cause it to tear.

4.5 Physical Parameters

4.5.1 The Effect of GDL Porosity on Cell Performance

The GDL porosities both anode and cathode were 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6. The results are shown in Figure 4.23.

Figure 4.23: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different GDL porosity of both anode and cathode.

It can be observed from Figure 4.23, that as the porosity increases from 0.1 to 0.6,

the current density at 0.53V increases from 0.92A/cm² to 1.75A/cm², the maximum power density increases from 0.543W/cm² to 1.049W/cm². This is due to the limited transportation of oxygen towards the catalyst layer as the porosity reduces. This trend is consistent with the studies conducted by Gurau et al. [11]. For porosity 0.5 and above, the current density at 0.53V becomes constant at 1.74A/cm² and the maximum power density at 1.043W/cm². This is because of the efficiency of the transport of oxygen is at its maximum. Larger porosity no longer improves its transport.

Next, the cathode GDL porosity is fixed at 0.4, while the anode GDL porosity is varied between 0.1 to 0.6. The results are shown in Figure 4.24.

Figure 4.24: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different GDL porosity of both anode and cathode.

Figure 4.24 shows that the current density remains the same at 1.85A/cm² for 0.51V even though the porosity increases from 0.1 to 0.6, and the maximum power density too

remains at $1.029\text{W}/\text{cm}^2$.

Then, the anode GDL porosity is fixed at 0.4, while the cathode GDL porosity is varied between 0.1 to 0.6. The results are shown in Figure 4.25.

Figure 4.25: The comparison of polarization curves (solid lines) and power density curves (dash lines) for different cathode GDL porosity.

Figure 4.25 shows that the current density at 0.53V increases from $0.92\text{A}/\text{cm}^2$ to $1.75\text{A}/\text{cm}^2$, when the porosity increases from 0.1 to 0.6, and the maximum power density increases from $0.543\text{W}/\text{cm}^2$ to $1.049\text{W}/\text{cm}^2$. Same as above, for porosity 0.5 and above, the current density at 0.53V becomes constant at $1.74\text{A}/\text{cm}^2$ and the maximum power density at $1.043\text{W}/\text{cm}^2$.

This shows that changing the anode GDL porosity have no effect on the performance while changing the cathode GDL porosity affect the performance of the fuel cell. For the effect of the GDL porosity on the fuel cell performance, the cathode GDL porosity is the

only contributor. Therefore, the fuel cell performance can be improved by increasing only the cathode GDL porosity. For porosity 0.5 and above, the improvement is negligible.

Chapter 5

Sensitivity Analysis

This chapter provides a sensitivity analysis for the fuel cell model. The result of the sensitivity analysis will show which parameter is more sensitive in affecting the performance of the fuel cell. This is necessary to give a rough idea on which parameter should be focused on during the design phase before fabricating the fuel cell, which will save time and cost instead of trying to change one parameter after another experimentally.

5.1 ANOVA

Analysis of variance (ANOVA) is a probabilistic sensitivity analysis method. It is used to determine whether an output and the inputs are statistically associated. ANOVA tests the hypothesis that the means among two or more groups are equal, assuming that the populations distribute normally. For studies of the effect of one factor (input) on the response variable (output), single-factor ANOVA is used. While for two or more factors, multi factor ANOVA is used. The effect of interactions between factors can also be determined. ANOVA is used to determine whether the changes in the input are associated to the output by observing whether the output's mean values changes in a statistically significant manner when the inputs' values changes. If the output's mean response does not have a significant association with the changes in the inputs, the change in the output is considered as random. Whether there is a significant difference between the inputs and

output, is being determined by using F-test. If the null hypothesis (no difference among interactions) is accepted, there may be no relation exists between the inputs and the output. If the F-test rejects the null hypothesis, further analysis of the inputs should be undertaken. The statistical significance of the inputs is being determined based on the F-values. From the F-values, the inputs can be ranked based on their relative magnitude. If the input's F-value is high, it is more sensitive to the output. Inputs with higher F-values are ranked higher. The input's sum of squares can be considered as an alternative to the measure of sensitivity. However, the F-value is preferred as it accounts for not only the sum of squares but also the degree of freedom associated with the input. The F-values calculated for each input indicate the statistical sensitivity of the respective inputs.

