

Modeling of PEM Fuel Cell Heat and Pressure

4.1 Fuel Cell Thermodynamics

Thermodynamics is the study of energy changing from one state to another. The predictions that can be made using thermodynamic equations are essential for understanding and modeling fuel cell performance since fuel cells transform chemical energy into electrical energy. Basic thermodynamic concepts allow one to predict states of the fuel cell system, such as potential, temperature, pressure, volume, and moles in a fuel cell.

4.1.1 Entropy of H₂, O₂, and Water in the PEM fuel cell

1. Entropy

Entropy can be defined loosely as the amount of “disorder” in a system, and can be expressed as:

$$S_2 - S_1 = \left[\int_1^2 \frac{\delta Q}{T} \right]_{\text{int rev}} \quad (4.1)$$

This is valid for any reversible process that links two states. Entropy is calculated in the same way that enthalpy was calculated using the properties v , u , and h . When dealing with two-phase liquid-vapor mixtures as in fuel cells, the specific entropy can be calculated in the same manner as enthalpy:

$$S = (1 - X)S_f + XS_g = S_f + X(S_g - S_f) \quad (4.2)$$

Like enthalpy, the values for v , u , and h vary only slightly with changes in pressure at a fixed temperature; therefore, the following can be assumed for most engineering calculations:

$$S(T, p) \approx s_f(T) \quad (4.3)$$

When a pure, compressible system undergoes an internally reversible process in the absence of gravity and overall system motion, an energy balance can be written as:

$$\delta Q_{\text{int rev}} = dU + \delta W_{\text{int rev}} \quad (4.4)$$

In a simple compressible system, the work can be defined as:

$$\delta W_{\text{int rev}} = p \cdot dV \quad (4.5)$$

Substituting previous two equations, one obtains:

$$Tds = dU - pdV = dh - Vdp \quad (4.6)$$

When the ideal gas model is used, the specific entropy depends only upon temperature and can be derived from above Equation, therefore:

(4.7)

(4.8)

Determination of the absolute entropy of H_2 , O_2 , and water (H_2O) at the pressure of 1 atm at a temperature of 300 to 1000 K using increments of 50, using following equations. Plotting of the hydrogen and oxygen enthalpy as a function of temperature by Calculation of the absolute enthalpy for the vapor and liquid form if applicable. The MATLAB code can be used to plot the hydrogen and oxygen Enthalpy as a function of temperature: (Appendix C-C-4)

