HIGH TEMPERATURE PROTON EXCHANGE MEMBRANE FUEL CELL

OPTIMIZATION OF FLOW CHANNEL GEOMETRY

by

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ABSTRACT

Several groups are studying and researching major factors which influence high temperature proton exchange membrane fuel cells. These factors include material type, temperature, and fuel cell lifespan. Only a few groups research the optimization of the size of the fuel channels within the fuel cell. For channel optimization, a model was created to find the optimum flow channel and rib widths. The approach used was to code the losses due to activation, concentration, and ohmic polarizations to yield the fuel cell voltage and power expected from the fuel cell itself. The model utilizes the specified cell parameters including the material properties, fuel cell temperature, and channel size. This method gives an initial view of how a fuel cell will perform given specific parameters. It is not limited to one fuel cell size, allowing future research efforts to utilize this model to optimize flow channels in a variety of fuel cells.
1 BACKGROUND

High temperature proton exchange membrane (PEM) fuel cells have been studied in more recent history. Low temperature PEM fuel cells have an operation temperature below 100°C, whereas high temperature PEM fuel cells work above this 100°C threshold. The majority of these high temperature fuel cells are operated in the 120°C to 180°C range (Ubong, 2009). High Temperature PEM fuel cells have been found to tolerate some levels of carbon monoxide. (Kwon, 2008) This tolerance allows for the hydrogen fuel to be reformed from other fuel sources such as methane. Other reasons high temperature PEM fuel cells are being researched and used are due to their improved water management and faster electrochemical kinetics (Shao, 2007). When the system is maintained above 100°C the water produces is in the form of vapor. This reduces the chance of flooding, a major problem with low temperature PEM fuel cells. This flooding blocks the flow of the reactant gasses and reduces the performance of the fuel cell. Just as there are advantages to using high temperature PEM fuel cells, there are also drawbacks. This includes increased chances of membrane dehydration, decreased proton conduction, and cell degradation. (Zhang, 2006) These drawbacks must be closely watched to ensure the high temperature fuel cell does not fall below acceptable operating levels. Polybenzimidazole (PBI) membranes are being doped with different acids to improve the conductivity. One commonly used acid is Phosphoric acid (PA). It was found that doping the PBI membrane with about 500mol% of PA resulted in a good operation for the fuel cell. (Kwon, 2009)
Current research is concentrating on optimizing membranes, temperatures, and fuel channel types, presenting the opportunity to take the established systems and optimize the fuel channels to achieve the best performance. This is especially important because once all of the major aspects have been chosen, optimizing the flow channels won’t change the overall design but will improve the performance of the system. Achieving the best performance for the system at hand is necessary to make fuel cells an efficient source of electricity.
2 LITERATURE REVIEW

2.1 Experimental

Multiple experiments have been conducted to test the performance of high temperature proton exchange membrane fuel cells to not only see what the physical performance is, but also to acquire comparative data for numerical models. Depending on the temperature of the fuel cell, membrane used, backpressure, flow channel design, and other variables, a variety of results can be found.

In the journal article “Experimental Factors that influence carbon monoxide tolerance of high-temperature proton-exchange membrane fuel cells” by Kyungjung Kwon, a phosphoric acid doped PBI membrane was used with parallel serpentine flow channels. Figure 1 displays the performance curve at different temperatures with two different feed modes: constant flow rate (cfr) and constant utilization (cu). This experimental test displays how better performance can be achieved with a higher temperature which is also seen in other research works. The main range of temperatures being tested are from 140 to 190 °C. (Kwon, 2008) With advancements in materials research groups hope to get the temperature even above 200°C.
Within this work they tested various carbon monoxide percentages in the hydrogen fuel to discover the tolerance with respect to temperature, fuel feed mode, and the platinum loading. In Figure 2, only the temperature of the fuel cell and the fuel modes are being investigated. The results show that the higher the temperature, the higher the CO tolerance. The use of constant utilization instead of constant flow rate for the fuel mode results in a higher CO tolerance as well. For the other variable the research work found that a higher Platinum loading on the catalyst leads to a higher CO tolerance. (Kwon, 2008)

Figure 1: I-V performance of .5mg cm⁻² Pt loaded anode with pure hydrogen.
As it has been discussed, the advantages of high temperature PEM fuel cells are the improved kinetics, water management, and carbon monoxide tolerance. The major drawback to high temperature PEM fuel cells is the cell degradation which can be seen in the research work “Influence of operating temperature on cell performance and endurance of high temperature proton exchange membrane fuel cells” by Yuka Oono. Within this research work, long term tests were conducted with phosphoric acid-doped PBI electrolyte membranes and were stopped when the voltage dropped by 10% from its peak value. In Figure 3, it can be seen that as the temperature is raised the cell life is decreased. This was discovered to be due to aggregation of the electrode catalyst particles in the early stages, and due to the depletion of phosphoric acid. (Onno, 2009) This means that raising the temperature to try to achieve optimal performance can be
harmful by reducing the life of the fuel cell. Both performance and fuel cell life should be taken into consideration when designing a high temperature proton exchange membrane fuel cell.

Figure 3: Time course of cell voltages and internal resistances of three cells operated at 0.2 A cm$^{-2}$ at cell temperatures of 150, 170, and 190°C.
For contact resistances the relationship between interfacial resistance and clamping pressure was given in Muhammad Hadi Akbari’s journal article, “Numerical investigation of flow field configuration and contact resistance for PEM fuel cell performance.” This graph can be seen in Figure 4 and can be later used to determine the contact resistance to be applied to the model. (Muhammad 2008)

![Graph showing the variation of interfacial contact resistance over a range of clamping pressures.](image)

Figure 4: Variation of the interfacial contact resistance over a range of clamping pressures.
2.2 Modeling Equations

For numerical models of fuel cells, many equations need to be used to be able to calculate the expected performance of the fuel cell. Before these equations can be used, assumptions need to be made for the system to create a solvable model. From many different works the following assumptions are common between each source:

- Water is in the vapor state
- Laminar flow
- Incompressible flow
- Gases are treated as ideal

Some assumptions that are only seen in some of the sources are as follows:

- Isothermal
- Isotropic homogeneous porous region
- Membrane impermeable to gases
- Steady state
- Anode overpotential neglected

With the assumptions of laminar and incompressible flow the continuity and Navier-Stokes equations apply in equations (1) and (2).

\[ \nabla \cdot (\rho u) = Q \quad (1) \]

\[ \rho (u \cdot \nabla) u + \nabla p - \nabla \cdot \mu (\nabla u + (\nabla u)^T) = 0 \quad (2) \]
Then the Maxwell-Stefan equation is used for the transport of multi-component gas species in the porous material in equation (3). (Cheddie, 2006)

\[ \nabla m_i = \sum_{j=1}^{n} \frac{m_i N_j - m_j N_i}{\rho D_{i,j}^{\text{eff}}} \]  \hspace{1cm} (3)

The effective diffusivity is calculated using the Bruggemann’s relationship for the diffusivity in porous media in equation (4). (Su, 2009)

\[ D_{i,j}^{\text{eff}} = \varepsilon_g^{1.5} D_{i,j} \]  \hspace{1cm} (4)

Reversible cell potential with \( T=298 \) K with 1.185V is given in the equation (5). (Cheddie, 2006)

\[ E_r = E_r^0 + \frac{\Delta S}{nF} (T - T_0) + \frac{2RT}{nF} \ln \left( \frac{p_{H_2} \cdot p_{O_2}^{0.5}}{p_w} \right) \]  \hspace{1cm} (5)

The entropy change is given in equation (6). (Cheddie, 2006)

\[ \frac{\Delta S}{n} = -18.449 - 0.01283(T) \]  \hspace{1cm} (6)

Activation overpotential in most of the research work utilized the Butler-Volmer equations (7) and (8). (Sohn, 2011).

\[ i_a = i_{o,a}^{\text{ex}} \left( \frac{C_{H_2}}{C_{H_2}^{\text{ref}}} \right)^{1/2} \frac{2F}{RT} \eta_a \]  \hspace{1cm} (7)
\[ i_c = i_{0,c}^{ex} \left( \frac{C_{O_2}}{r_{O_2}^{ref}} \right) \exp \left( - \frac{\alpha_c F}{RT} \eta_a \right) \] (8)

\( \eta \) is the overpotential at each electrode and is determined by equation (9).

\[ \eta = \varphi_s - \varphi_e - \varphi_{eq} \left( \varphi_{eq,a} = 0, \varphi_{eq,c} = V_0 \right) \] (9)

In one work the exchange current density for the cathode is determined by the Arrenius-like law in equation (10) where the reference temperature is 353K, the reference exchange current density is \( 1.78 \times 10^{-6} \) A m\(^{-2}\), and the \( E_{A,ex}/R \) is 16456 K. (Lobato, 2010)

\[ i_{0,c}^{ex} = i_{0,c,ref}^{ex} \exp \left[ - \frac{E_{A,ex}}{R} \left( \frac{1}{T} - \frac{1}{T_{ref,i_c}} \right) \right] \] (10)

The cell operating potential can be seen below which incorporates the reversible cell potential, the activation overpotential and the ohmic overpotential in equation (11). (Cheddie, 2006)

\[ E_{cell} = E_r - E_{act} - E_{ohm} \] (11)

For one source, activation overpotential is calculated a different way than the Butler-Volmer equation where only the cathode layer is considered. The anode layer is neglected due to the kinetics for the hydrogen dissociation being so much faster than the oxygen reduction reaction. This is calculated using the Tafel relation in equation (12). (Cheddie, 2006)
The ohmic overpotential used by a single source can be seen in the equation (13), which simplifies the ohmic overpotential to allow for a simpler calculation. (Cheddie, 2006) This can be used to verify more complicated calculations to ensure they are on the correct order of magnitude.

\[ E_{\text{act}} = \frac{RT}{2\alpha F} \ln \left( \frac{I}{I_0} \right) \]  \hspace{1cm} (12)

\[ E_{\text{ohm}} = I \left( \frac{l_m}{\kappa m} + \frac{2l_d}{\sigma_d^{\text{eff}}} \right) \]  \hspace{1cm} (13)
2.3 Numerical Results

From the work conducted by O. Shamardina in “A simple model of a high temperature PEM fuel cell,” they created a two dimensional model with the assumptions of steady state and isothermal. Figure 5 displays their numerical model results compared to their experimental results. The main parameters are that the cell was at 433 K, a fixed flow rate was used, and pure hydrogen with dry air was used. (Shamardina, 2010)

![Current-voltage curves for the base case conditions](image)

In another work conducted by Young-Jun Sohn named “Numerical analysis of convection and diffusive fuel transports in high-temperature proton-exchange membrane fuel cells,” a two dimensional numerical model was created. (Sohn, 2011) This model was checked
versus the experimental data retrieved from Ubong et al.’s work from 2009. (Ubong, 2009) The temperature for this experiment was set to 453K with stoichiometric values of 1.2 for hydrogen and 2.0 for oxygen. The experimental and model results can be seen in Figure 6. (Sohn, 2011)

Figure 6-Validation of the present numerical model.