5.2 Methodology

ANOVA is used for the sensitivity analysis of the fuel cell model. The parameters temperature, concentration of hydrogen, concentration of oxygen, anode operating pressure, cathode operating pressure, stoichiometric flow ratio of air, channel height, anode GDL thickness, cathode GDL thickness and membrane thickness are used as inputs, while the output of interest are the current density and maximum power density. The parameters are classified into two different categories, the operational parameters and design parameters. The values of each parameters that are used in this analysis are displayed in Table 5.1 and Table 5.2. The values are randomly chosen.

Table 5.1: Values of operating parameters used for the ANOVA sensitivity analysis.

Factor	Value 1	Value 2
Temperature	70°C	80°C
Concentration of Hydrogen	30%	50%
Concentration of Oxygen	15%	20%
Operating Pressure (Anode)	2.0bar	3.0bar
Operating Pressure (Cathode)	2.0bar	3.0bar
Stoichiometric Flow Ratio of Air	3.0	4.0

Table 5.2: Values of design parameters used for the ANOVA sensitivity analysis.

Factor	Value 1	Value 2
Channel Height	0.8mm	1.0mm
GDL Thickness (Anode)	0.3mm	0.4mm
GDL Thickness (Cathode)	0.3mm	0.4mm
Membrane Thickness	50 μ m	108 μ m

All factors are given a sensitivity rank based on their respective F-values. The larger the magnitude of the F-values, the more sensitivity it is of that factor in effecting the fuel cell performance. The relativity of the F-values between factors indicates how significantly a factor is more sensitive than the other. Apart from single factors, sensitivity ranks are also given to the effect of the combination of any two factors on the performance of the fuel cell. Simulations are carried out using COMSOL for every combinations of condition based on Table 5.1 and Table 5.2. Then the resultant current densities at 0.6V and the maximum power densities of each category are analyze using ANOVA with the help of MATLAB.

5.3 Results and Discussion

The respective F-values and their ranks for the operating parameters are displayed in Table 5.3 and Table 5.4.

Table 5.3: ANOVA results and rankings for the operating parameters of the fuel cell model based on current density at 0.6V as the output.

Factor	F-Value	Rank
Temperature	19479.83	1
Concentration of Hydrogen	1423.47	5
Concentration of Oxygen	15075.24	3
Operating Pressure (Anode)	5083.65	4
Operating Pressure (Cathode)	16462.88	2
Stoichiometric Flow Ratio of Air	1284.12	6
Temperature & Concentration of Hydrogen	9.98	16
Temperature & Concentration of Oxygen	267.46	8
Temperature & Operating Pressure (Anode)	29.8	13
Temperature & Operating Pressure (Cathode)	289.61	7
Temperature & Stoichiometric Flow Ratio of Air	63.52	11
Concentration of Hydrogen & Concentration of Oxygen	4.56	18
Concentration of Hydrogen & Operating Pressure (Anode)	4.49	19
Concentration of Hydrogen & Operating Pressure (Cathode)	5.09	17
Concentration of Hydrogen & Stoichiometric Flow Ratio of Air	1.07	21
Concentration of Oxygen & Operating Pressure (Anode)	13.56	15
Concentration of Oxygen & Operating Pressure (Cathode)	181.58	9
Concentration of Oxygen & Stoichiometric Flow Ratio of Air	76.25	12
Operating Pressure (Anode) & Operating Pressure (Cathode)	15.17	14
Operating Pressure (Anode) & Stoichiometric Flow Ratio of Air	3.45	20
Operating Pressure (Cathode) & Stoichiometric Flow Ratio of Air	87.25	10

Table 5.4: ANOVA results and rankings for the operating parameters of the fuel cell model based on maximum power density as the output.

Factor	F-Value	Rank
Temperature	3370.19	4
Concentration of Hydrogen	248.1	11
Concentration of Oxygen	24303.13	2
Operating Pressure (Anode)	748.57	5
Operating Pressure (Cathode)	27290.93	1
Stoichiometric Flow Ratio of Air	7403.66	3
Temperature & Concentration of Hydrogen	0.03	21
Temperature & Concentration of Oxygen	609.52	7
Temperature & Operating Pressure (Anode)	0.06	20
Temperature & Operating Pressure (Cathode)	674.87	6
Temperature & Stoichiometric Flow Ratio of Air	286.15	9
Concentration of Hydrogen & Concentration of Oxygen	8.47	16
Concentration of Hydrogen & Operating Pressure (Anode)	2.02	19
Concentration of Hydrogen & Operating Pressure (Cathode)	10.34	15
Concentration of Hydrogen & Stoichiometric Flow Ratio of Air	3.24	18
Concentration of Oxygen & Operating Pressure (Anode)	20.23	14
Concentration of Oxygen & Operating Pressure (Cathode)	487.04	8
Concentration of Oxygen & Stoichiometric Flow Ratio of Air	224.7	12
Operating Pressure (Anode) & Operating Pressure (Cathode)	23.69	13
Operating Pressure (Anode) & Stoichiometric Flow Ratio of Air	8.07	17
Operating Pressure (Cathode) & Stoichiometric Flow Ratio of Air	252.21	10

