CHAPTER 6

Numerical simulation of proton exchange membrane fuel cell

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Abstract

This chapter presents general mathematical models and numerical simulation for proton exchange membrane fuel cell (PEMFC) to evaluate the effects of various designs and operating parameters on the PEMFC performance. Both one and two-dimensional models are presented; the advantages and weaknesses of using one-dimensional and two-dimensional models are discussed in detail. Subsequently, a general three-dimensional model is developed and described in detail. This three-dimensional general model accounts for electrochemical kinetics, current density distribution, hydrodynamics, and multi-component transport. It starts from basic transport equations including mass conservation, momentum equations, energy balance, and species concentration in different elements of the fuel cell sandwich, as well as the equations for the phase potential in the membrane and the catalyst layers. These governing equations are coupled with chemical reaction kinetics by introducing various source terms. It is found that all these equations are in a very similar form except the source terms. Based on this observation, all the governing equations can be solved using the same numerical formulation in a single domain without prescribing the boundary conditions at interfaces between different elements of the fuel cell. Detailed numerical formulations are presented in this chapter. Various parameters, such as velocity field, local current density distribution, species concentration variation along the flow channel, under various operation conditions are computed by solving these governing equations in a single domain consisting of gas channel, catalyst layer and membrane. The performance of the PEMFC affected by various parameters such as temperature, pressure, and the thickness of the membrane is investigated. The numerical results are further validated with experimental data, which are available in the literature. This general three-dimensional model can be used for the optimization of PEMFC design and operation. It can also serve as a building block for the modeling and understanding of PEMFC stacks and systems.
1 Introduction

Although the fuel cell has received much attention in recent years, the underlying concept is still under heavy investigations [1]. The general concept of fuel cell operations can be characterized as gas-mixtures transport and transformation of species by electrochemical reactions. Therefore, one of the most challenging problems in fuel cell research is to predict the performance of the fuel cell. Using a mathematical model with numerical procedures to simulate the transport phenomena is a powerful tool to understand the fundamental physical and chemical processes of a fuel cell. Thus, reliable mathematical models are essential for fuel cell design, operation and optimization.

2 One-dimensional (1-D) model

The earliest attempts to simulate the phenomena in PEM fuel cells were mainly using 1-D models. The pioneering work in 1-D modeling includes Savinell and Fritts [2], Ridge [3], Fritts and Savinell [4], Yang [5], Verbrugge and Hill [6], Bernardi and Verbrugge [7], and Springer [8]. These earliest works mostly considered water and thermal management. During PEM fuel cell operations, water molecules are carried from the anode side to cathode side of the membrane by electro-osmosis. If this transport rate of water is higher than that by back diffusion of water, the membrane will become dehydrated and too resistive to conduct current. On the other side, if there is too much water, i.e. cathode side flooding may occur in the pores of the gas diffuser and hinder the transportation of reactants to the catalyst side. Consequently, proper water management is required to maintain high membrane conductivity and prevent flooding. Moreover, the effect of reacting gas dilution by high vapor pressure must be taken into consideration [1]. Thus, the water management is critical for efficient performance. Verbrugge and Hill [6] have carried out extensive modeling of transport properties in perfluorosulfonate ionomers based on dilute solution theory. False [9] reported an isothermal water map based on hydraulic permeability and electro-osmotic drag data. Fuller and Newman [10] applied concentrated solution theory and employed literature data on transport properties to produce a general description of water transport in fuel cell membranes. Bernardi and Verbrugge [7] took a different approach, in which transport through the gas diffusion electrodes was considered. They assumed the membrane to be uniformly hydrated, corresponding to an “ultra-thin membrane” case. Springer [8] presents an isothermal model, which includes transport through the porous electrodes. Their model required inputs from calculated diffusivities, which are needed to correct for porosity, and from experimentally determined transport parameters for the transport through the membrane. Most of these models treated flow channel as being perfectly well fixed, with no pressure and concentration difference along the gas channel. These research works were particularly useful in classifying the different models for porous gas diffusion electrodes and providing the key properties of the membrane required for numerical simulation. These 1-D models provided the sub-model bases for many following 2-D or 3-D research works.
Here, we introduce a general 1-D PEM fuel cell model based on the research work by Bernardi and Verbrugge [7].

2.1 General 1-D model

2.1.1 Model description

The fuel cell consists of a membrane sandwiched between two gas-diffusion electrodes as shown in Fig. 1. The gas-diffusion electrodes are porous composites made of electronically conductive material mixed with hydrophobic polytetrafluorethylene and supported on carbon cloth. The gaseous reactants can transport through the electrodes during operation. The electrochemical reactions occur in the catalyst layer. Humidified hydrogen enters anode gas chamber, transports through the anode gas diffuser, and dissolves into catalyst layer. Hydrogen molecule is oxidized and generates protons and electrons. Protons go into membrane and electrons are received by carbon conductor. The overall electrochemical reaction can be expressed as:

\[
2H_2 \leftrightarrow 4H^+ + 4e^-.
\]  

(1)

Gaseous reactant \( O_2 \) from air, usually mixed with \( H_2O \), enters into cathode gas channel, transports through porous gas diffuser, and dissolves into cathode catalyst layer. Hydrogen protons diffuse into the cathode catalyst layer from anode catalyst layer through the membrane. On the surface of the catalyst particles, the oxygen is consumed along with the protons and electrons, and the product, \( H_2O \), is produced along with the waste heat. The overall electrochemical reactions occurring at the reaction site may be represented as:

\[
4H^+ + 4e^- + O_2 \rightarrow 2H_2O + \text{heat}.
\]  

(2)

Therefore, the overall electrochemical reaction of the PEM fuel cell is:

\[
2H_2 + O_2 \rightarrow 2H_2O + \text{heat} + \text{electric energy}.
\]  

(3)

Figure 1: Schematic diagram of PEMFC.
The proton, dissolved oxygen, and dissolved hydrogen concentrations depend on the kinetic expressions of four-electron-transfer reaction for oxygen reduction and the proton-transfer reaction for hydrogen oxidation.

### 2.1.2 Model assumptions

The cell is assumed to operate at steady state conditions. Since the cell thickness is very small compared with the other dimensions of the cell, a one-dimensional approximation is used in the model formulation. The entire system is taken to be at constant temperature, and the gases are assumed to be ideal and well mixed in the chambers. The steady state and isothermal assumptions are valid because these conditions are often achieved in a small single-cell experimental investigation. The model requires some properties inputs such as water-diffusion coefficients, electro-osmotic drag coefficients, water sorption isotherms, and membrane conductivities, which are all measured in single-cell experimental studies. The temperature of fuel cell is assumed to be well controlled. The heat transfer is supposed to be very efficient so that the heat generation, which is due to the irreversibility of the electrochemical reaction, ohmic resistance, as well as mass transport overpotentials, can be taken out quickly. The inlet gaseous temperature is assumed to be preheated to the cell temperature. Fully hydrated membrane, wet gas diffuser, and saturated chamber gases are considered.

The total gas pressure within the gas channel is assumed to be constant and same as the pressure in gas diffuser since the gas velocity is very slow, the pressure variation can be neglected along the gas channel. However, the pressure can vary between anode and cathode.