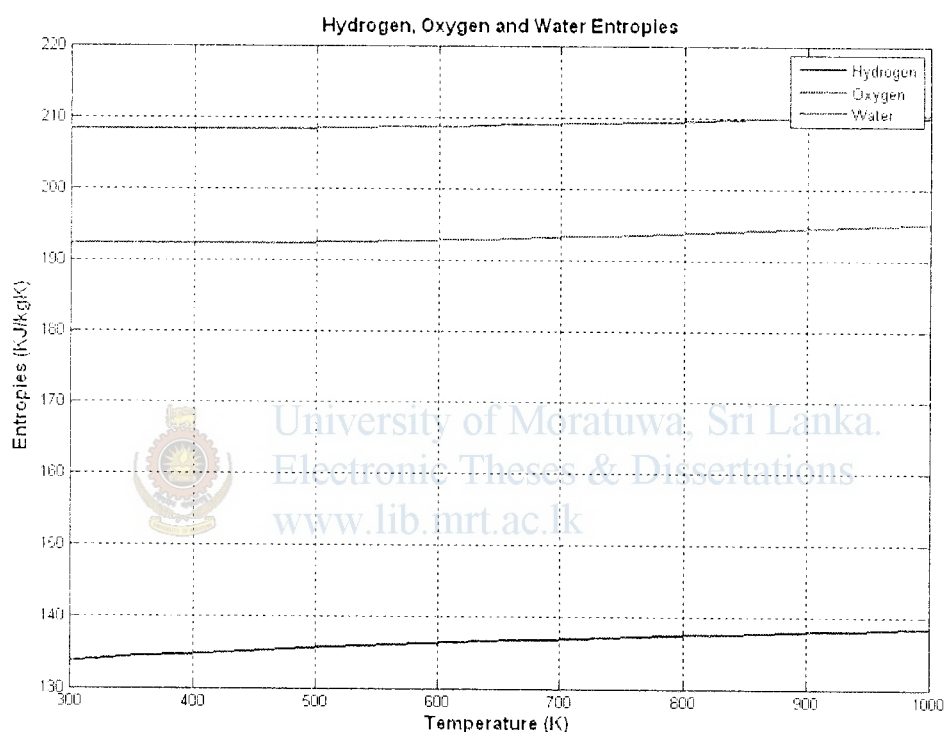


Figure 4.1- Hydrogen and oxygen entropies as a function of temperature.

4.2 Heat Transfer of Fuel cell

Temperature in a fuel cell is not always uniform, even when there is a constant mass flow rate in the channels. Uneven fuel cell stack temperatures are due to a result of water phase change, coolant temperature, air convection, the trapping of water, and heat produced by the catalyst layer. In order to precisely predict temperature-dependent parameters and rates of reaction and species transport, the heat distribution throughout the stack needs to be determined accurately [11] [12]. The determination of the heat distribution in a fuel cell stack is to perform energy balances on the system. The total energy balance around the fuel cell is based upon the power produced, the fuel cell reactions, and the heat loss that occurs in a fuel cell. Convective heat transfer occurs between the solid surface and the gas streams, and conductive heat transfer occurs in the solid and/or porous structures. The reactants, products, and electricity generated are the basic components to consider in modeling basic heat transfer in a fuel cell, as shown in Figure 4.2.

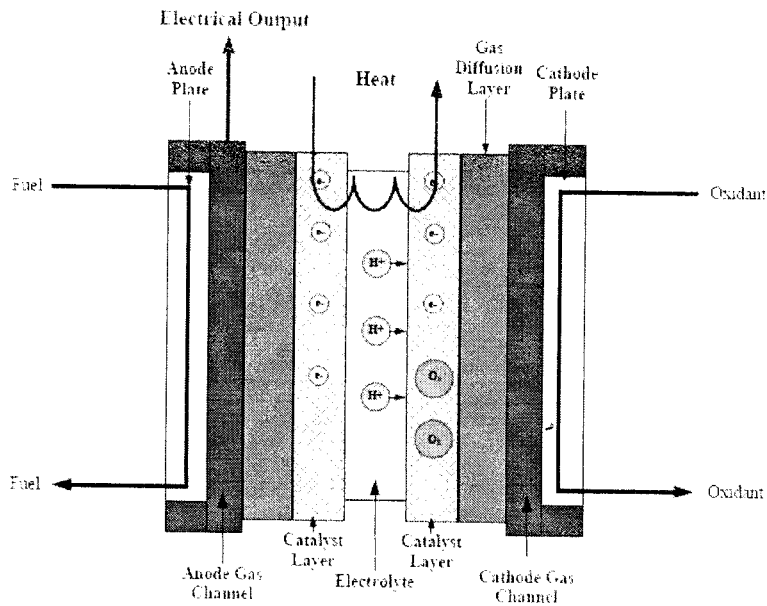


Figure 4.2- Stack illustration for heat flow study

The general energy balance states that the enthalpy of the reactants entering the cell equals the enthalpy of the products leaving the cell plus the sum of the heat generated by the power output, and the rate of heat loss to the surroundings. The basic heat transfer calculations will aid in predicting the temperatures and heat in overall fuel cell stack and stack components. The rate of heat transfer in the x-direction through a finite cross-sectional area, A , is known as Fourier's law, and can be expressed as:

$$(4.9)$$

Where k is the thermal conductivity, $W/(m \cdot K)$.