From Table 5.3, the most sensitive factor in effecting the fuel cell performance based on the current density at 0.6V, is the temperature, which is followed by the cathode operating pressure and concentration of oxygen. Anode operating pressure, concentration for hydrogen and stoichiometric flow ratio of air are 4th, 5th and 6th respectively. The com-

binations of two factors are statistically insensitive in effecting the fuel cell performance. Consider the F-values, temperature is 1.18 times more sensitive than cathode operating pressure, cathode operating pressure is 1.09 times more sensitive than concentration of oxygen, concentration of oxygen is 2.97 times more sensitive than anode operating pressure, anode operating pressure is 3.57 times more sensitive than concentration for hydrogen and concentration for hydrogen is 1.11 times more sensitive than stoichiometric flow ratio of air. It can be concluded that the first three factors are statistically more sensitive than the other three. Therefore, in the actual experiment, to improve the current density of the fuel cell at a certain voltage, the three factors first to increase are temperature, cathode operating pressure and concentration of oxygen before considering adjusting other parameters.

From Table 5.4, the most sensitive factor in effecting the fuel cell performance based on the maximum power density is the cathode operating pressure, followed by the concentration of oxygen, stoichiometric flow ratio of air, temperature and anode operating pressure. Concentration of hydrogen is ranked below some of the combinations of two factors, which makes it insensitive in effecting the maximum power density. Concentration of hydrogen and all the combinations of two factors are statistically insignificant in effecting the fuel cell performance, Based on the F-values, cathode operating pressure is 1.12 times more sensitive than concentration of oxygen, concentration of oxygen is 3.28 times more sensitive than stoichiometric flow ratio of air, stoichiometric flow ratio of air is 2.20 times more sensitive than temperature, temperature is 4.50 times more sensitive than anode operating pressure. Statistically, cathode operating pressure and concentration of oxygen is the two most sensitive factors in effecting the maximum power density. Therefore, in order to increase the maximum power density of the fuel cell, one need to increase the cathode operating pressure and concentration of oxygen first, before considering adjusting other parameters.

In conclusion, in order to improve the current density of the fuel cell at the operating phase, the temperature of the fuel cell and the humidifying temperature need to be increased first, as it is the most sensitive factor, followed by increasing the cathode

operating pressure and concentration of oxygen in the air supplied in cathode channel. In order to improve the maximum power density of the fuel cell at the operating phase, the cathode operating pressure need to be increased, followed by increasing the concentration of oxygen. This is consistent with the fact that cathode side's gas is slow and sluggish in transport and chemical reaction, inefficient, which leave a lot of room for improvement, i.e. increasing the pressure or the concentration of the oxygen. While the anode side, hydrogen's transport and reaction is fast and efficient, not much room for improvement. The respective F-values and their ranks for the design parameters are displayed in Table 5.5 and Table 5.6.

Table 5.5: ANOVA results for the fuel cell model based on current density at 0.51V as the output for design parameters.

Factor	F-Value	Rank
Channel Height	189.69	6
GDL Thickness (Anode)	8159.38	3
GDL Thickness (Cathode)	14437.66	2
Membrane Thickness	234253.49	1
Channel Height & GDL Thickness (Anode)	1	9
Channel Height & GDL Thickness (Cathode)	0.07	10
Channel Height & Membrane Thickness	23.46	8
GDL Thickness (Anode) & GDL Thickness (Cathode)	33.39	7
GDL Thickness (Anode) & Membrane Thickness	385.78	5
GDL Thickness (Cathode) & Membrane Thickness	876.78	4

Table 5.6: ANOVA results for the fuel cell model based on maximum power density as the output for design parameters.