In the work “Mathematical model of a PEMFC using a PBI membrane” by Denver Cheddie the numerical results are compared with Wang et al.’s experimental results at 423K with both an air supply and an oxygen supply. The current density to potential can be seen in Figure 7 and the current density to potential and power can be seen in Figure 8. This article also investigates the overpotentials that contribute to voltage loss as
current density is increased. This can be seen for the oxidant air in Figure 9. (Cheddie, 2006)

Figure 7- IV curves for model and experimental data (a) model curve for oxidant = oxygen and (b) model curve for oxidant = air

Figure 8- Power density vs. current density (a) cell voltage for oxidant = oxygen; (b) cell voltage for oxidant = air; (c) power density for oxidant = oxygen and (d) power density for oxidant = air
Figure 9 – Overpotentials for oxidant = air. (a) Cell potential; (b) activation overpotential; (c) ohmic overpotential and (d) concentration overpotential.
3 METHODOLOGY

After researching current knowledge in the field of High Temperature PEM fuel cells, it was found that very few models exist to optimize the flow channel and rib width geometry. This is why a numerical model was created to predict the results of a fuel cell with given parameters. This numerical model was programmed into Matlab with all fuel cell parameters set as variables within the code itself. Upon modifying the variables within the matlab code, a new result can be displayed for any dimensional configuration. The following sections talk about how the model goes about calculating the final voltage of the fuel cell. The overall sequence of the code is to first calculate the concentration of hydrogen that yields the partial pressure of hydrogen on the anode side of the fuel cell. Second, the concentrations on the cathode side are calculated yielding the oxygen and water partial pressures. The three partial pressures in combination with the standard state electromotive force are used to calculate the electromotive force available. The activation polarization is then calculated and subtracted from the electromotive force which yields the modified electromotive force used in the ohmic calculation. Once the ohmic polarization is calculated the final cell voltage is found. The numerical model runs through a range of different current densities to give the performance of the cell over this range. This overall process is visually shown in the process flow diagram in Figure 10. The processes for the calculations of the anode and cathode concentrations can be seen in Figure 11 and Figure 12, respectively.
Figure 10: Flow Diagram Overall Process
Figure 11: Anode Process Flow Diagram
Figure 12: Cathode Process Flow Diagram

1. Mass Transfer in Bulk
2. Bulk Concentration
3. Diffusivity
4. Mole Fractions of Species
5. Initial Int and Cathode Concentrations
6. Mix Bulk Diffusivity
7. Mix GDL and Electrode Diffusivity
8. Effective Diffusivity
9. Average Concentrations for GDL and Cathode
10. Modified Effective Diffusivity
11. New int Concentration
12. Cathode Concentration
13. New Mole Fractions of Species
14. Partial Pressures
### 3.1 Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A )</td>
<td>Interface area</td>
</tr>
<tr>
<td>( P_{\text{channel}} )</td>
<td>Perimeter of channel</td>
</tr>
<tr>
<td>( A_{\text{channel}} )</td>
<td>Cross sectional area of channel</td>
</tr>
<tr>
<td>( a_w )</td>
<td>Water activity</td>
</tr>
<tr>
<td>( D )</td>
<td>Diffusion coefficient ((m^2/s))</td>
</tr>
<tr>
<td>( F )</td>
<td>Faraday constant ((96493 \text{ C/mol}))</td>
</tr>
<tr>
<td>( I )</td>
<td>Current ((A))</td>
</tr>
<tr>
<td>( i )</td>
<td>Current density ((A/m^2))</td>
</tr>
<tr>
<td>( M )</td>
<td>Species molecular weight ((\text{kg/mol}))</td>
</tr>
<tr>
<td>( J )</td>
<td>Species mass flux ((\text{kg/s}))</td>
</tr>
<tr>
<td>( j )</td>
<td>Species mass flux in unit area ((\text{kg/(s m^2)}))</td>
</tr>
<tr>
<td>( n )</td>
<td>Species molar consumption flux ((\text{mol/s}))</td>
</tr>
<tr>
<td>( n )</td>
<td>Number of water transport coefficient in the membrane</td>
</tr>
<tr>
<td>( P )</td>
<td>Pressure ((\text{Pa}))</td>
</tr>
<tr>
<td>( R )</td>
<td>Universal gas constant ((\text{J/(mol K)}))</td>
</tr>
<tr>
<td>( T )</td>
<td>Temperature ((\text{K}))</td>
</tr>
<tr>
<td>( v )</td>
<td>Diffusion velocity</td>
</tr>
<tr>
<td>( X )</td>
<td>Species mole fraction</td>
</tr>
</tbody>
</table>
Greek symbols

\( \rho \) Species mass concentration

\( \eta \) Species utilization

\( \delta \) Thickness of gas diffusion layer and electrode layer

\( \lambda \) Water content

Subscript

s Interface between channel and gas diffusion layer

int Interface between gas diffusion layer and electrode layer

ia Interface between anode layer and membrane

ic Interface between cathode layer and membrane
3.2 Schematic

Equations (14) and (15) represent the two electrochemical half equations that make up the reaction of the PEM Fuel Cell. Equation (14) occurs on the anode side of the system, while equation (15) occurs on the cathode side. (Mench, 2008) This separation of the reactions with a membrane between, formally known as an electrolyte, causes the electrons to run through an external circuit. This allows the system to be used as an electrical power source. This process can be seen in Figure 13.

\[ H_2 \rightarrow 2H^+ + 2e^- \quad (14) \]

\[ \frac{1}{2} O_2 + 2H^+ + 2e^- \rightarrow H_2O \quad (15) \]

Figure 13: Fuel Cell Schematic for High Temperature Proton Exchange Membrane Fuel Cell
There are two area calculations used for the total area $B$ and the effective area $A$. These can be seen in equations (16) and (17). The total current ($I$) is calculated using the total area ($B$) and the current density ($i$). This can be seen in equation (18). The character $w$ stands for the width and $l$ is for the length of the system.

$$B = l_{\text{channel}} \times (w_{\text{channel}} + w_{\text{rib}}) \quad (16)$$

$$A = l_{\text{channel}} \times w_{\text{channel}} \quad (17)$$

$$I = ixB \quad (18)$$

For this analysis the model schematic can be seen in Figure 14. This displays all the material included in the analysis, and how the rib is in two halves on either side of the channel. This rib and channel relationship is better seen in Figure 15.
Figure 14: Model Schematic for Analysis

Figure 15: Representation of Channel and Ribs
3.3 Mass transfer in bulk flow

Similar to the way heat transfer has a coefficient with the variable $h$, mass transfer has a similar coefficient $h_m$ with the subscript of mass to signify its use. This coefficient can be calculated using the Sherwood number as seen in equation (19). The Sherwood number can be determined from the channel geometry and orientation when simplified by assuming laminar flow. The value is determined using Table 1 and calculating $\alpha$, which is the ratio of the width of the channel ($b$) to the height of the channel ($a$) ($\alpha = b/a$). To calculate the mass transfer coefficient the hydraulic diameter and diffusivity are also needed. The calculation for the hydraulic diameter uses the cross sectional area and the perimeter of the channel in equation (20). The diffusivity calculations are seen in equations (37) and (39) for a two species mix and a three or more species mix, respectively. (O’Hayre, 2009)

$$h_{mass,i} = Sh \frac{D_i \text{mix}}{D_h}$$  \hspace{1cm} (19)

<table>
<thead>
<tr>
<th>Cross Section $\alpha$</th>
<th>0.4</th>
<th>0.7</th>
<th>1.0</th>
<th>2.0</th>
<th>2.5</th>
<th>5.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sh$_D$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sh$_F$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sh$_D$</td>
<td>4.4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sh$_F$</td>
<td>3.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sh$_D$</td>
<td>3.7</td>
<td>3.1</td>
<td>3.0</td>
<td>3.4</td>
<td>3.7</td>
<td>4.8</td>
</tr>
<tr>
<td>Sh$_F$</td>
<td>4.5</td>
<td>3.8</td>
<td>3.6</td>
<td>4.1</td>
<td>4.5</td>
<td>5.7</td>
</tr>
<tr>
<td>Sh$_D$</td>
<td>1.4</td>
<td>2.0</td>
<td>2.4</td>
<td>3.2</td>
<td>3.4</td>
<td>3.9</td>
</tr>
<tr>
<td>Sh$_F$</td>
<td>1.6</td>
<td>2.3</td>
<td>2.7</td>
<td>3.5</td>
<td>3.8</td>
<td>4.4</td>
</tr>
</tbody>
</table>

Table 1: Sherwood Number for Laminar Flows in Circular, Rectangular, and Three-sided Closed Rectangular Ducts (O’Hayre, 2009)

$$D_h = \frac{4 * A_{channel}}{P_{channel}}$$  \hspace{1cm} (20)
3.4 Anode Concentration

Because the anode will have a mixed input of hydrogen and water vapor, the unit area mass flux of hydrogen and water are needed at each interface. For the purpose of this research an interface is the contact surface between two materials. For the interface between the gas diffusion layer and the bulk flow channel the calculations can be seen in equations (21) and (22). (O’Hayre, 2009)

\[ j_{H_2} = h_{mass,H_2} \left( \rho_{\infty}^{H_2} - \rho_s^{H_2} \right) \]  \hspace{1cm} (21)

\[ j_{H_2O,a} = h_{mass,H_2O} \left( \rho_{\infty}^{H_2O} - \rho_s^{H_2O} \right) \]  \hspace{1cm} (22)

Where \( \rho_{\infty} \) is the average mass concentration of hydrogen in the bulk flow and \( \rho_s \) is the average mass concentration of hydrogen at the interface between gas diffusion layer and the bulk flow. The unit area mass consumption rate of hydrogen relates to the current density in the form of equation (23). To get to a usable flow rate for the inlet fuel, the mole flow rate, utilization, and mole fraction of hydrogen in the fuel are needed. Two different flow rates can be used which are constant utilization and fixed flow rates. The equation for constant utilization flow rate can be seen in equation (25) where \( u_{H_2} \) is the utilization ratio used to supply enough fuel for the system to avoid a depletion of fuel. The equation for the fixed flow rate is in equation (26) where the maximum expected current is used to supply enough fuel for the entire range of current densities. For this study, only constant flow rate cases are used, but both are built into...
the numerical model for further use. Equation (24) gives the molar flow rate of the reaction for hydrogen which is used in concentration calculations. (Mench, 2008)

\[ j_{H_2} = \frac{i}{2F} M_{H_2} \]  \hspace{1cm} (23)

\[ \dot{n}_{H_2} = \frac{i}{2F} \]  \hspace{1cm} (24)

\[ \dot{n}_{H_2}^{in} = \frac{i}{2F \eta_{H_2}} \]  \hspace{1cm} (25)

\[ \dot{n}_{H_2}^{in} = \frac{i_{max}}{2F} \]  \hspace{1cm} (26)

Where \( M_{H_2} \) is the molecular weight of hydrogen used in the mass consumption rate calculation. To find the concentration of hydrogen and water in the bulk flow, the average of the inlet and outlet concentrations is used and can be seen in equation (27).