With these assumptions the cell model is formulated with transport equations for the electrodes, catalyst layers and membrane as described below.

### 2.1.3 Governing equations

The governing equations constituting the mathematical model of the PEM fuel cell are derived by applying the conservation equations for an ideal gas in porous medium, the Butler-Volmer equations, and the Stefan-Maxwell equation for gas-phase transport.

**Electrodes:**

**Continuity:**

\[
\frac{d}{dx}(\rho v) = 0. \tag{4}
\]

**Species:**

\[
\frac{d}{dx}(\rho_i v + \rho_i V_i) = m_i. \tag{5}
\]

**Potential:**

\[
\frac{d}{dx}(\Phi_e) = -\frac{I}{\sigma_{\text{eff}}}. \tag{6}
\]

where \( \rho_i \) is the partial density of species \( i \), \( \rho \) is average density, \( v \) is the mass-averaged velocity in \( x \) direction, \( V_i \) is the species \( i \) diffusion velocity, \( m_i \) is the mass...
of species $i$, $\Phi_s$ is the electrical potential in the solid matrix of the electrode, $I$ is cell current density, and $\sigma_{\text{eff}}$ is the effective electrical conductivity. The diffusion velocity $V_i$ can be determined from the Stefan-Maxwell equation for multi-component gas diffusion,

$$\nabla x_i = \sum_j \left( \frac{x_i x_j}{D_{ij}^{\text{eff}}} \right) (V_j - V_i), \quad (7)$$

where $D_{ij}^{\text{eff}}$ is the effective binary diffusion coefficient for species $i$ in $j$, and $x_i$ is the mole fraction for species $i$. Species $i$ for cathode electrode can be taken as $O_2$, $N_2$ and $H_2O$; species $i$ for anode electrode can be taken as $H_2$ and $H_2O$.

### 2.1.4 Catalyst layers

The catalyst layers are very thin compared to the other components in PEMFC, but they are the heart of the fuel cell. Electrochemical reaction occurs in this region to produce electrical energy and products. In this region, the transfer of mass and energy is coupled with reaction kinetics when the cell is loaded and results in a potential difference between electrodes. How this potential difference varies as functions of mass transfer, electrode kinetics, and energy flux determines the fuel cell performance. The mathematical description of the active-catalyst-layer region is based on Butler-Volmer relations \[13, 14\] for electrochemical reaction and species diffusion. The macro-homogeneous approach is used in developing the governing equations. Current in the catalyst layer can transfer to electronically-conductive solid portion of the catalyst layer (carbon and catalyst particles). The rate of electrochemical reaction is given by the Butler-Volmer expression \[13, 14\]. The mass transfer is modeled by using species conservation and Fick’s Law of diffusion. The governing equations can be expressed as follows:

$$\frac{di}{dx} = -aj_{0}^{\text{ref}} \left( \frac{C_{O_2}}{C_{O_2}^{\text{ref}}} \right) \exp \left( -\frac{\alpha_c F \eta_c}{RT} \right), \quad (8)$$

where $i$ is the current density, $a$ is the catalyst reactive surface area per unit volume, $j_{0}^{\text{ref}}$ is the reference exchange current density at the reference concentration $C_{\text{ref}}$, $C_{O_2}$ is the oxygen concentration, $\alpha_c$ is the transfer coefficients in Butler-Volmer relation, $F$ is the Faraday’s number, $R$ is the universal gas constant, $\eta_c$ is the over-potential at cathode side, and $T$ is the reaction temperature.

From the material balance based on standard porous-electrode theory, we have:

$$\frac{dN_i}{dx} = -s_i \frac{di}{nF dx}, \quad (9)$$

where $N_i$ is the superficial flux of species $i$, and $s_i$ is the stoichiometric coefficient for species $i$ in the cathode reaction and anode reaction. The right hand side of eqn (9) is the source term for the species conservation equation as shown below.

For hydrogen:

$$D_{H_2}^{\text{eff}} \frac{d^2C_{H_2}}{dx^2} = v \frac{dC_{H_2}}{dx} + \frac{di}{dx} \left( s_{H_2} \right). \quad (10)$$
For oxygen:
\[
D_{\text{eff}} \frac{d^2 C_{\text{O}_2}}{dx^2} = v \frac{dC_{\text{O}_2}}{dx} + \frac{di}{dx} \left( \frac{\text{sO}_2}{n\text{F}} \right),
\]  
(11)

For H\text{H}_2\text{O}:
\[
D_{\text{H}_2\text{O}} \frac{d^2 C_{\text{H}_2\text{O}}}{dx^2} = v \frac{dC_{\text{H}_2\text{O}}}{dx} + \frac{di}{dx} \left( \frac{-s\text{H}_2\text{O}}{n\text{F}} \right).
\]  
(12)

Potential:
\[
i = -\sigma_{\text{eff}} \frac{d\Phi}{dx},
\]  
(13)

where \(i\) is the current density in the electron-conducting solid, and \(\sigma_{\text{eff}}\) is the conductivity of the electronically conductive catalyst layer.

### 2.1.5 Membrane

The membrane of PEM fuel cell acts as the hydrogen proton conductor. The transport processes in the membrane can be described by the conservation of species. The flux of species in the membrane is determined by the net effect of electro-osmotic drag, diffusion due to concentration gradient, and the convection due to a pressure gradient. A form of the Nernst-Planck equation is used to describe the flux of species in the membrane [15, 16].

\[
N_i = -z_i F \frac{D_i}{RT} \frac{dC_i}{dx} = D_i \frac{dC_i}{dx} + v C_i,
\]  
(14)

where \(N_i\) is the superficial flux of species \(i\), \(z_i\) is charge number of species \(i\), \(C_i\) is the concentration of species \(i\), and \(D_i\) is the diffusion coefficient of species \(i\), and \(\Phi_m\) is electrical potential in membrane. \(v\) is the velocity of H\text{H}_2\text{O}, which is generated by electric potential and pressure gradient, and can be described by a form of Schögl’s equation:

\[
v = \frac{k_\Phi}{\mu} z_f c_f F \frac{d\Phi_m}{dx} - \frac{k_p}{\mu} \frac{dp}{dx},
\]  
(15)

where \(k_\Phi\) is electro-kinetic permeability, \(\mu\) is pore-fluid viscosity, \(z_f\) is fixed-site charge, \(c_f\) is fixed-charge concentration, and \(k_p\) is hydraulic permeability.

Current conservation:
\[
\frac{di}{dx} = 0.
\]  
(16)

Mass conservation for liquid flow:
\[
\frac{dv}{dx} = 0.
\]  
(17)

Electric potential:
\[
\frac{d\Phi}{dx} = -\frac{i}{\sigma} + \frac{F}{\sigma} c_{H^+},
\]  
(18)

\[
\sigma = \frac{F^2}{RT} D_{H^+} c_{H^+}.
\]  
(19)
Numerical simulation of proton exchange membrane fuel cell

Furthermore, the potential and pressure profiles throughout the membrane region are assumed to be linear with constant velocity. This is basically true for fully-developed porous media case.

2.1.6 Boundary conditions

Before solving the governing equations, appropriate boundary conditions must be specified. The temperature, pressure, relative humidity, flow rate, compositions of the reactant gases both in anode and cathode channels are specified according to the cell operation condition.