Factor	F-Value	Rank
Channel Height	329.37	5
GDL Thickness (Anode)	2679.56	3
GDL Thickness (Cathode)	7640.42	2
Membrane Thickness	80764.67	1
Channel Height & GDL Thickness (Anode)	3.23	9
Channel Height & GDL Thickness (Cathode)	0.99	10
Channel Height & Membrane Thickness	73.07	6
GDL Thickness (Anode) & GDL Thickness (Cathode)	19.58	8
GDL Thickness (Anode) & Membrane Thickness	68.04	7
GDL Thickness (Cathode) & Membrane Thickness	557.97	4

Table 5.5 shows that membrane thickness is the most sensitive factor in effecting the fuel cell performance, current density as the output, followed by cathode GDL thickness and anode GDL thickness. Channel height is ranked below some of the combinations of the two factors. From their F-values, membrane thickness is 16.22 times more sensitive than cathode GDL thickness and cathode GDL thickness is 1.77 times more sensitive than anode GDL thickness. Anode GDL thickness is 9.31 times more sensitive than the others. Therefore, the only factors that are statistically sensitive in affecting the fuel cell current density are membrane thickness, cathode GDL thickness and anode GDL thickness. In order to improve the fuel cell current density, it is best to first choose a thinner membrane, thinner GDLs for both cathode and anode, before considering other factors.

Table 5.6 shows that the top 3 most sensitive factors in effecting the fuel cell performance, maximum power density as the output, are the same as the one with the current density as the output, that are membrane thickness, cathode GDL thickness and anode GDL thickness. The channel height is also ranked below some combinations of the two

factors. Based on the F-values, membrane thickness is 10.57 times more sensitive than cathode GDL thickness and cathode GDL thickness is 2.85 times more sensitive than anode GDL thickness. Anode GDL thickness is 4.80 times more sensitive than the others. Statistically, the channel height and the other combination of two factors are insensitive. Therefore, like the above, the only factors that are most sensitive in affecting the fuel cell maximum power density are membrane thickness, cathode GDL thickness and anode GDL thickness. In order to improve the fuel cell maximum power density, it is best to first choose a thinner membrane, thinner GDLs for both cathode and anode, before considering other factors.

In conclusion, in order to improve the current density and the maximum current density of a fuel cell at the design phase, the thickness of the membrane and GDLs of both sides need to be reduced, in other words, choose a thinner membrane and GDLs. Although it is to note that very thin membrane or GDL are bound to tearing, this makes assembling the fuel cell very challenging.

Chapter 6

Conclusions and Recommendations

6.1 Conclusions

A two-dimensional, steady-state and isothermal model has been developed and validated with experimental results from the literature. This is used to investigate the effects of the temperature, concentration of hydrogen, concentration of oxygen, operating pressure, stoichiometric flow ratio of air, channel height, gas diffusion layer (GDL) thickness, membrane thickness and GDL porosity. The results are summarized in Table 6.1. Table 6.1 list out the maximum and minimum value for each factors that was used in the simulation, the resultant current density at the specified voltage and the maximum power density for the specified two values, and the effect of the respective factor based on the current density and maximum power density.

Table 6.1: Summary of the parametric studies.

<i>Range</i>	<i>Current Density</i> (A/cm ²)	<i>Maximum Power</i> <i>Density (W/cm²)</i>	<i>Effect</i>
Temperature of fuel cell and gas humidification at both anode and cathode flow channels			
50°C to 80°C	(at 0.51V) 1.40 to 1.85	0.755 to 1.029	Increase performance

Concentration of hydrogen at the inlet of the anode flow channel			
10% to 90%	(at 0.51V) 1.74 to 1.88	0.971 to 1.044	Increase performance
Concentration of oxygen in air at the inlet of the cathode flow channel			
5% to 30%	(at 0.61V) 0.87 to 1.24	0.545 to 1.072	Increase performance
Pressure of both flow channels			
1.0bar to 4.0bar	(at 0.51V) 1.53 to 1.94	0.803 to 1.077	Increase performance
Pressure at the cathode flow channel			
1.0bar to 4.0bar	(at 0.51V) 1.53 to 1.77	0.803 to 0.996	Increase performance
Pressure at the anode flow channel			
1.0bar to 4.0bar	(at 0.51V) 1.53 to 1.64	0.803 to 0.847	Increase performance
Stoichiometric flow ratio of hydrogen and air at both flow channels inlet			
1.0 to 9.0	(at 0.62V) 0.98 to 1.19	0.609 to 1.041	Increase performance
Stoichiometric flow ratio of hydrogen at anode flow channel inlet			
1.0 to 9.0	No effect	No effect	No effect
Stoichiometric flow ratio of air at cathode flow channel inlet			
1.0 to 9.0	(at 0.62V) 0.98 to 1.18	0.609 to 1.031	Increase performance
Channel height (anode and cathode)			
0.4mm to 1.6mm	(at 0.51V) 1.78 to 1.86	0.939 to 1.036	Increase performance