The inlet concentration and outlet concentration calculations of hydrogen can be seen in equation (28) and (29). Similar calculations are done for the water on the anode side and can be seen in equations (30), (31) and (32). (O’Hayre, 2009)

\[ \rho_{H_2}^{in} = \frac{(\rho_{H_2}^{in} + \rho_{H_2}^{out})}{2} \]  \hspace{1cm} (27)

\[ \rho_{H_2}^{in} = \frac{\dot{m}_{H_2}^{in}}{V_{total}} = \frac{\dot{n}_{H_2} M_{H_2} P_{\text{fuel}}}{\dot{m}_{fuel}^{in} \eta_{H_2} RT} \]  \hspace{1cm} (28)

\[ \rho_{H_2}^{out} = \frac{\dot{m}_{H_2}^{out}}{V_{total}} = \frac{(\dot{n}_{fuel}^{in} - \dot{n}_{H_2}) M_{H_2} P_{\text{fuel}}}{(\dot{n}_{H_2} / \eta_{H_2} - \dot{n}_{H_2}) RT} \]  \hspace{1cm} (29)
There are three parts that contribute to the mole flux by the Nernst-Planck equation found in equation (33). (Mench, 2008)

\[ N_i = -z_i u_i F \nabla \Phi - D_i \nabla c_i + c_i v \]  

(33)

The first term includes \( z_i \) which is the charge number, \( c_i \) which is concentration of the \( i \)th species, and \( u_i \) which is mobility. These make up the migration portion which represents the motion of charged species and results when there is a potential gradient. If neglecting the gradient influence (\( \Phi \)), then the remaining two terms make up the mass transfer in a porous media. These are the mass diffusion, caused by a concentration gradient term, and the convection term. The convection term denotes the motion of the species as the bulk motion moves it along. This then leads to the equations for unit area species mass transfer fluxes in the gas diffusion layer as seen in equations (34) and (35). (O’Hayre, 2009)

\[ j_{H_2} = -D_{H_2(\text{eff})} \nabla \rho_{\text{GDL}}^{H_2} + \rho_{\text{GDL}}^{H_2} v_{\text{GDL}} \]  

(34)

\[ j_{H_2O,a} = -D_{H_2O(\text{eff})} \nabla \rho_{\text{GDL}}^{H_2O} + \rho_{\text{GDL}}^{H_2O} v_{\text{GDL}} \]  

(35)
Within the unit area species mass transfer fluxes $v$ is the diffusion velocity that is caused by the mass diffusion of the species, $\rho^i$ is the average mass concentrations of species in the gas diffusion layer, and $\nabla \rho^i$ is the gradient of the concentration of species across the porous layer. For these equations it is defined as if the mass flux towards the bulk flow is positive.

The effective diffusivity is calculated using the Bruggemann’s relationship for the diffusivity in porous media seen in equation (36). (Su, 2009) This utilizes the ordinary diffusivity ($D_{i,j}$) and the porosity ($\varepsilon_g$) for the mix of one species $i$ and a second species $j$.

$$D_{i,j(\text{eff})} = \varepsilon_g^{1.5} D_{i,j}$$ (36)

To find the ordinary diffusivity the temperature ($T$), molecular weight ($M$), molecular volume ($V$), and Pressure ($P$) are needed as seen in equation (37). Equations (38) and (39) are used when the mix of species is greater than two as in the case of the mix on the cathode side of air. (Mench, 2008)

$$D_{i,j} = \frac{0.01013T^{1.75} \left( \frac{1}{M_i} + \frac{1}{M_j} \right)^{0.5}}{P \left[ V_i^{1/3} + V_j^{1/3} \right]^2}$$ (37)

$$X_i = \frac{(\rho_i/M_i)}{\sum_{j\neq i} (\rho_j/M_j)}$$ (38)
For the diffusivity calculation on the anode side, since there are only two components in the fuel, only equation (37) needs to be utilized. This calculation can be seen in equation (40) where the diffusivity for hydrogen in water is the same as the diffusivity for water in hydrogen \( D_{H_2 \cdot H_2O} = D_{H_2 \cdot H_2} \). If one gas diffuses a certain amount into another gas that means that second gas is diffusing into the first as well. The values of diffusion volumes can be retrieved in Table 2. The effective diffusivity calculation for hydrogen and water are in equations (41) and (42) which are then used in the modified effective diffusivity calculations.

<table>
<thead>
<tr>
<th>Formula</th>
<th>V (unit less)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>7.07</td>
</tr>
<tr>
<td>H₂O (Vapor)</td>
<td>12.7</td>
</tr>
</tbody>
</table>

Table 2: Diffusion Volumes Anode (Mench, 2008)

\[
D_{H_2,H_2O,a} = \frac{0.01013T^{1.75}\left(\frac{1}{M_{H_2}} + \frac{1}{M_{H_2O}}\right)^{0.5}}{P_a \left[V_{H_2}^{1/3} + V_{H_2O}^{1/3}\right]^2}
\]  

(40)

\[
D_{H_2(\text{eff})} = \varepsilon^\frac{1.5}{g}D_{H_2,H_2O,a}
\]  

(41)

\[
D_{H_2O(\text{eff})_{a,H_2}} = \varepsilon^\frac{1.5}{g}D_{H_2O,a,H_2}
\]  

(42)
The modified effective diffusivities in the gas diffusion layer and anode are seen in equations (43) and (44). This incorporates the component of the Nernst-Planck equation (33) for mass diffusion due to the flow of the species. This new diffusivity can then be used to find the new concentration of each species at the new location. These equations will be used to calculate the modified diffusivities at different locations in the anode. (Mench, 2008)

\[ D_{a,H_2\text{(eff)}} = D_{H_2\text{(eff)}} \frac{\rho^{H_2} + \rho^{H_2O}}{\rho^{H_2O}} \]  

(43)

\[ D_{a,H_2O\text{(eff)}} = D_{H_2O\text{(eff)},a} \frac{\rho^{H_2} + \rho^{H_2O}}{\rho^{H_2O}} \]  

(44)

The modified effective diffusion equations allow the mass flux equations to be expressed in more compact forms as seen in equation (45).

\[ j_{H_2} = -D_{a,H_2\text{(eff)}} \nabla \rho^{H_2} \]  

(45)

Mass transfer flux and diffusivity in the electrode layer follow the same pattern as shown in the gas diffusion layers. Eventually, at any given current density i, the molar concentrations of species at the interface between the electrode and membrane are obtained. The partial pressures of reactants and production species at the interface are found and the calculation can be seen in equation (46).” (Mench, 2013)

\[ P_{\text{int}}^{H_2} = \frac{\rho_{\text{int}}^{H_2}}{\rho_{\text{int}}^{H_2} + \rho_{\text{int}}^{H_2O,a}} P_{\text{anode}} \]  

(46)
For the anode side calculations of the concentration of each species need to be made at the two interfaces. The interface between the gas diffusion layer and electrode layer (int) and the interface between anode (ia) and the membrane. For this calculation an iteration process is implemented. With using set values for the concentrations as the starting conditions the iteration process can commence and find the needed concentrations at each location.

The surface concentration can be calculated on the anode side without being included in the iteration process. The calculations for both hydrogen and water at the surface between the channel and gas diffusion layer can be seen in equations (47) and (48), respectively. (O’Hayre, 2009)

\[
\rho_s^{H_2} = \rho_{\infty}^{H_2} - \frac{\dot{n}_{H_2} M_{H_2}}{A h_{mass,H_2}} \tag{47}
\]

\[
\rho_s^{H_2O,a} = \rho_{\infty}^{H_2O,a} \tag{48}
\]

The iteration process for the anode side takes in initial values, calculates average concentrations of the surface and int interfaces and again for the int and ia interfaces. It then calculates the effective diffusivity considering velocity. Using this new effective diffusivity the model calculates the new int interface concentration, and then calculates the new ia interface concentration. The new int and ia concentrations are then used as the initial values for the next iteration. This process is then repeated until the values for the int and ia concentrations converge. Once the final concentrations are achieved the values for the fraction of hydrogen at the interface between the cathode and
membrane (ia) is calculated and this allows for the pressure due to hydrogen at this interface to be calculated. Equations (49) through (60) displays one iteration to find the concentrations needed.

The process first begins with the calculation of the average concentrations for both hydrogen and water at the gas diffusion layer and the anode seen in equations (49) through (52).

\[
\rho_{GDL_{AVE}}^{H_2} = \frac{(\rho_{s}^{H_2} + \rho_{int}^{H_2})}{2} \tag{49}
\]

\[
\rho_{anode_{AVE}}^{H_2} = \frac{(\rho_{int}^{H_2} + \rho_{ia}^{H_2})}{2} \tag{50}
\]

\[
\rho_{GDL_{AVE}}^{H_2O_{a}} = \frac{(\rho_{s}^{H_2O_{a}} + \rho_{int}^{H_2O_{a}})}{2} \tag{51}
\]

\[
\rho_{anode_{AVE}}^{H_2O_{a}} = \frac{(\rho_{int}^{H_2O_{a}} + \rho_{ia}^{H_2O_{a}})}{2} \tag{52}
\]

The process then calculates the effective diffusivity considering convective velocity at the gas diffusion layer and the electrode for both hydrogen and oxygen seen in equations (53) through (56).

\[
D_{a,H_2(\text{eff})}^{GDL} = D_{H_2(\text{eff})}^{GDL} \frac{\rho_{GDL_{AVE}}^{H_2} + \rho_{GDL_{AVE}}^{H_2O_{a}}}{\rho_{GDL_{AVE}}} \tag{53}
\]

\[
D_{a,H_2(\text{eff})}^{\text{electrode}} = D_{H_2(\text{eff})}^{\text{electrode}} \frac{\rho_{anode_{AVE}}^{H_2} + \rho_{anode_{AVE}}^{H_2O_{a}}}{\rho_{anode_{AVE}}} \tag{54}
\]
After the diffusivities are calculated the interface between the gas diffusion layer and electrode layer (int) concentrations are calculated using the calculations seen in equations (57) and (58) for hydrogen and water, respectively. (O’Hayre, 2009)

\[
D_{a,H_2O(\text{eff})}^{\text{GDL}} = D_{H_2O(\text{eff})}^{\text{GDL}} \frac{\rho_{H_2} \times \rho_{H_2O.a}^{\text{GDL,AVE}} + \rho_{H_2O.a}}{\rho_{H_2O.a}^{\text{GDL,AVE}}} \quad (55)
\]

\[
D_{a,H_2O(\text{eff})}^{\text{electrode}} = D_{H_2O(\text{eff})}^{\text{electrode}} \frac{\rho_{\text{anode,AVE}} \times \rho_{H_2O.a}^{\text{anode,AVE}} + \rho_{H_2O.a}}{\rho_{H_2O.a}^{\text{anode,AVE}}} \quad (56)
\]

Finally the concentrations at the interface between the anode and membrane (ia) are calculated using the calculations seen in equations (59) and (60) for hydrogen and water, respectively.

\[
\rho_{\text{int}}^{H_2} = \rho_{\text{s}}^{H_2} - \frac{\dot{n}_{H_2} M_{H_2}}{A} \times \frac{t_{\text{GDL}}^{\text{GDL}}}{D_{a,H_2(\text{eff})}^{\text{GDL}}} \quad (57)
\]

\[
\rho_{\text{int}}^{H_2O,a} = \rho_{\text{s}}^{H_2O} + \frac{\dot{n}_{H_2} M_{H_2}}{A} \times \frac{t_{\text{GDL}}^{\text{GDL}}}{D_{a,H_2O(\text{eff})}^{\text{GDL}}} \quad (58)
\]

Finally the concentrations at the interface between the anode and membrane (ia) are calculated using the calculations seen in equations (59) and (60) for hydrogen and water, respectively.