In the following model description, \( c_- \) is the anode catalyst layer, \( c_+ \) is the cathode catalyst layer, \( d_- \) is the anode gas diffuser; \( d_+ \) is the cathode gas diffuser, and \( m \) is membrane. \( l_{c_-} \) is the thickness of anode catalyst layer, \( l_{c_+} \) is the thickness of cathode catalyst layer, \( l_m \) is the thickness of membrane, \( l_{d_-} \) is the thickness of anode gas diffuser, \( l_{d_+} \) is the thickness of cathode gas diffuser. At the interface between the anode gas diffuser and catalyst layer, the solid phase potential gradient is related to the cell operating current density by Ohm’s law:

\[
i = \left. \frac{d\Phi_m}{dx} \right|_{c_-} \sigma_{c_-}^\text{eff}, \tag{20}\]

where \( \sigma_{c_-}^\text{eff} \) is electronic conductivity of anode catalyst layer.

The membrane concentration of oxygen set to be zero as,

\[
c_{O_2} = 0. \tag{21}\]

Since the hydraulic pressure distribution throughout the anode gas diffuser is linear, we can impose the boundary condition of pressure at the interface between anode gas diffuser and catalyst layer as:

\[
p_o = p_- - \frac{\mu}{k_p} l_{d_-} v_{s}^{d_-}, \tag{22}\]

where \( p_- \) is the pressure in anode gas chamber, \( k_p \) is anode gas diffuser permeability, and \( v_{s}^{d_-} \) is water velocity in anode gas diffuser.

Because the total water flux is continuous, we have

\[
C_w v_{s}^{d_-} + N_w^{d_-} = C_w \varepsilon_m \varepsilon_w v_{c_-} c_{c_-}, \tag{23}\]

where \( N_w^{d_-} \) is water vapor flux from Stefan-Maxwell equation [17], which is

\[
N_w^{d_-} = -\frac{I}{2F} \left. \frac{x_{w,\text{sat}}}{1 - x_{w,\text{sat}}^m} \right|_{c_-}, \tag{24}\]

where

\[
x_{w,\text{sat}} = \frac{p_{w,\text{sat}}}{p_-}. \tag{25}\]
The concentration of hydrogen is given by

\[ c_{H_2}^{\text{sat}} = (1 - x_m^{\text{sat}}) \frac{P}{K_{H_2}}. \]  

(26)

At the interface between the membrane and anode catalyst-layer, the current continuity should be satisfied:

\[ \sigma_m \frac{d \Phi}{dz} \bigg|_{m} = \sigma_{c+}^{\text{eff}} \frac{d \Phi}{dz} \bigg|_{c+}. \]  

(27)

The superficial flux of liquid water is continuous:

\[ v_m = \varepsilon_m^{c+} v_{c+}. \]  

(28)

and the flux of dissolved hydrogen is continuous through the internal boundary:

\[ D_{H_2} \frac{dc_{H_2}}{dx} \bigg|_{m} = D_{H_2}^{\text{eff}} \frac{dc_{H_2}}{dx} \bigg|_{c+}. \]  

(29)

At the membrane/cathode-catalyst-layer interface, the current, superficial flux of liquid water, and the flux of dissolved oxygen are continuous, and the dissolved hydrogen concentration is zero.

\[ \sigma_m \frac{d \Phi}{dz} \bigg|_{m} = \sigma_{c+}^{\text{eff}} \frac{d \Phi}{dz} \bigg|_{c+}, \]  

(30)

\[ v_m = \varepsilon_m^{c+} v_{c+}. \]  

(31)

\[ D_{O_2} \frac{dc_{O_2}}{dx} \bigg|_{m} = D_{O_2}^{\text{eff}} \frac{dc_{O_2}}{dx} \bigg|_{c+}, \]  

(32)

\[ c_{H_2} = 0. \]  

(33)

At the cathode-catalyst-layer/gas-diffuser interface, the current in the solid phase is continuous.

\[ \sigma_{c+}^{\text{eff}} \frac{d \Phi_{\text{solid}}}{dx} \bigg|_{c+} = \sigma_{d+} \frac{d \Phi_{\text{solid}}}{dx} \bigg|_{d+}. \]  

(34)

and the superficial flux of water is given by

\[ \rho v_d^{d+} + h_d^{d+} = \rho \varepsilon_m^{c+} \varepsilon_m^{w} v_{c+}, \]  

(35)

where

\[ N_{w}^{d+} = \frac{I}{4F} \frac{x_{w}^{\text{sat}}}{1 - x_{w}^{\text{sat}} - x_{N_2} + \frac{x_{N_2}}{r_w}}. \]  

(36)

and \( r_w \) is the diffusivity ratio given by

\[ r_w = \frac{D_{w-N_2}}{D_{w-O_2}}. \]  

(37)
Numerical simulation of proton exchange membrane fuel cell

The concentration of dissolved-oxygen in the catalyst layer is given by

\[ c_{\text{sat}}^\text{O}_2 = (1 - x_{\text{N}_2} - x_{\text{w}}}^\text{sat} p_+ K_{\text{O}_2}, \tag{38} \]

where \( K_{\text{O}_2} \) is Henry's constant, and

\[ x_{\text{w}}}^\text{sat} = \frac{p_{\text{w}}}^\text{sat} p_+. \tag{39} \]

2.1.7 Results and discussion

Ticianelli et al. [11] and Srinivasan et al. [18] published their experimental results respectively. Their experimental data have been used extensively as standard validation by many numerical studies such as Bernardi and Verbrugge [7]. Since most of the numerical simulation parameters and properties are based on their experimental results, these parameters and properties are adopted in this chapter. Table 1 shows the detailed physical parameters and properties.

Figure 2 shows the comparison of Bernardi and Verbrugge’s [7] calculated results with Ticianelli’s experimental data [11]. Note that, in their model the exchange-current density \( a_+ r^\text{ref} \) was adjusted to yield model results that are suitable mimic the experimental results. With this one adjustable parameter, the agreements between model and experimental results are quite good.

Figure 3 shows the components of the overall cell polarization for the base case. At the low current densities (less than 100 mA/cm\(^2\)), the activation overpotential of the oxygen reduction reaction is almost entirely responsible for the potential losses of the cell. For current densities greater than 200 mA/cm\(^2\), the ohmic potential loss due to the membrane and electrodes become more significant, and the cathode activation overpotential reaches a relatively constant value.

Figure 4 shows the effect of membrane thickness on the potential. Generally, the electronic conductivity is proportional to the thickness of the membrane. The results show the fuel cell potential increases as the membrane thickness decreases from 7 mil (1 mil = 1/1000 inch) to 2 mil under dry membrane state.

The modeling value for the wet membrane thickness was obtained by assuming that the ratio of the wet to dry thickness was a constant. The comparison between experimental results (not shown) and model predictions is generally satisfactory.

The effect of cathode pressurization on the fuel cell potential is depicted in Fig. 5. When the cathode pressure decreases from 5 to 3 atm, the open-circuit potential is only slightly affected by the change in cathode pressure. The cell potential decrease is primarily due to oxygen mole fraction decreased because of lower pressure; this leads to the increase in cathode activation overpotential loss.