4.3 Energy Balances for Fuel Cell Layers

Energy balances can be defined around each of the fuel cell layers to enable the study of the diffusion of heat through a particular layer as a function of time or position. Figure 3.9 shows an example of a fuel cell layer as a control volume. This section describes the mode of heat diffusion in each layer, and calculates the energy balances for the end plate, gasket, contact, flow field, GDL, catalyst, and membrane layers [11]. The end plate is typically made of a metal or polymer material, and is used to uniformly transmit the compressive forces to the fuel cell stack. The end plate must be mechanically sturdy enough to support the fuel cell stack, and be able to uniformly distribute the compression forces to all of the major surfaces of each layer within the fuel cell stack. Depending upon the stack design, there also may be contact and gasket layers in the fuel cell stack. The gasket layers help to prevent gas leaks and improve stack compression. The contact layers or current collectors are used to collect electrons from the bipolar plate and gas diffusion layer (GDL). Since there is typically no gas or liquid flows in the end plates, gaskets, or contact layers, conduction is the only mode of heat transfer. One side of each of these layers is exposed to an insulating material (or the ambient environment), and the other side is exposed to a conductive current collector plate or insulating material.

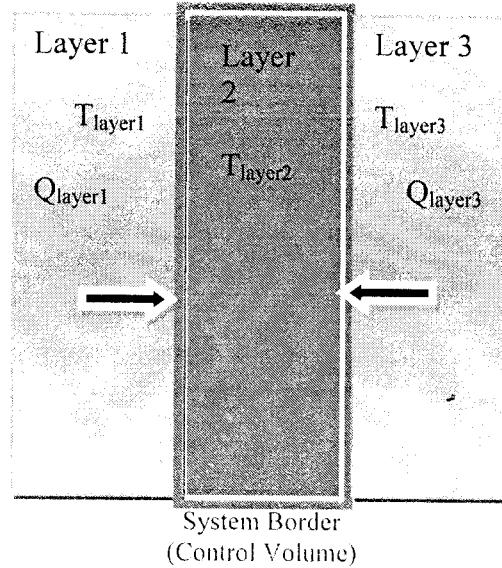


Figure 4.3- fuel cell layer as a control volume

The general energy balance for the end plate, contact, and GDL layers can be written as:

$$(\rho_{\text{Layer2}} A_{\text{Layer2}} t_{\text{layer2}} c_{p\text{Layer2}}) \frac{dT_{\text{Layer2}}}{dt} = Q_{\text{Layer1}} + Q_{\text{Layer3}} \quad (4.10)$$

Where, ρ_{Layer2} is the density of Layer2, A_{Layer2} is the area of Layer2, $c_{p\text{Layer2}}$ is the specific heat capacity of Layer2, Q_{Layer1} is the heat flow from Layer1, and Q_{Layer3} is the heat flow from Layer3.

The derivative on the left side is the rate of change of control volume temperature (dT_{Layer2}/dt). The heat flow from Layer1 to Layer2 is:

$$Q_{\text{Layer1}} = U_{\text{Layer1}} A (T_{\text{Layer1}} - T_{\text{Layer2}}) \quad (4.11)$$

Where U_{Layer1} is the overall heat transfer coefficient for Layer1, A is the area of the layer, and T is the temperature of the layer. The heat flow from Layer3 to Layer2 can be expressed as:

$$Q_{\text{Layer3}} = U_{\text{Layer3}} A (T_{\text{Layer3}} - T_{\text{Layer2}}) \quad (4.12)$$