\[
\rho_{\text{int}}^{H_2} = \rho_{\infty}^{H_2} - \frac{\dot{n}_{H_2} M_{H_2}}{A} \left[ \frac{t_{\text{GDL}}^{\text{GDL}}}{D_{a,H_2(\text{eff})}^{\text{GDL}}} + \frac{t_{\text{electrode}}^{\text{GDL}}}{D_{a,H_2(\text{eff})}^{\text{electrode}}} + \frac{1}{h_{\text{mass,}H_2}} \right] \quad (59)
\]

\[
\rho_{\text{int}}^{H_2O,a} = \rho_{\text{int}}^{H_2O,a} + \frac{\dot{n}_{H_2} M_{H_2}}{A} \times \frac{t_{\text{electrode}}^{\text{electrode}}}{D_{a,H_2O(\text{eff})}^{\text{electrode}}} \quad (60)
\]

This ends the iteration and the int and ia concentrations are used as the initial values for the next iteration. Once the iteration is complete the fraction amounts at each interface are calculated as well as the pressure due to hydrogen. The fractions at the surface, int,
and ia can be seen in equations (61), (62), and (63) respectively. The pressure due to hydrogen calculation can be seen in equation (64).

\[
X_{s}^{H_2} = \frac{\rho_s^{H_2}}{\rho_s/M_{H_2} + \rho_s^{O_2,a}/M_{H_2O}}
\]

(61)

\[
X_{int}^{H_2} = \frac{\rho_{int}^{H_2}}{\rho_{int}/M_{H_2} + \rho_{int}^{O_2,a}/M_{H_2O}}
\]

(62)

\[
X_{ia}^{H_2} = \frac{\rho_{ia}^{H_2}}{\rho_{ia}/M_{H_2} + \rho_{ia}^{O_2,a}/M_{H_2O}}
\]

(63)

\[
P_{ia}^{H_2} = X_{ia}^{H_2} \times P_{fuel}
\]

(64)

This ends the concentration calculations done on the anode side. A similar iteration process is done for the cathode side and the process is explained below, needing more calculations due to the presence of three species in the flow.
3.5 Cathode Concentration

The cathode will also have a mixed input of air which will include oxygen, nitrogen, and water vapor. The unit area mass flux of oxygen, nitrogen, and water are needed at each interface. For the interface between the gas diffusion layer and the bulk the calculation can be seen in equations (65), (66), and (67). (O’Hayre, 2009)

\[ j_{O_2} = h_{mass,O_2}(\rho_{\infty}^{O_2} - \rho_s^{O_2}) \]  
\[ j_{N_2} = h_{mass,N_2}(\rho_{\infty}^{N_2} - \rho_s^{N_2}) \]  
\[ j_{H_2O,c} = h_{mass,H_2O}(\rho_{\infty}^{H_2O} - \rho_s^{H_2O}) \]

The unit area mass consumption rate of oxygen relates to the current density in the form of equation (68). (Mench, 2008 or O’Hayre, 2009)

\[ j_{O_2} = \frac{i}{4F} M_{O_2} \]

Where \( M_{O_2} \) is the molecular weight of oxygen. This relationship is used in combination with the unit area mass flux to find the concentration at the surface between the channel and the gas diffusion layer.

The reaction rate for oxygen and the production rate of water are in the calculations in equations (69) and (70), respectively. The flow rate provided for the cathode side uses constant utilization or constant flow rate just as was seen for the anode. The calculation for constant utilization is seen in equation (71) where \( \eta_{O_2} \) is the utilization of oxygen. The equation used for this research is the constant flow rate in equation (72). Utilizing
the inlet flow rate of oxygen, the inlet flow rate of nitrogen and water vapor are calculated in equations (73) and (74), respectively. (O’Hayre, 2009)

\[ \dot{n}_{o_2} = \frac{I}{4F} \]  
\[ \dot{n}_{H_2O} = \frac{I}{2F} \]  
\[ \dot{n}_{o_2}^{in} = \frac{I}{4F\eta_{o_2}} = \frac{\dot{n}_{o_2}}{\eta_{o_2}} \]  
\[ \dot{n}_{o_2}^{in} = \frac{I_{max}}{4F} \]  
\[ \dot{n}_{N_2}^{in} = \dot{n}_{o_2}^{in} \cdot \frac{.79}{.21} \]  
\[ \dot{n}_{H_2O}^{in} = \frac{\dot{n}_{o_2}^{in} \cdot X_{H_2O,c}}{.21 \cdot (1 - X_{H_2O,c})} \]  

Note that \( X_{H_2O,c} \) is the mole fraction at the inlet surface of the cathode, also known as the inlet humidity of H\(_2\)O vapor mole fraction. To find the concentration of oxygen, nitrogen, and water in the bulk flow the average of the inlet and outlet concentrations are used with the calculation for oxygen seen in equation (75). The inlet concentration and outlet concentration calculations of oxygen can be seen in equations (76) and (77). Similar calculations are done for the nitrogen and water and can be seen in equations (78) through (83). (O’Hayre, 2009)

\[ \rho_{o_2}^{\infty} = \frac{\rho_{in}^{o_2} + \rho_{out}^{o_2}}{2} \]
The unit area species mass transfer fluxes in the gas diffusion layer for the cathode side are seen in equations (84), (85), and (86) where they come from the Nernst-Planck equation found in equation (33). (Mench, 2008)

\[ j_{O_2} = -D_{O_2(\text{eff})} \nabla \rho_{GDL}^{O_2} + \rho_{GDL}^{O_2} v_{GDL} \]  
(84)

\[ j_{N_2} = -D_{N_2(\text{eff})} \nabla \rho_{GDL}^{N_2} + \rho_{GDL}^{N_2} v_{GDL} \]  
(85)

\[ j_{H_2O,c} = -D_{H_2O(\text{eff})} \nabla \rho_{GDL}^{H_2O} + \rho_{GDL}^{H_2O} v_{GDL} \]  
(86)
The ordinary diffusivity for the cathode components is first calculated by finding the two component mix diffusivity. There are three equations to calculate all the ordinary diffusivities seen in equations (87) through (89). The values of diffusion volumes can be retrieved in Table 2. The two species diffusivity calculations are same for one species into the second to the second species into the first where \( D_{O_2,N_2} = D_{N_2,O_2} \), \( D_{O_2,H_2O,c} = D_{H_2O,c,O_2} \), and \( D_{N_2,H_2O,c} = D_{H_2O,c,N_2} \). (Mench, 2008)

<table>
<thead>
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<td>O(_2)</td>
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<tr>
<td>N(_2)</td>
<td>17.9</td>
</tr>
<tr>
<td>H(_2)O (Vapor)</td>
<td>12.7</td>
</tr>
</tbody>
</table>

Table 3: Diffusion Volumes Cathode (Mench, 2008)

\[
D_{O_2,N_2} = \frac{0.01013T^{1.75} \left( \frac{1}{M_{O_2}} + \frac{1}{M_{N_2}} \right)^{0.5}}{P_c \left[ \frac{1}{V_{O_2}} + \frac{1}{V_{N_2}} \right]^{2}}
\] (87)

\[
D_{O_2,H_2O,c} = \frac{0.01013T^{1.75} \left( \frac{1}{M_{O_2}} + \frac{1}{M_{H_2O}} \right)^{0.5}}{P_c \left[ \frac{1}{V_{O_2}} + \frac{1}{V_{H_2O}} \right]^{2}}
\] (88)

\[
D_{N_2,H_2O,c} = \frac{0.01013T^{1.75} \left( \frac{1}{M_{N_2}} + \frac{1}{M_{H_2O}} \right)^{0.5}}{P_c \left[ \frac{1}{V_{N_2}} + \frac{1}{V_{H_2O}} \right]^{2}}
\] (89)
The fuel on the cathode side contains three components which require a mix diffusivity to be calculated. The percentage of the bulk flow due to each component can be calculated and will be used to calculate the mix diffusion by using equation (38). This is done for oxygen, nitrogen, and water seen in equations (90), (91), and (92) respectively.

\[
X^{O_2}_\infty = \frac{\rho^{O_2}_\infty / M_{O_2}}{\left(\frac{\rho^{O_2}_\infty / M_{O_2} + \rho^{N_2}_\infty / M_{N_2} + \rho^{H_2O_{-c}}_\infty / M_{H_2O}}{M_{H_2O}}\right)} \tag{90}
\]

\[
X^{N_2}_\infty = \frac{\rho^{N_2}_\infty / M_{N_2}}{\left(\frac{\rho^{O_2}_\infty / M_{O_2} + \rho^{N_2}_\infty / M_{N_2} + \rho^{H_2O_{-c}}_\infty / M_{H_2O}}{M_{H_2O}}\right)} \tag{91}
\]

\[
X^{H_2O_{-c}}_\infty = \frac{\rho^{H_2O_{-c}}_\infty / M_{H_2O}}{\left(\frac{\rho^{O_2}_\infty / M_{O_2} + \rho^{N_2}_\infty / M_{N_2} + \rho^{H_2O_{-c}}_\infty / M_{H_2O}}{M_{H_2O}}\right)} \tag{92}
\]

The mix diffusion in the bulk flow of the cathode utilizes equations (90) through (92), the ordinary diffusivity in equation (37), and the mix diffusion in equation (39). These diffusivity calculations are shown in equations (93) through (95).

\[
D^{\infty}_{O_2, mix} = \frac{1 - X^{O_2}_\infty}{\left(\frac{X^{N_2}_\infty / D^{\infty}_{O_2,N_2} + X^{H_2O_{-c}}_\infty / D^{\infty}_{O_2,H_2O}}{D^{\infty}_{O_2,N_2} + D^{\infty}_{O_2,H_2O}}\right)} \tag{93}
\]
To get to the effective diffusivity, equation (36) is used and is calculated in equations (96) through (98). Utilizing the effective diffusivities, the modified effective diffusivity can be calculated. (Sohn, 2011)

\[
D_{N_2,\text{mix}}^\infty = \frac{(1 - X_{N_2}^{\infty})}{\left(\frac{X_{N_2}^{\infty}}{D_{N_2,O_2}} + \frac{X_{H_2O,c}^{\infty}}{D_{N_2,H_2O}}\right)} 
\]

(94)

\[
D_{H_2O,c,\text{mix}}^\infty = \frac{(1 - X_{H_2O,c}^{\infty})}{\left(\frac{X_{N_2}^{\infty}}{D_{H_2O,N_2}} + \frac{X_{O_2}^{\infty}}{D_{H_2O,O_2}}\right)} 
\]

(95)

The modified effective diffusivities in the gas diffusion layer, anode, and cathode are seen in equations (43) through (101). This incorporates the component of the Nernst-Planck equation (33) for mass diffusion due to the flow of the species. This new diffusivity can then be used to find the new concentration of each species at the new location. These equations will be used to calculate the modified diffusivities at different locations in both the anode and cathode calculations. (Mench, 2008)

\[
D_{O_2(\text{eff})} = \varepsilon_g^{1.5} D_{O_2,\text{mix}}^\infty 
\]

(96)

\[
D_{N_2(\text{eff})} = \varepsilon_g^{1.5} D_{N_2,\text{mix}}^\infty 
\]

(97)

\[
D_{H_2O(\text{eff}),c} = \varepsilon_g^{1.5} D_{H_2O,c,\text{mix}}^\infty 
\]