2.1.8 Summary

1-D model provides a good preliminary foundation for PEM fuel cell modeling. These 1-D models base on the fundamental transport properties where the potential losses incurred by the activation overpotential of the anode and cathode reactions,
Table 1: The values of the parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wet membrane thickness, ( l_m )</td>
<td>0.023 cm</td>
</tr>
<tr>
<td>Gas diffuser thickness, ( l_d )</td>
<td>0.026 cm</td>
</tr>
<tr>
<td>Catalyst layer thickness, ( l_c )</td>
<td>0.001 cm</td>
</tr>
<tr>
<td>Relative humidity of inlet air</td>
<td>100%</td>
</tr>
<tr>
<td>Relative humidity of inlet hydrogen</td>
<td>100%</td>
</tr>
<tr>
<td>Inlet fuel and air temperature, ( T_0 )</td>
<td>105 °C</td>
</tr>
<tr>
<td>Cell temperature, ( T )</td>
<td>80 °C</td>
</tr>
<tr>
<td>Inlet nitrogen-oxygen mole ratio</td>
<td>0.79/0.21</td>
</tr>
<tr>
<td>Air-side pressure, ( p_+ )</td>
<td>5 atm</td>
</tr>
<tr>
<td>Fuel-side pressure, ( p_- )</td>
<td>3 atm</td>
</tr>
<tr>
<td>Thermodynamic open-circuit potential, ( U )</td>
<td>1.194 V</td>
</tr>
<tr>
<td>Estimated proton diffusion coefficient, ( D_{H^+} )</td>
<td>( 4.5 \times 10^{-5} ) cm²/s</td>
</tr>
<tr>
<td>Estimated ionic conductivity, ( \sigma_m )</td>
<td>0.17 ohm/cm</td>
</tr>
<tr>
<td>Fixed charge site concentration, ( c_f )</td>
<td>( 1.2 \times 10^{-3} ) mol/cm³</td>
</tr>
<tr>
<td>Charge of fixed site, ( z_f )</td>
<td>-1</td>
</tr>
<tr>
<td>Dissolved oxygen diffusivity, ( D_{O_2} )</td>
<td>( 1.2 \times 10^{-6} ) cm²/s</td>
</tr>
<tr>
<td>Electrokinetic permeability, ( k_{\Phi} )</td>
<td>( 1.13 \times 10^{-15} ) cm²</td>
</tr>
<tr>
<td>Hydraulic permeability, ( k_p )</td>
<td>( 1.58 \times 10^{-14} ) cm²</td>
</tr>
<tr>
<td>Pore-fluid (water) viscosity, ( \mu )</td>
<td>( 3.565 \times 10^{-4} ) kg/m·s</td>
</tr>
<tr>
<td>Pore-fluid (water) density, ( \rho )</td>
<td>( 0.054 ) mol/cm³</td>
</tr>
<tr>
<td>Saturated water vapor pressure, ( \rho_{sat} )</td>
<td>0.467 atm</td>
</tr>
<tr>
<td>Henry’s law constant for oxygen in membrane, ( K_{O_2} )</td>
<td>( 2 \times 10^5 ) atm·cm³/mol</td>
</tr>
<tr>
<td>Henry’s law constant for hydrogen in membrane, ( K_{H_2} )</td>
<td>( 4.5 \times 10^4 ) atm·cm³/mol</td>
</tr>
<tr>
<td>Volume fraction membrane in active layer, ( \epsilon_{m,c} )</td>
<td>0.5</td>
</tr>
<tr>
<td>Volume fraction water in membrane, ( \epsilon_{w,m} )</td>
<td>0.28</td>
</tr>
<tr>
<td>Electronic conductivity, ( \sigma_{eff}^d = \sigma_{eff}^c )</td>
<td>0.53 ohm/cm</td>
</tr>
<tr>
<td>Reference kinetic parameter of anode, ( a_{g_{H^+}}^{ref} )</td>
<td>( 1.4 \times 10^5 ) A/cm³</td>
</tr>
<tr>
<td>Reference kinetic parameter of cathode, ( a_{f_{O_2}}^{ref} )</td>
<td>( 1 \times 10^{-5} ) A/cm³</td>
</tr>
<tr>
<td>Cathodic transfer coefficient, ( \alpha_c )</td>
<td>2</td>
</tr>
<tr>
<td>Anodic transfer coefficient, ( \alpha_a )</td>
<td>( 1/2</td>
</tr>
<tr>
<td>( H^+ ) reference concentration, ( c_{H^+}^{ref} )</td>
<td>( 1.2 \times 10^{-3} ) mol/cm³</td>
</tr>
<tr>
<td>( O_2 ) reference concentration, ( c_{O_2}^{ref} )</td>
<td>( 3.39 \times 10^{-6} ) mol/cm³</td>
</tr>
<tr>
<td>( H_2 ) reference concentration, ( c_{H_2}^{ref} )</td>
<td>( 5.64 \times 10^{-3} ) mol/cm³</td>
</tr>
</tbody>
</table>

and the ohmic losses incurred by the membrane. The membrane is assumed fully hydrated and the cell is assumed isothermal. However, it cannot model the depletion of the reactants and the accumulation of products in the flow direction.

### 2.2 General 2-D model

Two-dimensional (2-D) models are developed to improve the earlier 1-D models. Fuller and Newman [19] modeled and solved the transport across the fuel cell...
Figure 2: Model and experimental data for fuel cell at 80 °C, $p_+ = 5$ atm, $p_- = 3$ atm.

Figure 3: The contribution of fuel cell.

sandwich at certain location along the gas channel and then integrated in the second direction. In this 2-D model, the gas outside the gas diffusers was assumed to have uniform composition in the direction across the cell. Nguyen and White [20], Amphlett et al. [21], and Yi and Nguyen [22] developed pseudo 2-D models accounting for composition changes along the flow path. These models are useful for small single cells, however, when it is applied to large-scale fuel cells, particularly under high fuel utilization conditions, the applicability is limited.
Later, Gurau et al. [23] presented a 2-D model of transport phenomena in PEM fuel cells. They developed a model to understand the transport phenomena such as the oxygen and water distributions. They considered the interaction between the gas channels and the rest of the fuel cell sandwich. Yi and Nguyen [24] also formulated a 2-D model to explore hydrodynamics and multi-component transport in the cathode.
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Figure 6 shows a typical 2-D PEM fuel cell. It includes the collector plates, fuel and gas channels, gas-diffusers, catalyst layers and membrane. Hydrogen and water vapor flow through anode fuel channel and humidified air is fed into the cathode channel. Assume that hydrogen oxidation and oxygen reduction reactions occur only within active catalyst layers.

Additional assumptions of this 2-D model are described below:

- The gas mixtures including anode channel and cathode channel are ideal gases. The density is treated as constant.
- The gas flows are laminar and incompressible.
- The electrodes, gas diffusers, catalyst layers, and membrane are isotropic and homogeneous.
- The heat generated under reversible condition is neglected.
- Only steady state condition is considered.
- Cell temperature is held constant.
- The contact electrical potential drop of different cell components is negligible.