Thickness of GDL (anode and cathode)			
0.1mm to 1.0mm	(at 0.51V) 2.22 to 1.20	1.257 to 0.641	Decrease performance
Thickness of anode GDL			
0.1mm to 1.0mm	(at 0.51V) 2.00 to 1.49	1.111 to 0.819	Decrease performance
Thickness of cathode GDL			
0.1mm to 1.0mm	(at 0.51V) 2.04 to 1.40	1.147 to 0.738	Decrease performance
Thickness of the membrane			
10 μ m to 300 μ m	(at 0.51V) 2.80 to 1.15	1.515 to 0.623	Decrease performance
GDL porosity of anode and cathode			
0.1 to 0.6	(at 0.53V) 0.92 to 1.75	0.543 to 1.049	Increase performance
GDL porosity of anode			
0.1 to 0.6	No effect	No effect	No effect
GDL porosity of cathode			
0.1 to 0.6	(at 0.53V) 0.92 to 1.75	0.543 to 1.049	Increase performance

The factors were then categorized into two groups, operating parameters and design parameters. Operating parameters consist of temperature, concentration of hydrogen, concentration of oxygen, operating pressure and stoichiometric flow ratio of air and design parameters consist of channel height, gas diffusion layer (GDL) thickness, membrane thickness and GDL porosity. Their sensitivity towards the performance of the fuel cell for each group was ranked, using analysis of variance (ANOVA). The performance of

the fuel cell is characterized by the polarization curves and power density curves. The rankings for each case are shown in Table 6.2, Table 6.3 and Table 6.4. Table 6.2 shows the ranking for the operating parameters based on the current density of the fuel cell while Table 6.3 is based on maximum power density. Table 6.4 shows the ranking for the design parameters based on the current density and the maximum power density of the fuel cell.

Table 6.2: Ranking for each operating parameters based on their sensitivity response towards the current density of the fuel cell.

Rank	Operating Parameters
1	Temperature
2	Operating Pressure (Cathode)
3	Concentration of Oxygen
4	Operating Pressure (Anode)
5	Concentration of Hydrogen
6	Stoichiometric Flow Ratio of Air

Table 6.3: Ranking for each operating parameters based on their sensitivity response towards the maximum power density of the fuel cell.

Rank	Operating Parameters
1	Operating Pressure (Cathode)
2	Concentration of Oxygen
3	Stoichiometric Flow Ratio of Air
4	Temperature
5	Operating Pressure (Anode)
6	Concentration of Hydrogen

Table 6.4: Ranking for each design parameters based on their sensitivity response towards both the current density and maximum power density of the fuel cell.

Rank	Design Parameters
1	Membrane Thickness
2	GDL Thickness (Cathode)
3	GDL Thickness (Anode)
4	Channel Height

In brief, the performance of the fuel cell can be improved by increasing the temperature of the fuel cell and the humidification temperature of both hydrogen and air, the concentration of hydrogen, the concentration of oxygen, operating pressure (especially on the cathode flow channel), stoichiometric flow ratio of air, channel height and cathode GDL porosity, while reducing both the anode and cathode GDLs thickness and membrane thickness.

6.2 Recommendations

Following issues are recommendations that will further improve the simulation model.

1. Develop a single-phase transport, non-isothermal, two dimensional PEM fuel cell model, to investigate the effect of temperature on the fuel cell performance, and to observe the temperature distribution.
2. Develop a two-phase, non-isothermal, two dimensional PEM fuel cell model, to observe the flow field of liquid water and perform parametric study to investigate the effect of some parameters on the fuel cell performance. These include the effect of temperature, pressure, concentration of oxygen, thickness of membrane, catalyst layer and GDL and humidity of reactant gases.
3. Develop a two-phase, non-isothermal, three dimensional PEM fuel cell model.

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