(98)

\[
D_{c,O_2(\text{eff})} = D_{O_2(\text{eff})} \frac{\rho_{O_2}^{\infty} + \rho_{N_2}^{\infty} + \rho_{H_2O}^{\infty}}{\rho_{N_2}^{\infty} + \rho_{H_2O}^{\infty}} 
\]

(99)
With the modified effective diffusion equations it leads to the mass flux equations to be able to be expressed in more compact forms seen in equations (102) through (104).

\[
D_{c,N_2(\text{eff})} = D_{N_2(\text{eff})} \frac{\rho_{O_2}^0 + \rho_{N_2}^0 + \rho_{H_2O}^0}{\rho_{N_2}^0} 
\]

\[
D_{c,H_2O(\text{eff})} = D_{H_2O(\text{eff}),c} \frac{\rho_{O_2}^0 + \rho_{N_2}^0 + \rho_{H_2O}^0}{\rho_{N_2}^0 + \rho_{O_2}^0} 
\]

(Mench, 2008)

\[-\left(\frac{i}{2F} M_{H_2O}\right) \frac{\rho_{O_2}^0}{\rho_{N_2}^0 + \rho_{H_2O}^{\text{cathode}}} - \frac{i}{4F} M_{O_2} = D_{c,O_2(\text{eff})} \nabla \rho_{O_2}^0 \]  

(102)

\[
\frac{i}{4F} M_{O_2} - \frac{i}{2F} M_{H_2O} = D_{c,N_2(\text{eff})} \nabla \rho_{N_2}^0 
\]

(103)

\[
\frac{i}{2F} M_{H_2O} + \frac{\rho_{H_2O}^{\text{cathode}}}{\rho_{N_2}^0 + \rho_{O_2}^0} M_{O_2} \frac{i}{4F} = D_{c,H_2O(\text{eff})} \nabla \rho_{H_2O}^{\text{cathode}} 
\]

(104)

As was seen for the anode side it is also applied applicable to the cathode side that, the mass transfer flux and diffusivity in the electrode layer follow the same pattern as shown in the gas diffusion layers. Eventually, at any given current density I, the molar concentrations of species at the interface between the electrode and membrane are obtained for the cathode, and the partial pressures of reactants and production species at the interface are obtained for oxygen and the produced which can be seen in equations (105) and (106).

\[
p_{\text{int}}^{O_2} = \frac{\rho_{\text{int}}^{O_2}}{\rho_{\text{int}}^{O_2} + \rho_{\text{int}}^{N_2} + \rho_{\text{int}}^{H_2O,c} P_{\text{cathode}}} 
\]

(105)
To find the final partial pressures at the interface between cathode layer and membrane (ic) for oxygen and water on the cathode side the calculations must continue with finding the mix diffusivity in the gas diffusion layer. By utilizing the percentages of each component in the GDL and the ordinary diffusivities, the mix diffusivities can be found in equations (107), (108), and (109).

\[
P_{\text{int}}^{H_2O,c} = \frac{\rho_{\text{int}}^{H_2O,c}}{\rho_{\text{int}}^{\text{O}_2} + \rho_{\text{int}}^{\text{N}_2} + \rho_{\text{int}}^{H_2O,c}} P_{\text{cathode}}
\]  

To find the final partial pressures at the interface between cathode layer and membrane (ic) for oxygen and water on the cathode side the calculations must continue with finding the mix diffusivity in the gas diffusion layer. By utilizing the percentages of each component in the GDL and the ordinary diffusivities, the mix diffusivities can be found in equations (107), (108), and (109).

\[
D_{\text{O}_2,\text{mix}}^{\text{GDL}} = \frac{(1 - X_{\text{GDL}}^{\text{O}_2})}{\left(\frac{X_{\text{GDL}}^{\text{N}_2}}{D_{\text{O}_2,\text{N}_2}} + \frac{X_{\text{GDL}}^{H_2O,c}}{D_{\text{O}_2,H_2O}}\right)}
\]  

\[
D_{\text{N}_2,\text{mix}}^{\text{GDL}} = \frac{(1 - X_{\text{GDL}}^{\text{N}_2})}{\left(\frac{X_{\text{GDL}}^{\text{O}_2}}{D_{\text{N}_2,\text{O}_2}} + \frac{X_{\text{GDL}}^{H_2O,c}}{D_{\text{N}_2,H_2O}}\right)}
\]  

\[
D_{\text{H}_2\text{O},\text{mix}}^{\text{GDL}} = \frac{(1 - X_{\text{GDL}}^{H_2O,c})}{\left(\frac{X_{\text{GDL}}^{\text{N}_2}}{D_{\text{H}_2\text{O},\text{N}_2}} + \frac{X_{\text{GDL}}^{\text{O}_2}}{D_{\text{H}_2\text{O},\text{O}_2}}\right)}
\]  

The same process for finding the mix diffusivities is then repeated for the electrode on the cathode side of the fuel cell. This utilizes the electrode percentages and the same ordinary diffusivities used for the GDL. These electrode mix diffusivities are calculated in equations (110), (111), and (112).
Once the mix diffusivities are calculated the effective diffusivities need to be calculated for both the GDL and the electrode. The effective diffusivities utilize the general equation (36) where equations (113) through (115) are the calculations for the GDL, and equations (116) through (118) are the calculations for the electrode. (Sohn, 2011)

\[
D^{\text{Electrode}}_{O_2, \text{mix}} = \frac{\left(1 - X_{O_2}^{\text{Electrode}}\right)}{\left(X_{\text{Electrode}}^{N_2} + x_{\text{Electrode}}^{H_2O,c} / D_{O_2,N_2} + x_{\text{Electrode}}^{H_2O} / D_{O_2,H_2O}\right)}
\]  
\[
D^{\text{Electrode}}_{N_2, \text{mix}} = \frac{\left(1 - X_{N_2}^{\text{Electrode}}\right)}{\left(x_{\text{Electrode}}^{O_2} / D_{N_2,O_2} + x_{\text{Electrode}}^{H_2O,c} / D_{N_2,H_2O}\right)}
\]  
\[
D^{\text{Electrode}}_{H_2O,c, \text{mix}} = \frac{\left(1 - X_{H_2O,c}^{\text{Electrode}}\right)}{\left(x_{\text{Electrode}}^{N_2} / D_{H_2O,c,N_2} + x_{\text{Electrode}}^{O_2} / D_{H_2O,O_2}\right)}
\]

Before these effective diffusivities can be calculated the surface concentration must be calculated. This requires the mass transfer coefficient for both oxygen and water (on the
cathode side). This utilizes the general equation for the mass transfer equation (19), the general hydraulic diameter equation (20), and the bulk mix diffusivities in equations (93) and (95). These calculations are seen in equations (119) and (120) for oxygen and water, respectively. (O’Hayre, 2009)

\[ h_{\text{mass,}\text{O}_2} = Sh \frac{D_{\text{O}_2,\text{mix}}} {D_{h,c}} \]  \hspace{1cm} (119)

\[ h_{\text{mass,}\text{H}_2\text{O}} = Sh \frac{D_{\text{H}_2\text{O}\text{,c, mix}}} {D_{h,c}} \]  \hspace{1cm} (120)

Once the mass transfer coefficient is calculated for oxygen it can be used for the surface concentration calculation by the fact the unit area mass consumption rate of oxygen is equal in (65) and (68) which can be seen in equation (121). This allows for the surface concentration to be calculated for oxygen by rearranging the terms in equation (121) and by utilizing the equation (71) for \( \dot{n}_{\text{O}_2} \) to consolidate the equation. The end result would give the ratio of areas (B/A), due to the fact that the entire area (B) does not diffuse the fuel. The effective area (A) is incorporated so that the concentration at the surface is accurately calculated by increasing the concentration lost. This calculation is seen in equation (122). Since nitrogen is not consumed, the surface concentration is equal to the bulk flow concentration. The surface concentration of water on the cathode side uses the same relationship the oxygen does, but since water is being produced in this system it is added to the bulk flow as seen in equation (124). (O’Hayre, 2009)

\[ j_{\text{O}_2} = h_{\text{mass,}\text{O}_2} (\rho_{\text{O}_2} - \rho_{s,\text{O}_2}) = \frac{i}{4F} M_{\text{O}_2} \]  \hspace{1cm} (121)
For the average concentration calculations in the GDL and cathode for oxygen, nitrogen and water, the simple average calculations are completed in equations (125) through (126). These calculations utilize the surface (s), the interface between the gas diffusion layer and electrode layer (int), and the interface between the cathode layer and membrane (int). Since the calculation for the int concentration and ic concentration have not been done yet, an initial value is used. This requires the iteration process to be used which begins with equation (107) and ends with equation (148).

\[ \rho_{s}^{o_2} = \rho_{\infty}^{o_2} - \frac{\dot{n}_{o_2} M_{o_2}}{A h_{mass_{o_2}}} \]  \hspace{1cm} (122)

\[ \rho_{s}^{N_2} = \rho_{\infty}^{N_2} \]  \hspace{1cm} (123)

\[ \rho_{s}^{H_2O,C} = \rho_{\infty}^{H_2O,C} + \frac{\dot{n}_{H_2O,C} M_{H_2O}}{A h_{mass_{H_2O}}} \]  \hspace{1cm} (124)

\[ \rho_{GDL_{AVE}}^{o_2} = \frac{(\rho_{s}^{o_2} + \rho_{int}^{o_2})}{2} \]  \hspace{1cm} (125)

\[ \rho_{cathode_{AVE}}^{o_2} = \frac{(\rho_{int}^{o_2} + \rho_{ic}^{o_2})}{2} \]  \hspace{1cm} (126)

\[ \rho_{GDL_{AVE}}^{N_2} = \frac{(\rho_{s}^{N_2} + \rho_{int}^{N_2})}{2} \]  \hspace{1cm} (127)

\[ \rho_{cathode_{AVE}}^{N_2} = \frac{(\rho_{int}^{N_2} + \rho_{ic}^{N_2})}{2} \]  \hspace{1cm} (128)

\[ \rho_{GDL_{AVE}}^{H_2O,C} = \frac{(\rho_{s}^{H_2O,C} + \rho_{int}^{H_2O,C})}{2} \]  \hspace{1cm} (129)
To find the effective diffusivity in the gas diffusion layer with the convective velocity considered the generic equations (99), (100), and (101) are used. This is combined with the average concentration calculations in the GDL in equations (125), (126), and (127). The GDL effective diffusivity is calculated in equations (113), (114), and (115). These new effective diffusivities are calculated in equations (131), (132), and (133). This will be used to find the concentration between the GDL and cathode surface (int).

\[
\rho_{\text{cathode}_\text{AVE}}^{H_2O,C} = \frac{(\rho_{\text{int}}^{H_2O,C} + \rho_{\text{c}}^{H_2O,C})}{2}
\]  

(130)

\[
D_{c,O_2(\text{eff})}^{GDL} = D_{O_2(\text{eff})}^{GDL} \frac{\rho_{GDL,\text{AVE}}^{O_2} + \rho_{GDL,\text{AVE}}^{N_2} + \rho_{GDL,\text{AVE}}^{H_2O,C}}{\rho_{GDL,\text{AVE}}^{N_2} + \rho_{GDL,\text{AVE}}^{H_2O,C}}
\]  