2.2.2 Mathematical model

A single-domain approach developed by Um et al. [24] is used in this section to describe fuel cell transport processes. Therefore, no boundary conditions are required at the interface of different fuel cell components.
The governing equations can be written as:

**Mass conservation:**
\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \tag{40}
\]

**Momentum conservation:**
\[
\frac{1}{\varepsilon \rho} \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\varepsilon}{\varepsilon} \frac{\partial P}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + S_x, \tag{41}
\]
\[
\frac{1}{\varepsilon \rho} \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\varepsilon}{\varepsilon} \frac{\partial P}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + S_y. \tag{42}
\]

**Species conservation:**
\[
\frac{1}{\varepsilon} \left( u \frac{\partial X_k}{\partial x} + v \frac{\partial X_k}{\partial y} \right) = \varepsilon D_k \left( \frac{\partial^2 X_k}{\partial x^2} + \frac{\partial^2 X_k}{\partial y^2} \right) + S_k. \tag{43}
\]

**Charge conservation:**
\[
\frac{\partial}{\partial x} \left( \sigma_m \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \sigma_m \frac{\partial \Phi}{\partial y} \right) + S_{\Phi} = 0, \tag{44}
\]
where \( \varepsilon \) is porosity (for gas channel \( \varepsilon \) equals 1), \( S \) is the source term.

Table 2 shows the values for different region of fuel cell. \( X_k \) is the mole fraction of species \( k \), \( D_k \) is diffusivity of species \( k \).
Numerical simulation of proton exchange membrane fuel cell current densities defined by the Bulter-Volmer equations:

\[ j_a = a j_0^{\text{ref}} \left( \frac{X_{O_2}}{X_{O_2}^{\text{ref}}} \right) \left[ \exp \left( \frac{\alpha_a F}{RT} \eta_a \right) - \exp \left( -\frac{\alpha_a F}{RT} \eta_c \right) \right], \quad (45) \]

\[ j_c = a j_0^{\text{ref}} \left( \frac{X_{H_2}}{X_{H_2}^{\text{ref}}} \right)^{1/2} \left[ \exp \left( \frac{\alpha_a F}{RT} \eta_a \right) - \exp \left( -\frac{\alpha_c F}{RT} \eta_c \right) \right], \quad (46) \]

where \( \sigma_m \) is the proton conductivity in the membrane, which was correlated by Springer et al. [8] as:

\[ \sigma_m = \exp \left( 1268 \left( \frac{1}{303} - \frac{1}{T} \right) \right) (0.005139 \lambda - 0.00326). \quad (47) \]

The water content \( \lambda \), in eqn (47) can be expressed as follows [25]:

\[ \lambda = 0.043 + 17.81A - 39.85A^2 + 36A^3 \quad \text{for } 0 < A < 1, \]

\[ \lambda = 14 + 1.4(A - 1) \quad 1 \leq A \leq 3. \quad (48) \]

Note that \( A \) is defined as the vapor activity at the cathode gas diffuser catalyst layers interface assuming thermodynamic equilibrium, which is given by:

\[ A = \frac{X_m p}{p^{\text{sat}}}. \quad (49) \]

Here \( X_m \) is the water vapor molar fraction. The saturated water partial pressure, \( p^{\text{sat}} \) is expressed by the following empirical equation.

\[ \log_{10} p^{\text{sat}} = -2.1794 + 0.2953T - 9.1837 \times 10^{-5}T^2 + 1.4454 \times 10^{-7}T^3. \quad (50) \]

Once the electrical potential is determined in the membrane, the local current density can be calculated by:

\[ i(y) = -\sigma_m \frac{\partial \Phi_m}{\partial x} \big|_{\text{interface}}. \quad (51) \]

Then the averaged current density is determined as follows:

\[ i_{\text{avg}} = \frac{1}{L} \int_{\text{mem}} i(y) dy. \quad (52) \]

The cell voltage can be calculated as:

\[ E = E_0 - |\eta_a| - |\eta_c| - i_{\text{avg}}/\sigma_m, \quad (53) \]

where \( E_0 \) is the reference open-circuit potential of the fuel cell, which can be expressed as a function of temperature [25]:

\[ E_0 = 0.0025T + 0.2329. \quad (54) \]
2.2.3 Boundary conditions
The boundary conditions for \( u, v, p, X_{\text{H}_2}, X_{\text{H}_2O}, X_{\text{O}_2}, \Phi_c \) at inlet of the channel are fixed.

\[
\begin{align*}
    u_{\text{in,anode}} &= u_0^-, \quad v_{\text{in,anode}} = 0, \quad u_{\text{in,cathode}} = u_0^+, \quad v_{\text{in,cathode}} = 0, \\
    p_{\text{in,anode}} &= p_0^-, \quad p_{\text{in,cathode}} = p_0^+, \quad X_{\text{H}_2O,\text{anode}} = X_{\text{H}_2O}^o^- \\
    X_{\text{H}_2O,\text{cathode}} &= X_{\text{H}_2O}^o^+
\end{align*}
\]

where superscript or subscript \( o^- \) and \( o^+ \) represent inlet condition at anode and cathode, respectively.

All velocities at solid walls are set to be zero due to no-slip conditions. The boundary condition for the electric potential is no-flux everywhere along the boundaries of computational domain. At the outlet, both channels are assumed sufficiently long that the velocity and species concentration are fully developed.

2.2.4 Numerical procedures
Gurau et al. [23] solved these governing equations in three different domains: the cathode gas channel-gas diffuser-catalyst layer for air mixture, the cathode gas diffuser-catalyst layer-membrane-anode catalyst layer-gas diffuser for liquid water, and the anode gas channel-gas diffuser-catalyst layer for hydrogen. The continuity equations and momentum equations for the gas mixture were solved first in the coupled gas channel and gas diffuser domains. Then the species concentration equations together with the Butler-Volmer equations were solved iteratively. After convergence is achieved, the transport equations related to water vapor flow as well as the equations for cell potential and current density can be solved. Since the source term and boundary conditions for the two domains have to be matched at the interface, new level iterations have to be introduced. When they solved the electrochemical cell efficiency, they assumed the total overpotential first and then calculated the transfer current density together with other unknowns. Once the correct current density is found, the ohmic losses can be calculated, and the cell potential is set to be the open potential minus the sum of the total over-potential, and the total ohmic losses.

Um et al. [25] solved the governing equations in a single domain. Although some species are practically non-existing in certain regions of a fuel cell, the species transport equations can still be applied throughout the entire computational domain by using the large source term technique, which is often assigned a sufficiently large source term in this sub-region, that effectively freezes the non-exsiting species mole fraction to zero.

2.2.5 Results and discussion
Figure 7 shows the basic profile of fuel cell potential-current density characteristics for a 2-D model solution [26]. The potential loss generally has three sources: (1) activation polarization (act), (2) ohmic polarization (ohm), and (3) concentration polarization (conc). The activation polarization loss is dominant at low current...
Numerical simulation of proton exchange membrane fuel cell

Figure 7: Fuel cell voltage-current density.

Figure 8: Effect of the gas diffuser porosity on the voltage-current density characteristic.

density. At this point, electronic barriers have to be overcome prior to current and ion flow. Activation losses increase slightly as current increases. Ohmic polarization (loss) varies directly with current, increasing over the whole range of current because cell resistance remains essentially constant when temperature does not change too much. Gas transport losses occur over the entire range of current density, but these losses become prominent at high limiting currents where it becomes difficult to provide enough reactant flow to the cell reaction sites.