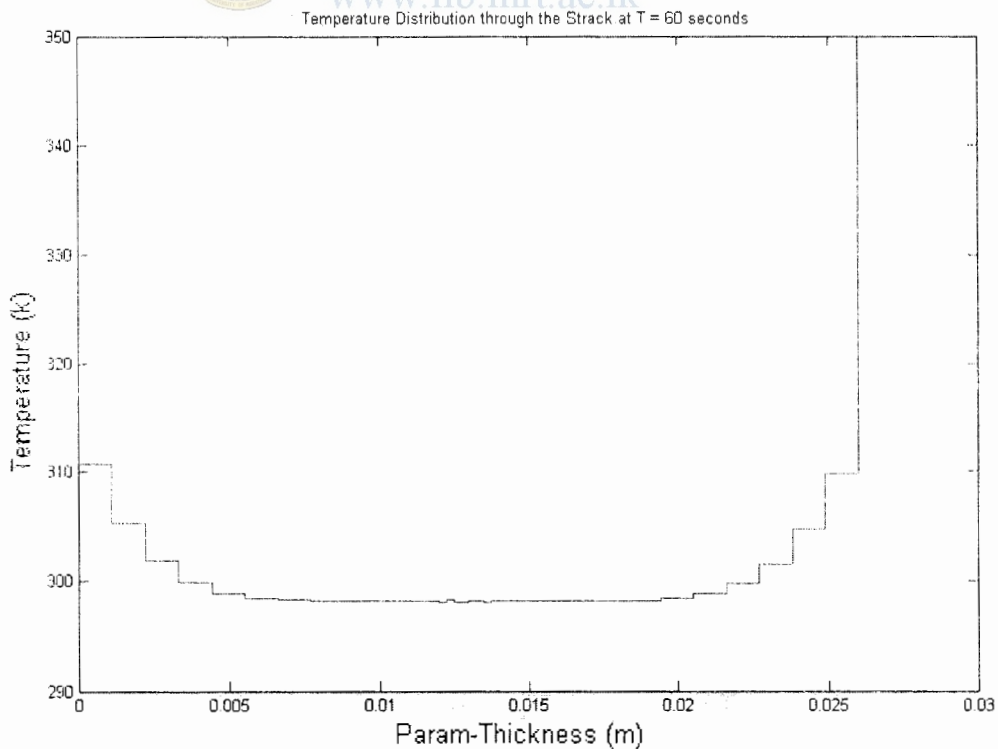
The overall heat transfer coefficient for the heat coming from Layer1 and layer 3

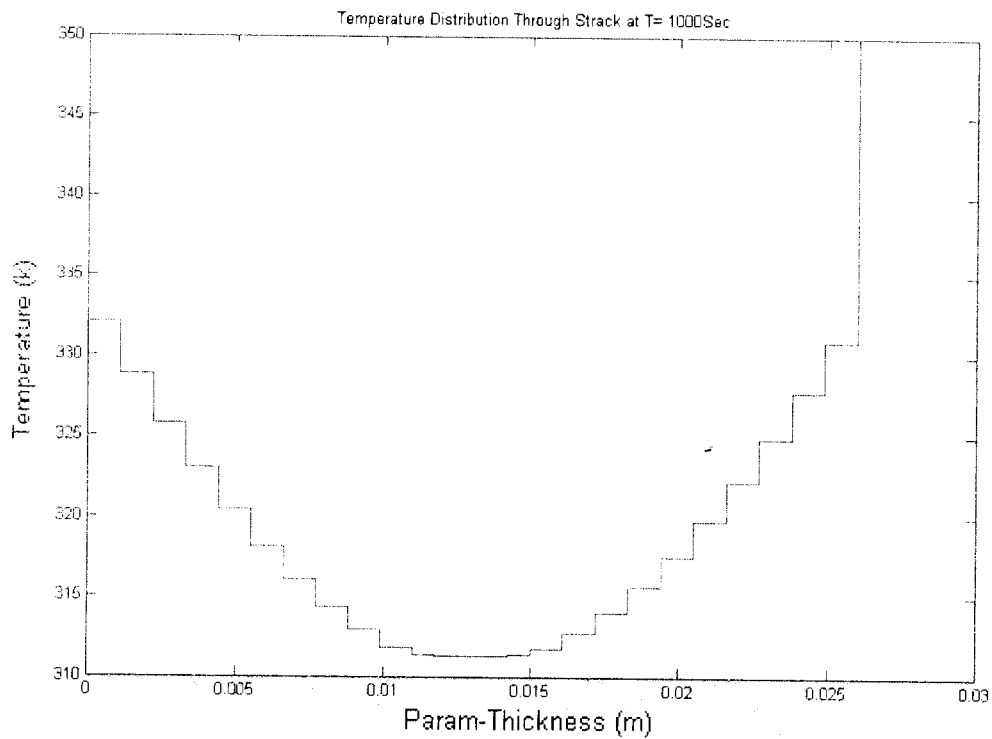
$$U_{\text{Layer1}} = \frac{1}{\frac{t_{\text{Layer2}}}{k_{\text{Layer2}}} + \frac{t_{\text{Layer1}}}{k_{\text{Layer1}}}} \quad U_{\text{Layer3}} = \frac{1}{\frac{t_{\text{Layer3}}}{k_{\text{Layer3}}} + \frac{t_{\text{Layer2}}}{k_{\text{Layer2}}}} \quad (4.13)$$