(131)

\[
D_{c,N_2(\text{eff})}^{GDL} = D_{N_2(\text{eff})}^{GDL} \frac{\rho_{GDL,\text{AVE}}^{O_2} + \rho_{GDL,\text{AVE}}^{N_2} + \rho_{GDL,\text{AVE}}^{H_2O,C}}{\rho_{GDL,\text{AVE}}^{N_2} + \rho_{GDL,\text{AVE}}^{H_2O,C}}
\]  

(132)

\[
D_{c,H_2O,C(\text{eff})}^{GDL} = D_{H_2O,C(\text{eff})}^{GDL} \frac{\rho_{GDL,\text{AVE}}^{O_2} + \rho_{GDL,\text{AVE}}^{N_2} + \rho_{GDL,\text{AVE}}^{H_2O,C}}{\rho_{GDL,\text{AVE}}^{O_2} + \rho_{GDL,\text{AVE}}^{N_2}}
\]  

(133)

The same process implemented for the GDL effective diffusivity in the cathode, which considers convective velocity, is also used for the electrode diffusivity by considering convective velocity. This utilizes the cathode average concentrations and electrode effective diffusivities to get the electrode diffusivity considering convective velocity seen in equations (134), (135), and (136).
To find the concentration at the int interface (surface between GDL and cathode) for oxygen, the bulk concentration is used minus the components from the convective mass transport and the diffusion through the GDL. The diffusion components take into account both the consumption of oxygen and production of water. This is calculated in equation (137). For nitrogen the int concentration is comprised of the bulk nitrogen concentration and then the addition from the fact oxygen is being consumed and the loss due to water being produced seen in equation (138). The last int concentration is for the water component. This takes the bulk flow of water and adds the convective mass transport of water, plus the diffusion through the GDL for both produced water and consumed oxygen. This calculation is seen in equation (139). (O’Hayre, 2009)

\[
D^\text{electrode}_{c,O_2(\text{eff})} = D^\text{electrode}_{O_2(\text{eff})} \frac{\rho_{c,O_2} \rho_{\text{cathode}_{AVE}} + \rho_{N_2} \rho_{\text{cathode}_{AVE}} + \rho_{H_2O,c} \rho_{\text{cathode}_{AVE}}}{\rho_{\text{cathode}_{AVE}}} \\
D^\text{electrode}_{c,N_2(\text{eff})} = D^\text{electrode}_{N_2(\text{eff})} \frac{\rho_{c,O_2} \rho_{\text{cathode}_{AVE}} + \rho_{N_2} \rho_{\text{cathode}_{AVE}} + \rho_{H_2O,c} \rho_{\text{cathode}_{AVE}}}{\rho_{\text{cathode}_{AVE}}} \\
D^\text{electrode}_{c,H_2O,c(\text{eff})} = D^\text{electrode}_{H_2O,c(\text{eff})} \frac{\rho_{c,O_2} \rho_{\text{cathode}_{AVE}} + \rho_{N_2} \rho_{\text{cathode}_{AVE}} + \rho_{H_2O,c} \rho_{\text{cathode}_{AVE}}}{\rho_{\text{cathode}_{AVE}} + \rho_{N_2}}
\]  

To find the concentration at the int interface (surface between GDL and cathode) for oxygen, the bulk concentration is used minus the components from the convective mass transport and the diffusion through the GDL. The diffusion components take into account both the consumption of oxygen and production of water. This is calculated in equation (137). For nitrogen the int concentration is comprised of the bulk nitrogen concentration and then the addition from the fact oxygen is being consumed and the loss due to water being produced seen in equation (138). The last int concentration is for the water component. This takes the bulk flow of water and adds the convective mass transport of water, plus the diffusion through the GDL for both produced water and consumed oxygen. This calculation is seen in equation (139). (O’Hayre, 2009)

\[
\rho_{\text{int}}^{O_2} = \rho_{\infty}^{O_2} - \frac{\dot{n}_{O_2} M_{O_2}}{A h_{\text{mass}_{O_2}}} - \frac{t_{GDL}^{c,O_2(\text{eff})}}{A D_{GDL}^{c,O_2(\text{eff})}} \left[ \frac{\dot{n}_{H_2O,c} M_{H_2O} \rho_{GDL_{AVE}}^{O_2}}{(\rho_{GDL_{AVE}} + \rho_{GDL_{AVE}}^{H_2O,c})} + \dot{n}_{O_2} M_{O_2} \right] \\
\rho_{\text{int}}^{N_2} = \rho_{\infty}^{N_2} + \frac{t_{GDL}^{c,N_2(\text{eff})}}{A D_{GDL}^{c,N_2(\text{eff})}} \left( \dot{n}_{O_2} M_{O_2} - \dot{n}_{H_2O,c} M_{H_2O} \right)
\]
To find the concentration of oxygen at the interface between the cathode and the membrane (ic) the int concentration is used minus the loss due to the electrode thickness. This loss includes the diffusion component with the rate of oxygen consumed and the component with the rate of water produced. This is due to the concentration loss across a material which is the contribution due to diffusion through a material. This calculation is displayed in equation (140). The concentration of nitrogen at the ic surface uses the concentration of nitrogen at the int surface, and the components due to diffusion through the electrode layer. In the case of nitrogen, the component from the rate of oxygen consumed is added while the component from the rate of water produced is subtracted. The calculation of nitrogen at the ic surface is shown in equation (141). The last concentration is for water at the ic surface. Just like oxygen and nitrogen, the concentration starts with the previous concentration at the int surface for water with the modification due to diffusion through the electrode layer. With this case, both the components of diffusion due to water and oxygen are added. This is due to the fact that water is being produced at the cathode and that oxygen is being consumed which causes the other concentrations to increase in reference. This calculation is shown in equation (142). (O’Hayre, 2009)
Once the concentration has been calculated in the GDL and \( \text{ic} \), the new fraction of each component can be calculated in the GDL as seen in equations (143), (144), and (145) for oxygen, nitrogen, and water respectively. This can also be done for the electrode where the calculations are displayed in equations (146), (147), and (148). These are the last calculations included in the iteration process. The system goes through twenty iterations to ensure the concentrations converge on a single value. There are checks taken in the calculations to ensure the values don’t diverge.

\[
\rho_{\text{ic}}^{O_2} = \rho_{\text{int}}^{O_2} - \frac{t_{\text{electrode}}^{c, O_2(\text{eff})}}{AD_{\text{electrode}}^{c, O_2(\text{eff})}} \left[ \frac{\dot{n}_{H_2O,c}^{O_2} M_{H_2O} \rho_{\text{cathode AVE}}^{O_2}}{(\rho_{\text{cathode AVE}}^{N_2} + \rho_{\text{cathode AVE}}^{H_2O,c})} + \dot{n}_{O_2} M_{O_2} \right] \tag{140}
\]

\[
\rho_{\text{ic}}^{N_2} = \rho_{\text{int}}^{N_2} + \frac{t_{\text{electrode}}^{c, N_2(\text{eff})}}{AD_{\text{electrode}}^{c, N_2(\text{eff})}} \left( \dot{n}_{O_2} M_{O_2} - \dot{n}_{H_2O,c} M_{H_2O} \right) \tag{141}
\]

\[
\rho_{\text{ic}}^{H_2O,c} = \rho_{\text{int}}^{H_2O,c} + \frac{t_{\text{electrode}}^{c, H_2O,c(\text{eff})}}{AD_{\text{electrode}}^{c, H_2O,c(\text{eff})}} \left[ \dot{n}_{H_2O,c} M_{H_2O} + \frac{\dot{n}_{O_2} M_{O_2} \rho_{\text{cathode AVE}}^{H_2O,c}}{(\rho_{\text{cathode AVE}}^{N_2} + \rho_{\text{cathode AVE}}^{O_2})} \right] \tag{142}
\]

\[
X_{\text{GDL}}^{O_2} = \frac{\rho_{\text{GDL AVE}}^{O_2} / M_{O_2}}{\rho_{\text{GDL AVE}}^{O_2} / M_{O_2} + \rho_{\text{GDL AVE}}^{N_2} / M_{N_2} + \rho_{\text{GDL AVE}}^{H_2O,c} / M_{H_2O}} \tag{143}
\]

\[
X_{\text{GDL}}^{N_2} = \frac{\rho_{\text{GDL AVE}}^{N_2} / M_{N_2}}{\rho_{\text{GDL AVE}}^{O_2} / M_{O_2} + \rho_{\text{GDL AVE}}^{N_2} / M_{N_2} + \rho_{\text{GDL AVE}}^{H_2O,c} / M_{H_2O}} \tag{144}
\]
Calculation of the fraction at ic for oxygen, water, and nitrogen are then computed and are displayed in equations (149), (150), and (151). These fraction calculations are then used to find the partial pressure due to oxygen and water seen in equations (152) and (153). This is simply the fraction multiplied by the total pressure in the cathode and these will be used in combination with the hydrogen pressure to find the electromotive force calculated in equation (158).
\[ X_{lc}^{O_2} = \frac{\rho_{lc}^{O_2}}{\rho_{lc}^{O_2} + \rho_{lc}^{N_2}/M_{N_2} + \rho_{lc}^{H_2O,c}/M_{H_2O}} \] (149)

\[ X_{lc}^{N_2} = \frac{\rho_{lc}^{N_2}}{\rho_{lc}^{O_2}/M_{O_2} + \rho_{lc}^{N_2}/M_{N_2} + \rho_{lc}^{H_2O,c}/M_{H_2O}} \] (150)

\[ X_{lc}^{H_2O,c} = \frac{\rho_{lc}^{H_2O,c}}{\rho_{lc}^{O_2}/M_{O_2} + \rho_{lc}^{N_2}/M_{N_2} + \rho_{lc}^{H_2O,c}/M_{H_2O}} \] (151)

\[ P_{lc}^{O_2} = X_{lc}^{O_2} \ast P_c \] (152)

\[ P_{lc}^{H_2O,c} = X_{lc}^{H_2O,c} \ast P_c \] (153)

<table>
<thead>
<tr>
<th>Physical property or Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas diffusion layer thickness</td>
<td>380 micrometers</td>
</tr>
<tr>
<td>Electrode layer thickness</td>
<td>10 micrometers</td>
</tr>
<tr>
<td>Membrane thickness</td>
<td>60 micrometers</td>
</tr>
<tr>
<td>GDL Porosity</td>
<td>0.7</td>
</tr>
<tr>
<td>Electrode Porosity</td>
<td>0.4</td>
</tr>
<tr>
<td>Faraday Constant, F</td>
<td>96485 C/mol</td>
</tr>
<tr>
<td>Cas Constant, R</td>
<td>8.314 J/mol/K</td>
</tr>
</tbody>
</table>

Table 4: Physical Properties and parameters
3.6 Activation Polarization

Activation overpotential in most of the research work referenced utilized the Butler-Volmer equation seen in equations (154) and (155). (Sohn, 2011)

\[ i_a = i_{0,a}^{ex} \left( \frac{C_{H_2}}{C_{H_2}^{ref}} \right)^{1/2} \frac{2F}{RT} \eta_a \]  (154)

\[ i_c = i_{0,c}^{ex} \left( \frac{C_{O_2}}{C_{O_2}^{ref}} \right) \exp \left( - \frac{\alpha_c F}{RT} \eta_c \right) \]  (155)

\( \eta \) is the overpotential at each electrode and is determined by the relationship seen in equation (156). (Sohn, 2011)

\[ \eta = \varphi_s - \varphi_e - \varphi_{eq} \left( \varphi_{eq,a} = 0, \varphi_{eq,c} = V_0 \right) \]  (156)

In the journal article “Three-dimensional model of a 50 cm² high temperature PEM fuel cell Study of the flow channel geometry influence,” by J. Lobato the exchange current density for the cathode is determined by the Arrenius-like law where the reference temperature is 353K, the reference exchange current density is \( 1.78 \times 10^{-6} \) A m\(^{-2} \), and the \( E_{A,ex}/R \) is 16456 K which is visible in equation (157). (Lobato, 2010)

\[ i_{0,c}^{ex} = i_{0,c,ref}^{ex} \exp \left[ - \frac{E_{A,ex}}{R} \left( \frac{1}{T} - \frac{1}{T_{ref,i_c}} \right) \right] \]  (157)
3.7 Ohmic Polarization

The ohmic polarization inside the fuel cell is due to the layer resistances and the contact resistances that exist. The current conduction route from a typical anode-side current collector to a cathode-side current collector can be discretized into multiple segments, and an equivalent network circuit can be created as shown in Figure 16. This is used to calculate the ohmic losses in the fuel cell. This method is similar to the one used for the solid oxide fuel cell.