Figure 8 demonstrated the effect of gas diffuser porosity on fuel cell performance presented by Gurau et al. [23]. In their work, an isothermal condition at $T = 353 \, K$ and an inlet air velocity $U_0 = 0.35 \, m/s$ with 100% humidity were assumed. For lower values of porosity, lower values of the limiting current density were found. The cell performance in the region where the concentration over-potentials are predominant was also predicted.
Figure 9: Effect of the air inlet velocity on the performance.

Figure 9 presents the current density for different air inlet velocity at the cathode gas channel, assuming the gas diffuser porosity $\varepsilon = 0.4$ and a constant temperature $T = 353$ K with 100% humidity. For higher inlet air velocity, more oxygen is fed; therefore, more oxygen is likely to arrive at the catalyst layer, with the result of a higher limiting current density. This is explained by the fact that for the same pressure field, the axial momentum transfer across the gas channel-gas diffuser interface becomes more important for higher velocities. This is a consequence when more “fresh” air is able to arrive at the catalyst layer. For the inlet air velocity higher than approximately 2 m/s, the limiting current becomes constant, which shows that there is a limiting effect of the momentum transfer across the gas channel-gas diffuser interface.

Figure 10 shows the oxygen mole fraction field in the cathode gas channel-gas diffuser coupled domain for a case of current density $I_{\text{avg}} = 2.89 \times 10^{3}$ A/m², $U_i = 0.35$ m/s, and $T = 353$ K (iso-thermal case) with humidity = 100%. The oxygen is consumed in the catalyst layer. The mole fraction is decreased along the flow direction. The oxygen consumption depends on the operating current density. The higher current density, the more oxygen is consumed, thus, the faster mole fraction decreases along the flow direction. A limiting current density may occur when the oxygen or hydrogen is completely depleted at the reaction surface. The hydrogen mole fraction field in the anode gas channel-gas diffuser coupled domain has a similar distribution as the oxygen distribution in cathode side. In the present model, it is assumed that water only exists in the vapor state. However, if the electrochemical reaction rate is sufficiently high, the amount of water produced is condensed into liquid phase. Under this situation, two-phase flow model has to be considered.

2.2.6 Concluding remarks
The 2-D model is a significant improvement over the 1-D models and could provide simulations that are more realistic. It can predict the transport phenomena in the
numerical simulation of proton exchange membrane fuel cell 233

2.3 Three-dimensional (3-D) model

Recently, a few research groups extended 2-D model to 3-D model such as Shim-palee and Dutta [27], Zhou and Liu [28], Um and Wang [29], and Jen et al. [30]. One of the major improvements of the 3-D model over the 2-D model is its ability to study the blocking effect of the collector plates and the effectiveness of the interdigitated flow field [31]. Here we introduce a generalized 3-D model as well as some numerical approaches and results. To solve the 3-D model, many different numerical method have been used such as CD-Star [24], FLUENT [27], Semi-Implicit Method [28], and Vorticity-Velocity Method [30]. In this section, 3-D formulations are developed in such a way that they allow using the same code for solving the Navier-Stokes equations of the gas channel, gas diffuser and catalyst layers in a coupled domain. The potential equation and species concentration equations are solved in a single domain of the whole fuel cell. The solutions of the hydrodynamics of the flow and polarization curves are analyzed and presented in details. The results of this study may be beneficial for further and more complete analyses of the performance of fuel cells.

2.3.1 Model development

A typical PEM fuel cell configuration is shown in Fig. 11. The physical fuel cell model consists of anode gas channel, anode gas diffuser that formed by porous

Figure 10: Oxygen distribution in the cathode gas channel and gas diffuser.
media, anode catalyst layer, membrane, cathode catalyst layer, cathode gas diffuser, and cathode gas channel. In reality, when the fuel cell works, fuel and oxidant can be viewed as a steady, laminar, developing forced convection flow in an isothermal rectangular channel, and penetrating through the gas diffuser to catalyst layers. In the model presented here, the flow is assumed to be steady, constant properties, and incompressible. The viscous dissipation, compression work and buoyancy are assumed negligible. The gas mixtures are considered as perfect gases, and the species concentrations are considered as constant at the inlet of the channel. The concentrations along the gas channel and the gas-diffuser will vary due to diffusion-convection transport and electron kinetics in catalyst layers, and the distributions will depend on the gas properties and reaction rate. Water transport in and out of the electrodes is assumed to be in the form of vapor only. This assumption may be questionable in this model, in particular when the reactants flow into the gas channel under saturated conditions. The water generation rate is very likely to exceed its removal rate and thus condensation formed in the cathode. As a result, two-phase flow forms in the cathode channel. This complex case is, however, neglected in this chapter. The gas-diffuser, catalyst layers, and the membrane materials are considered as isotropic porous media. Contraction of the porous media is also neglected.

2.3.2 Mathematical model

The governing equations base on conservation of mass, momentum, energy and species.

The model governing equations can be written as:

Mass conservation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (55)$$
Momentum conservation:

\[
\frac{\rho}{\varepsilon} \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = -\varepsilon \frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + S_x,
\]

(56)

\[
\frac{\rho}{\varepsilon} \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = -\varepsilon \frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + S_y,
\]

(57)

\[
\frac{\rho}{\varepsilon} \left( u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = -\varepsilon \frac{\partial p}{\partial z} + \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + S_z.
\]

(58)

Species conservation:

\[
\frac{1}{\varepsilon} \left( u \frac{\partial X_k}{\partial x} + v \frac{\partial X_k}{\partial y} + w \frac{\partial X_k}{\partial z} \right) = \varepsilon D_k \left( \frac{\partial^2 X_k}{\partial x^2} + \frac{\partial^2 X_k}{\partial y^2} + \frac{\partial^2 X_k}{\partial z^2} \right) + S_k.
\]

(59)

Charge conservation:

\[
\frac{\partial}{\partial x} \left( \sigma_m \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \sigma_m \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \sigma_m \frac{\partial \Phi}{\partial z} \right) + S_\Phi = 0,
\]

(60)

where \( \varepsilon \) is porosity, for gas channel \( \varepsilon \) equals 1, for gas diffuser \( \varepsilon = \varepsilon_d \), for catalyst layer \( \varepsilon = \varepsilon_c \), and for membrane \( \varepsilon = \varepsilon_m \), and \( S \) is the source term. Table 3 shows the source terms for different region of fuel cell.

The parameters of above governing equations are the same as the 2-D model. The boundary conditions and numerical procedures are similar to the 2-D case and will not repeat here.

Here we introduce a new method, which was used by Jen et al. [30], to simplify the 3-D model by making the usual parabolic assumption. With the parabolic assumption, the diffusion term in axial direction such as \( \frac{\partial^2 u}{\partial z^2} \), \( \frac{\partial^2 v}{\partial z^2} \), \( \frac{\partial^2 w}{\partial z^2} \), as well as \( \frac{\partial^2 X_k}{\partial z^2} \) can be neglected. Furthermore, the modified pressure \( P \) may be defined as

\[
P(x, y, z) = p(z) + p^*(x, y),
\]

(61)

where \( p(z) \) is the pressure over the cross section at each axial location, and \( p^*(x, y) \) is the pressure variation in the \( x, y \) direction, which drives the secondary flow. Pressure gradient for axial direction:

\[
\frac{\partial P}{\partial z} = \frac{\partial p}{\partial z} + \frac{\partial p^*}{\partial z},
\]

(62)

where \( \frac{\partial p}{\partial z} \gg \frac{\partial p^*}{\partial z} \) is due to the useful parabolic assumption. So the axial pressure gradient can be written as:

\[
\frac{\partial P}{\partial z} = \frac{\partial p}{\partial z} = f(z).
\]

(63)
Table 3: Source terms for the above governing equations.