![Figure 16: PEM Fuel Cell Electrical Circuit](image-url)
The contact resistance is determined by the topography of the contacting pair of materials which will cause a voltage drop across the interface. The contact area between the two materials is directly affected by the roughness of the two contacting surfaces. Membrane ionic conductivity depends on the membrane being used and for the PBI membrane the ionic conductivity ranges from 1.7 to 9.825 depending on the amount of doping and the manufacturer. Before the cell voltage is calculated the electromotive force and the losses due to activation polarization are applied. Electromotive force is calculated through the Nernst equation in equation (158). (Mench, 2008)

\[
E = E^0 + \frac{RT}{2F} \ln \left[ \left( \frac{P_{H_2}}{P^0} \right) \left( \frac{P_{O_2}}{P^0} \right)^{0.5} \left( \frac{P_{H_2O}}{P^0} \right) \right] \tag{158}
\]

Where \( E^0 \) is the standard state electromotive force, and it is \( -\Delta G^0 \) related. We obtain a linear relationship between \( E^0 \) and temperature by curve fitting which can be seen in equation (159). (O’Hayre, 2009)

\[
E^0 = -0.000243 \times (T) + 1.257115 \tag{159}
\]

The potential gradient inside the membrane is taken as the electromotive force including both the standard state and the contribution due to partial pressure of each gas as well as the influence of activation polarization. This can be seen in equation (160) which is incorporated into the ohmic analysis.

\[
\bar{E} = E - \eta_{act,c} - \eta_{act,a} \tag{160}
\]
The actual output voltage of the fuel cell is the potential gradient between the cathode and anode current collectors. This is done by assuming the anode current collector potential is zero, calculating the network circuit node potential using Kirchhoff’s first law. To obtain the cell output voltage the cathode current collectors voltage is used. The numbered nodes can be seen in Figure 17. This final cell voltage takes into consideration concentration polarization, activation polarization, and ohmic polarization. The following equations (177) through (194) are the eighteen node analysis equations used to solve the ohmic circuit. With eighteen equations and eighteen unknowns (V1 through V18) this allows matrix analysis to be used to solve for the voltage at node 18 which is the cell’s output voltage. Before the eighteen node analysis occurs the values for the resistances must be defined or calculated. This begins with the definition that a resistance from node x to y is equal to the resistance from node y to x. This is visually represented in equation (161). In Table 5 the values for contact resistances used in the model are given. In Table 6 the values for resistivity used in the model are given. Both Table 5 and Table 6 are used to calculate the resistance from each node to another.
### Table 5: Contact Resistances

<table>
<thead>
<tr>
<th>Name of Contact Resistances</th>
<th>Value (ohm*m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{\text{con_current_GDL_a}}$</td>
<td>0.001e-6</td>
</tr>
<tr>
<td>$R_{\text{con_current_GDL_c}}$</td>
<td>0.001e-6</td>
</tr>
<tr>
<td>$R_{\text{con_GDL_anode}}$</td>
<td>0.001e-6</td>
</tr>
<tr>
<td>$R_{\text{con_GDL_cathode}}$</td>
<td>0.001e-6</td>
</tr>
</tbody>
</table>

### Table 6: Resistivity Values

<table>
<thead>
<tr>
<th>Name of Resistivity</th>
<th>Value (ohm*m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{\text{GDL_a}}$</td>
<td>0.0189e-2</td>
</tr>
<tr>
<td>$R_{\text{GDL_c}}$</td>
<td>0.0189e-2</td>
</tr>
<tr>
<td>$R_{\text{anode}}$</td>
<td>1.754e-2</td>
</tr>
<tr>
<td>$R_{\text{cathode}}$</td>
<td>1.754e-2</td>
</tr>
<tr>
<td>$R_{\text{electrolyte}}$</td>
<td>$\frac{1}{I_{\text{on_con}}}$</td>
</tr>
</tbody>
</table>

Each node resistance is calculated incorporating values from Table 5 or Table 6 and the dimensions of the channel that contribute to the resistance value. Reference to Figure 17 can help clarify the dimensions used for each calculation. All the resistance calculations can be seen in equations (162) to (176). Where equations (162), (163), (166), (167), (173), and (174) are the contact resistances and the rest are the resistances...
in the GDL, anode, cathode, and electrolyte. The calculations of the resistances close to the end have a dimension modifier of \( \text{lr}_a \) or \( \text{lr}_c \).

\[
R_{1.2} = \frac{R_{\text{con.current.GDL.a}}}{\text{lr}_a \times ll/2}
\]

\[
R_{17.18} = \frac{R_{\text{con.current.GDL.c}}}{\text{lr}_c \times ll/2}
\]

\[
R_{2.4} = R_{\text{GDL.a}} \times 0.5 \times \left( \frac{l_{w_a}/6 + \text{lr}_a/2}{t_{\text{GDL}} \times ll} \right)
\]

\[
R_{4.6} = R_{6.8} = R_{\text{GDL.a}} \times 0.5 \times \left( \frac{l_{w_a}/6}{t_{\text{GDL}} \times ll} \right)
\]

\[
R_{2.3} = \frac{R_{\text{con.GDL.anode}}}{ll \times 0.5 \times \left( l_{w_a}/6 + \text{lr}_a/2 \right)}
\]

\[
R_{4.5} = R_{6.7} = R_{8.9} = \frac{R_{\text{con.GDL.anode}}}{ll \times 0.5 \times l_{w_a}/3}
\]

\[
R_{3.5} = R_{\text{anode}} \times 0.5 \times \left( \frac{l_{w_a}/6 + \text{lr}_a/2}{t_{\text{electrode}} \times ll} \right)
\]
\[ R_{5.7} = R_{7.9} = R_{\text{anode}} \times \frac{(lw_a/6)}{(t_{\text{electrode}} \times ll)} \]  \hspace{1cm} (169)

\[ R_{9.10} = R_{7.12} = R_{5.14} = R_{\text{electrolyte}} \times \frac{t_{\text{electrolyte}}}{(ll \times lw_a/6)} \]  \hspace{1cm} (170)

\[ R_{10.12} = R_{12.14} = R_{\text{cathode}} \times \frac{(lw_c/6)}{(t_{\text{electrode}} \times ll)} \]  \hspace{1cm} (171)

\[ R_{14.16} = R_{\text{cathode}} \times 0.5 \times \frac{(lw_c/6 + lr_c/2)}{(t_{\text{electrode}} \times ll)} \]  \hspace{1cm} (172)

\[ R_{10.11} = R_{12.13} = R_{14.15} = \frac{R_{\text{con GDL cathode}}}{ll \times 0.5 \times (lw_c/3)} \]  \hspace{1cm} (173)

\[ R_{16.17} = \frac{R_{\text{con GDL cathode}}}{ll \times 0.5 \times (lw_c/6 + lr_c/2)} \]  \hspace{1cm} (174)
\[ R_{11,13} = R_{13,15} = R_{GDL,c} \times 0.5 \times \left( \frac{lw_c/6}{t_{GDL} \times ll} \right) \] (175)

\[ R_{15,17} = R_{GDL,c} \times 0.5 \times \left( \frac{lw_c/6 + lr_c/2}{t_{GDL} \times ll} \right) \] (176)

Figure 17: PEM Fuel Cell Electrical Circuit with numbered nodes
\[ V1 = 0 \] \tag{177} 

\[ \frac{1}{R_{1,2}} V1 - \left( \frac{1}{R_{1,2}} + \frac{1}{R_{2,3}} + \frac{1}{R_{2,4}} \right) V2 + \frac{1}{R_{2,3}} V3 + \frac{1}{R_{2,4}} V4 = 0 \] \tag{178} 

\[ \frac{1}{R_{2,3}} V2 - \left( \frac{1}{R_{2,3}} + \frac{1}{R_{3,5}} \right) V3 + \frac{1}{R_{3,5}} V5 = 0 \] \tag{179} 

\[ \frac{1}{R_{2,4}} V2 - \left( \frac{1}{R_{2,4}} + \frac{1}{R_{4,5}} + \frac{1}{R_{4,6}} \right) V4 + \frac{1}{R_{4,5}} V5 + \frac{1}{R_{4,6}} V6 = 0 \] \tag{180} 

\[ \frac{1}{R_{3,5}} V3 + \frac{1}{R_{4,5}} V4 - \left( \frac{1}{R_{4,5}} + \frac{1}{R_{5,7}} + \frac{1}{R_{5,14}} \right) V5 + \frac{1}{R_{5,7}} V7 + \frac{1}{R_{5,14}} V14 = \frac{1}{R_{5,14}} \bar{E} \] \tag{181} 

\[ \frac{1}{R_{4,6}} V4 - \left( \frac{1}{R_{4,6}} + \frac{1}{R_{6,7}} + \frac{1}{R_{6,8}} \right) V6 + \frac{1}{R_{6,7}} V7 + \frac{1}{R_{6,8}} V8 = 0 \] \tag{182} 

\[ \frac{1}{R_{5,7}} V5 + \frac{1}{R_{6,7}} V6 - \left( \frac{1}{R_{5,7}} + \frac{1}{R_{6,7}} + \frac{1}{R_{7,9}} + \frac{1}{R_{7,12}} \right) V7 + \frac{1}{R_{7,9}} V9 + \frac{1}{R_{7,12}} V12 = \frac{1}{R_{7,12}} \bar{E} \] \tag{183} 

\[ \frac{1}{R_{6,8}} V6 - \left( \frac{1}{R_{6,8}} + \frac{1}{R_{8,9}} \right) V8 + \frac{1}{R_{8,9}} V9 = 0 \] \tag{184} 

\[ \frac{1}{R_{7,9}} V7 + \frac{1}{R_{8,9}} V8 - \left( \frac{1}{R_{7,9}} + \frac{1}{R_{8,9}} + \frac{1}{R_{9,10}} \right) V9 + \frac{1}{R_{9,10}} V10 = \frac{1}{R_{9,10}} \bar{E} \] \tag{185} 

\[ \frac{1}{R_{9,10}} V9 - \left( \frac{1}{R_{9,10}} + \frac{1}{R_{10,11}} + \frac{1}{R_{10,12}} \right) V10 + \frac{1}{R_{10,11}} V11 + \frac{1}{R_{10,12}} V12 = -\frac{1}{R_{9,10}} \bar{E} \] \tag{186}
\frac{1}{R_{10,11}} V_{10} - \left( \frac{1}{R_{10,11}} + \frac{1}{R_{11,12}} \right) V_{11} + \frac{1}{R_{11,12}} V_{12} = 0 \quad (187)