<table>
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<tr>
<th>Source Term</th>
<th>Value</th>
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And we also have:

\[
\frac{\partial P}{\partial x} = \frac{\partial p^*}{\partial x},
\]

(64)

\[
\frac{\partial P}{\partial y} = \frac{\partial p^*}{\partial y},
\]

(65)

With the above parabolic flow assumptions, it is now possible to simply march through the computational domains in the main flow direction without worrying about the downstream conditions as those in elliptic flow cases. A novel vorticity-velocity method was used here to solve this problem. The axial vorticity function can be defined as:

\[
\zeta = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x},
\]

(66)

Applying it to continuity eqn (55) for \( u \) and \( v \), respectively.

\[
\nabla^2 u = \frac{\partial \zeta}{\partial y} - \frac{\partial^2 w}{\partial x \partial z},
\]

(67)

\[
\nabla^2 v = -\frac{\partial \zeta}{\partial x} - \frac{\partial^2 w}{\partial y \partial z}.
\]

(68)

Cross differentiation of \( x \) and \( y \) momentum equations of gas channel to eliminate pressure terms yield:

\[
\frac{\partial \zeta}{\partial x} + \frac{\partial \zeta}{\partial y} + \frac{w \partial \zeta}{\partial z} + \zeta \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{\partial w}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \frac{\partial v}{\partial z} = \frac{\mu}{\rho} \left( \frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 \zeta}{\partial y^2} \right),
\]

(69)

Using the same method we can get similar equation for gas diffuser

\[
\frac{1}{\epsilon} \left( \frac{\partial \zeta}{\partial x} + \frac{\partial \zeta}{\partial y} + \frac{w \partial \zeta}{\partial z} + \zeta \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{\partial w}{\partial y} \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \frac{\partial v}{\partial z} \right) + \frac{\epsilon^2 \mu}{\kappa} \zeta = \frac{\mu}{\rho} \left( \frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 \zeta}{\partial y^2} \right).
\]

(70)

An additional constraint, which will be used to determine \( f(z) \), is that global mass conservation must be satisfied as follows:

\[
\int \int w \text{d}x \text{d}y = U_{in} D_e^2 \frac{(1 + r)^2}{4r},
\]

(71)

where \( r = \frac{a}{b} \) is the aspect ratio of the gas channel, \( U_{in} \) is inlet velocity, \( D_e \) is hydraulic diameter (4A/S).
2.3.3 Boundary conditions

Boundary conditions at the gas channel entries, such as gas mixture velocities, pressure, and component concentrations, are specified. No slip boundary conditions are specified at the gas channel walls. At the interface between the gas channel and electron collectors, the boundary conditions of components concentration are assumed as:

$$\frac{\partial X_i}{\partial n} = 0. \quad (72)$$

For the membrane potential equations, the boundary conditions are:

$$\frac{\partial \Phi}{\partial y} = 0. \quad (73)$$

This means that no proton current leaves top and bottom boundary. In $x$-direction,

$$\Phi \bigg|_{\text{anode catalyst surface}} = 0, \quad \frac{\partial \Phi}{\partial x} \bigg|_{\text{cathode catalyst surface}} = 0. \quad (74)$$

No boundary conditions are needed at the interface between gas channel and gas diffuser because they are coupled in a single domain.

2.3.4 Discretization strategies

In order to solve the above equations, some terms need to be discretized furthermore. The strategies of discretization is as follows:

The values of $\frac{\partial u}{\partial x}$, $\frac{\partial v}{\partial x}$, $\frac{\partial u}{\partial z}$, and $\frac{\partial v}{\partial z}$ are discretized using central differencing at each grid point. The values of $\frac{\partial u}{\partial z}$ and $\frac{\partial v}{\partial z}$, $\frac{\partial \Phi}{\partial z}$ are computed by two points backward differencing. The values of $\frac{\partial^2 w}{\partial x \partial z}$, $\frac{\partial^2 w}{\partial y \partial z}$, $\frac{\partial \zeta}{\partial x}$, and $\frac{\partial \zeta}{\partial y}$ are calculated by using backward differences axially and central differences in the transverse directions.

The values of vorticity on the boundary walls can be evaluated by following equations.

$$\zeta_{1.5j} = \frac{1}{2} (\zeta_{1,j} + \zeta_{2,j}) = \frac{1}{2 \Delta y} (u_{1.5,j+1} - u_{1.5,j-1}) - \frac{v_{2,j}}{\Delta x}, \quad (75)$$

$$\zeta_{1,j} = -2 v_{2,j}/\Delta y + (u_{2,j+1} - u_{2,j-1})/(2 \Delta y) - \zeta_{2,j}, \quad (76)$$

where $u_{1.5,j+1} = \frac{1}{2} u_{2,j+1}$, $u_{1.5,j-1} = \frac{1}{2} u_{2,j-1}$

2.3.5 Solution algorithms

1. Solve velocity and pressure field for anode domain first. The initial values of the unknowns $u$, $v$, and $\zeta$ are assigned to be zero at the entrance, $z = 0$. Uniform inlet axial velocity (i.e., $w = 1$) is used. Note that $\zeta = 0$ at $z = 0$ results from the vorticity definition.

2. Discretizing eqns (69), (70) with power-law scheme [33] and solving them in the coupled domain. Vorticity $\zeta$ can be calculated for gas channel, gas diffuser and catalyst layer.
3. The elliptic-type eqns (67) and (68) are solved for \( u \) and \( v \) iteratively. During the iteration process, the values of vorticity on the boundaries are evaluated using eqn (76).

4. Using control volume method with power-law scheme to discretize momentum equation in \( z \) direction, plug in new values \( u \) and \( v \) solved in step 2, one can solve axial velocity \( w \) in coupled domain with constraint (71) to meet the requirement of the constraint flow rate.

5. Steps 3 – 4 are repeated at a cross section until the following convergence criterion is satisfied for the velocity components \( u \) and \( v \):

\[
\frac{\max |u^{n+1}_{i,j} - u^n_{i,j}|}{\max |u^n_{i,j}|} < 10^{-5},
\]

(77)

where \( n \) is the \( n \)th iteration of steps 3 – 4.

6. Repeat steps 1 – 5 for cathode domain. One can calculate velocity distributions for gas channels, gas diffusers and catalyst layers in cathode domain.

7. With obtained solutions \( u, v, \) and \( w \) for both anode and cathode channels, species concentration equations and potential equations for a single domain from anode electrolyte to cathode electrolyte can be solved iteratively. These steps are repeated until the following convergence criterion is satisfied:

\[
\max \left( \frac{\max |X^{m+1}_k - X^m_k|}{\max |X^m_k|}, \frac{\max |\Phi^{m+1}_k - \Phi^m_k|}{\max |\Phi^m_k|} \right) < 10^{-6},
\]

(78)

where \( m \) is the \( m \)th iteration of step 6, and \( k \) is the \( k \)th species.

8. Steps 3 – 7 are repeated at the next axial location until the final \( z \) location is reached.

9. Once the electrolyte potential is obtained, the local current density can be calculated along the axial direction using following equation:

\[
I(y,z) = -\sigma_m \frac{\partial \Phi}{\partial x}.
\]

(79)

The average current density is then determined by

\[
I_{\text{avg}} = \frac{1}{bL} \int_0^b \int_0^L I(y,z)dz.
\]

(80)

2.3.6 Results and discussion

3-D models are generally more accurate and more detailed in transport phenomena than 2-D models. Jen et al. [30] investigated the secondary flow patterns in fuel cell channels. Zhou and Liu [28] analyzed detailed temperature distribution in fuel cell. Um and Wang [29] studied the effectiveness of the interdigitated flow field on fuel cell performance. Figure 12 shows the comparison of Zhou and Liu’s [28] 3-D model numerical results with experimental data [32]. The operating conditions are: cathode flow rate is 1200 cm³/s; anode flow rate is 1200 cm³/s; cathode temperature
is 60°C; anode temperature is 60°C; cathode pressure is 3 atm; anode pressure is 1 atm. It can be found that the 3-D model numerical results for the polarization curve agree well with the experimental data except in the region of the concentration polarization loss dominate. Even if some discrepancies can be seen in this region, the basic trend is still good. Note that the polarization of concentration region was not given in Ticianelli et al. [11, 12] experimental investigations. Most early 1-D or 2-D models did not investigate this region because no experimental data are available for this region.

2.3.6.1 Secondary flow pattern In Jen et al.’s 3-D model [30], a general secondary flow pattern in fuel cell channel were also investigated as shown in Fig. 13. At the location $\bar{z} = 0.0005$, as shown in Fig. 13(a), the secondary flow moves out from porous media in the core region. This is simply due to the acceleration of the core gas channel flow and the strong porous media resistance to push the fluid out of the gas diffuser in the early entrance region. Figure 13(b) shows the vector secondary flow pattern at $\bar{z} = 0.008$, which has two pairs of vortices, with one small pair counter rotating cells near the corner of the gas channel. It is observed that, near the core region, a fairly uniform secondary flow running from the left side to right side into the gas diffuser, and there are outflows from the gas diffuser to gas channel near the top and bottom wall. It is also interesting to see two counter rotating cells at the top and bottom left corner, which are generated due to the corner effect of the gas channel. In nearly fully developed region at $\bar{z} = 0.2$ (Fig. 13(c)), the secondary flow strength has decreased significantly, and the effect of cross-sectional convection is negligible.

2.3.6.2 Temperature distributions Zhu and Liu [28] analyzed the temperature distribution in PEMFC. The temperature distributions across the whole fuel cell
sandwich depend on the heat generation of the chemical reaction, Joule heating of the current, and cooling from channel walls. Due to very effective cooling, constant cell wall temperature is assumed; the typical temperature distribution is shown in Fig. 14 as an illustrative case. The inlet temperature of the air and fuel are both assumed to be 82 °C, inlet pressure at anode/cathode is 1 atm/3 atm. The major heat source is the chemical reaction and Joule heating in the cathode side catalyst layer. The maximum temperatures are located within the cathode side catalyst layer near air entrance region, as shown in Fig. 14. This is due to the high chemical reaction rate. The outer walls of the gas channels are kept at the constant temperature of 82 °C, heat is transferred out of the fuel cell effectively by the cooling along the outer walls of the gas channel so the inside of the fuel cell is prevented from overheating. The temperature distribution profiles can be used to improve fuel cell design to avoid membrane burning and drying out.

2.3.6.3 Water concentration variation Water management is very important for PEM fuel cell performance. During fuel cell operation, water within membrane is driven from the anode side to the cathode side by electro-osmosis, and at the same time it is driven in the opposite direction by diffusion [28]. If the water generation is more than water transport from the cathode, it causes cathode side flooding. On the other hand, if the water loss from anode is more than water supplies, it causes membrane dehydration which leads to high ohmic losses. The conductivity of the polymer electrolyte is a strong function of the degree of hydration, and flooding of
the cathode. It is common practice to saturate inlet fuel and air streams. However, due to the water generation along the cathode and electrical-osmosis drag from the anode to cathode, the water vapor concentration increases along the cathode channel. As the inlet cathode stream is already fully saturated, the added water from the chemical reaction and osmosis drag causes the cathode side to become over-saturated. In other words, liquid water exists along the cathode side and this could lead to flooding. To avoid this phenomenon, it is then suggested that the water content in the cathode inlet stream should be reduced. Figures 15 and 16 show the water vapor distributions along the cathode side and anode side when the hydrogen stream at the anode is fully saturated and the inlet air stream at the cathode is completely dry. Water vapor concentration along the cathode is increased due to the combined effect of water generation from the chemical reaction and electrical-osmosis drag from the anode to cathode as shown in Fig. 15. Under such operation conditions, the water vapor concentration along the anode is reduced due to the electrical-osmosis drag as shown in Fig. 16. Under this operation condition, membrane flooding can be avoided. However, the water vapor concentration near the inlet of the cathode is very low, the membrane dehydration may occur. Therefore, a proper water vapor added to the cathode stream and fully saturated anode stream are beneficial for fuel cell performance.

2.3.6.4 The effect of the flow fields

Um and Wang [29] investigated the effects of conventional flow fields and interdigitated flow fields on fuel cell performance. Conventional flow is usually straight streamtraces due to them all having open inlet and outlet. In contrast to conventional flow fields, interdigitated flow channels indicate that air comes in along the lower channel, penetrates through the porous backing layer and
Figure 15: Water vapor mole fraction varies along the flow direction in cathode channel.

Figure 16: Water vapor mole fraction varies along the flow direction in the anode channel.

exits through the upper channel. During the process, more oxygen is brought to the cathode catalyst reaction site by the forced convection, which results in better cell performance. Figure 17 shows the effect of the interdigitated flow field on the cell performance. There is a little difference in the current densities until cell potential reaching 0.55 V because the cell potential loss for current densities below 1 A/cm² is primarily dominated by the ohmic resistance. However, for $I_{\text{avg}} > 1$ A/cm², the cell polarization curve begins to be limited by mass transport. In this region the positive
role of the interdigitated flow field becomes apparent. It is seen that the mass transport limiting current density is much improved by the use of interdigitated flow field.

2.4 Summary and conclusion

The numerical simulation presented here enables prediction of phenomena in the entire fuel cell sandwich, including the two gas flow channels, two gas diffusers, two catalyst layers and membrane. It is able to predict detailed distributions of velocity fields, species concentration, current density, temperature, and polarization curves. It can be used to understand the interacting, complex electrochemical and transport phenomena that cannot be visualized experimentally. It also provides the ways to increase fuel cell power output for future fuel cell design, such as increase cell temperature, pressure, decrease the membrane thickness, choosing proper water vapor contents, and flow fields etc.

References


Transport Phenomena in Fuel Cells