\frac{1}{R_{7,12}} V_{7} + \frac{1}{R_{10,12}} V_{10} - \left( \frac{1}{R_{7,12}} + \frac{1}{R_{10,12}} + \frac{1}{R_{12,13}} + \frac{1}{R_{12,14}} \right) V_{12}
+ \frac{1}{R_{12,13}} V_{13} + \frac{1}{R_{12,14}} V_{14} = -\frac{1}{R_{7,12}} \bar{E} \quad (188)

\frac{1}{R_{11,13}} V_{11} + \frac{1}{R_{12,13}} V_{12} - \left( \frac{1}{R_{11,13}} + \frac{1}{R_{12,13}} + \frac{1}{R_{13,15}} \right) V_{13} + \frac{1}{R_{13,15}} V_{15} = 0 \quad (189)

\frac{1}{R_{5,14}} V_{5} + \frac{1}{R_{12,14}} V_{12} - \left( \frac{1}{R_{5,14}} + \frac{1}{R_{12,14}} + \frac{1}{R_{14,16}} + \frac{1}{R_{14,15}} \right) V_{14}
+ \frac{1}{R_{14,15}} V_{15} + \frac{1}{R_{14,17}} V_{17} = -\frac{1}{R_{5,14}} \bar{E} \quad (190)

\frac{1}{R_{13,15}} V_{13} + \frac{1}{R_{14,15}} V_{14} - \left( \frac{1}{R_{13,15}} + \frac{1}{R_{14,15}} + \frac{1}{R_{15,17}} \right) V_{15}
+ \frac{1}{R_{15,17}} V_{17} = 0 \quad (191)

\frac{1}{R_{14,16}} V_{14} - \left( \frac{1}{R_{14,16}} + \frac{1}{R_{16,17}} \right) V_{16} + \frac{1}{R_{16,17}} V_{17} = 0 \quad (192)

\frac{1}{R_{15,17}} V_{15} + \frac{1}{R_{16,17}} V_{16} - \left( \frac{1}{R_{15,17}} + \frac{1}{R_{16,17}} + \frac{1}{R_{17,18}} \right) V_{17} + \frac{1}{R_{17,18}} V_{18} = 0 \quad (193)
\[
\frac{1}{R_{17.18}} V_{17} - \frac{1}{R_{17.18}} V_{18} = I 
\]
4 RESULTS

4.1 Model Verification

To verify the numerical model, a comparison to data from “A Mathematical model of a PEMFC using a PBI membrane” by Denver Cheddie was used. (Cheddie, 2006) The model closely represents the experimental data given. Figure 18 shows the performance of the PEMFC with only an air source and utilizes the parameters given by the reference paper. The model slightly underestimates the performance in the lower currents while closely modeling the performance at higher currents. The largest error from the model value to the experimental data was about 4.4%. With error being built into the actual data itself this 4.4% error can be expected and should not hurt the validity of the model. Overall from this validation with existing data the model can then be used to optimize the channels.

![Model vs Cheddie](image)

Figure 18: IV Curve for verification of model versus (Cheddie, 2006) experimental data
4.2 Model Channel Optimization

For testing the numerical model for optimization the first step was to begin with a one to one ratio of the rib width to the channel width. With the inclusion of the capabilities for machining in house with a limit to a channel about .8 or larger, three different sizes were chosen being 1mm, 1.5mm and 2mm. The I vs. V curve with a constant flow rate can be seen in Figure 19 where the best output was due to the smallest size of 1mm rib to 1mm channel. It is also known that larger pressure drops can occur in serpentine flow channels, so by the channel size, the pressure drop that can occur will be limited. With this same output the power curve was plotted and can be seen in Figure 20, which also demonstrates that the smallest size is optimum for the fuel cell. Other factors can be investigated as well in terms of channel optimization.

![Current vs. Voltage (50% channel to rib)](image)

Figure 19: Voltage Output for 1:1 ratio of channel width to rib width
From Figure 19 and Figure 20 it was found that the smaller the channel the better, we can then test the ratio of the rib to the channel. When the one to one ratio was used, that graph gave the best case as a total width of 2.0mm, which was applied to the model parameters. For this set of analysis the total width 2.0mm is fixed but the rib to total width percentage is varied. The one to one ratio is applied again (50% rib) as well as a 40% rib and a 60% rib. This can be seen in Figure 21 for the I vs V curve where this makes a much more substantial impact to the results than the width alone. The overall trend is smaller the rib with a larger channel gives improved performance while still keeping the total width on the smaller side. This is a 40% rib (.8mm) and a 60% channel.
(1.2mm). This result can also be seen in the power graph showing the 40% rib greatly exceeding the 50% rib result in Figure 22.

Figure 21: Voltage Output for varying ratio of rib to channel with total being 2.0mm

Figure 22: Power Output for varying ratio of rib to channel with total being 2.0mm
To even further investigate what ratio and channel size would optimize the system, the size limit of both the rib and channel must be considered. There are manufacturing and pressure limits for the channel width and there are structural integrity limits for the rib size. As stated before, the limit for the channel is .8mm due to the manufacturability in our machine shop and the limit for the rib is .6mm. With improved manufacturing abilities these limits could be modified, but pressure must still be kept in mind. In Figure 23, a forty percent ratio of the rib width to total width (channel plus rib) is kept constant while the total width is adjusted. As the size gets smaller the performance improves, as we saw in the 50% ratio of Figure 19. This reaffirms the finding that the ratio of the rib width to the total width produces a more significant impact on the performance than the size of the channels alone. Figure 23 and Figure 24 are the I vs V and Power curves for the 40% ratio of rib to total width.
Figure 23: IV curve 40% ratio of rib to total with small rib sizes

Figure 24: Power curve 40% ratio of rib to total with small rib sizes
Since the ratio of rib to total area produces a larger impact on the performance of the fuel cell this could be even further optimized. In the final analysis for the given system the rib is fixed at .6mm (which is our set limit) and the percentage is adjusted from 40% to 30% by 5% increments. This analysis can be seen in Figure 25 and Figure 26 for the IV curve and Power curve, respectively. This shows how the smallest percentage of 30% gives the best result. However, the improvement from 50% to 40% in Figure 21 and Figure 22 is much more substantial than the improvement from 40% to 30% seen in Figure 25 and Figure 26. With this small improvement to 30%, further percentages do not need to be tried since the improvement will be minimal and the rib will become structurally unstable if made much smaller.

Figure 25: IV Curve .6mm rib varying ratio of rib to total
Figure 26: Power Curve .6mm rib varying ratio of rib to total.
4.3 Experimental Results

4.3.1 Setup

For the experimental setup of the testing materials and apparatus, the overall setup can be seen in Figure 27. This has the hydrogen tank flowing through the flow regulator to the mass flow meter. It then flows through metal tube into the oven to preheat the gas. From there it is sent through the distributor to then flow into the fuel cell. The other side is the filtered air which flows through the regulator to the mass flow meter. It then flows into the metal tube through the oven to be preheated. Upon leaving the oven it flows through the distributor, and into the fuel cell. The flow is setup to be countercurrent flow for this test. The two multi-meters are also connected to the system to measure the output voltage and current. Current is not measured directly, but by using a variable resistor and measuring the voltage the current is calculated. To get the current density the total current is divided by the active area of the fuel cell. The cell voltage is measured directly from the fuel cell to diminish losses through the wires of the other circuit.
For the fuel cell setup, the membrane, gasket, fuel channels, and current collectors are needed. The membrane can be seen in Figure 28 where the active area is $24\text{mm}^2$ and is a Celtec P membrane from BASF.
Figure 28: PBI Membrane

The fuel channels and gasket are pictured in Figure 29. The channel on the left is 1mm deep for the hydrogen flow on the anode side, and the channel on the right is 1.5mm deep for the air on the cathode side. The channel is machined into high grade graphite. The gasket is made of Viton from Eagle Elastomer and cut to fit the plates and membrane.
The pictures of the fuel cell assembly in Figure 30 and Figure 31 show the entire cell put together including the two graphite flow channels with gasket, the membrane, the current collector plates, and the outside backing plates.
Figure 30: Assembly Isometric View
Figure 31: Assembly Top View
Figure 32 shows one of the two mass flow meters used for measuring the flow of either hydrogen or air. This picture is taken while the system is off. In Figure 33 the multi-meters are shown where the unit on the left is used to find the current density, and the handheld unit is directly applied to the graphite plates to read the voltage of the cell.
In Figure 34, the metal tube setup in the oven is shown. The fuel cell sits atop the oven where a square whole is cutout and allows heat from the oven to stabilize the temperature of the fuel cell. Figure 35 further shows the assembly on top if the oven with the flow going through the distributors. The distributors allow for the flow to be split and run into a 4 fuel cell stack. It is plugged for this case to test a single fuel cell.
Figure 34: Flow Heating Setup with Assembly above
Figure 35: Assembly and Flow Distributors
4.3.2 Data Results

For this experimental setup, only low current densities could be tested with the resistance controller available. This test utilizes a total width of a fuel cell of 1.8mm with the rib being .8mm wide giving a percentage of 44%. This test is at 175°C with the air preheated before entering the heated fuel cell assembly. The results can be seen in Figure 36. With the model data versus the experimental data the largest percent error calculated is 2.8% which can be attributed to the uncertainty in the fuel cell temperature, mass flow meters, and multi-meters. This data helps verify again that the model does match physical experimental data for the performance of the fuel cell.

![Data vs Model](image)

Figure 36: Experimental Results versus model at 175°C
5 SUMMARY & CONCLUSION

In previous studies, it was found that using a temperature over 100°C with appropriate materials for a proton exchange membrane fuel cell can help with some issues found in the low temperature PEM fuel cells. Those being carbon monoxide poisoning of the fuel cell, water management, and fuel cell kinetics. Even though all of these have been improved with high temperature fuel cells, the cell degradation over time is still a major issue being worked on today by research which is developing more stable materials. Another study showed that the serpentine flow channel yields the best results, but causes significant pressure drops. Using serpentine flow channels and material properties from previous studies, a numerical model for the optimization of the geometry of the flow channels was developed.

Overall, the model was verified in two different methods. The first by checking the model to published experimental data, and the second by checking the model to an experiment conducted in-house. Both verified that the model can predict the performance of the high temperature fuel cell with small error. To further verify the model more experiments could be done in-house with more accurate equipment, improved materials, and with a fuel cell stack instead of a single cell test. Further research could include expanding the model to include prompted input of parameters from the user, expanding to display more results and calculate the results for a fuel cell stack.
The results show that, in general, the smaller the channel width, the higher the performance of the fuel cell will be. The more important result was that the percentage of the rib width to the total width affects the performance more than how small the channel is itself. It was found that about a 30% rib to total width gives the optimum performance for the fuel cell. By taking the smallest rib width manufacturable and making this 30% of the total width, optimum fuel cell performance will result. This optimization is for this specific fuel cell size, material, and temperature. The model can be modified for the fuel cell size, the material properties, and the temperature so it can work for many different fuel cell systems.
REFERENCES