Table 4.1- Material Properties Used for Heat Transfer Calculations

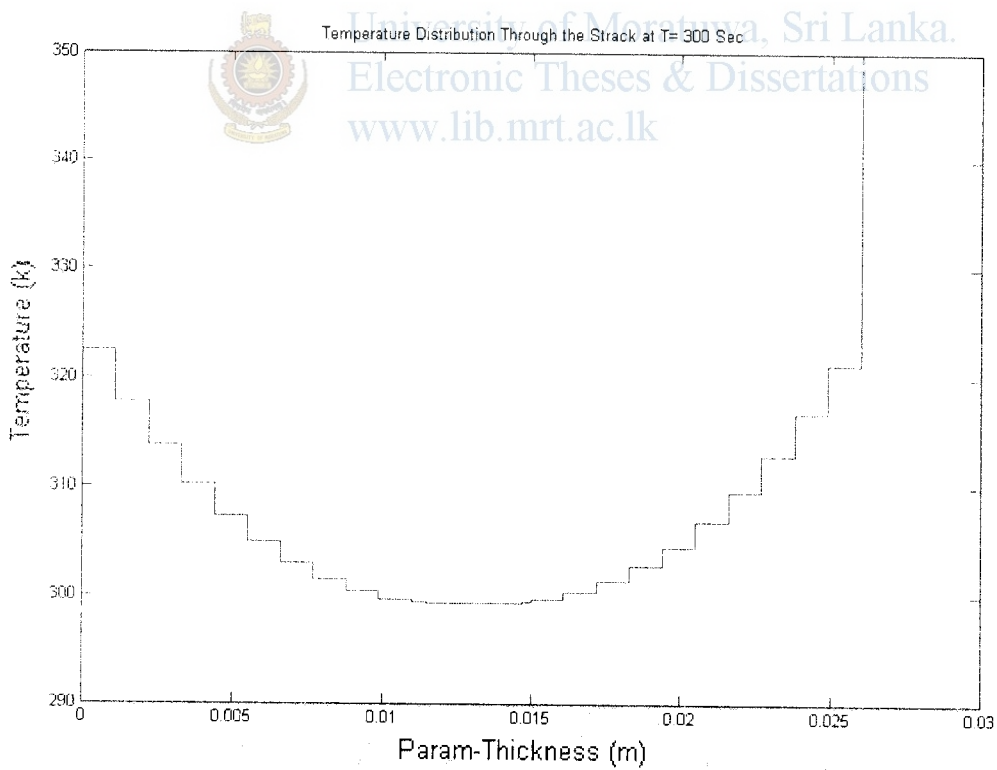
Fuel Cell Layer	Material	Thickness (m)	Area (m ²)	Density (kg/m ³)	Thermal Conductivity (W/m-K)	Specific Heat Capacity (J/kg-K)
End plate	Polycarbonate	0.01	0.0064	1300	0.2	1200
Gasket	Conductive rubber	0.001	0.001704	1400	1.26	1000
Flow field plate	Stainless steel	0.0005	0.003385	8000	65	500
MEA	Carbon cloth/ Pt/C/Nafion	0.001	0.0016	1300	26	864
Flow field plate	Stainless steel	0.0005	0.003385	8000	65	500
Gasket	Conductive rubber	0.001	0.001704	1400	1.26	1000
End plate	Polycarbonate	0.01	0.0064	1300	0.2	1200

Modeling example: A PEM hydrogen/air single cell fuel cell stack operates at an initial temperature of 298.15 K. There are seven layers in the stack: two polycarbonate end plates, two rubber gaskets, stainless steel flow field plates, and an MEA. The necessary material properties for heat transfer calculations for each layer are shown in Table 4.1. Using the equations in Section 3.3.3, plotting of the conductive heat transfer through the stack at 60 sec, 300 sec, and 1000 sec with one and 10 nodes per layer is shown in figure 4.4. Neglect heat generation and losses from thermal resistance, electrochemical reactions, and mass flows through the fuel cell. (Appendix C-C-5). when t=60 sec





When t =300 sec



When t= 1000 sec

Figure 4.4-Temperature plots for t = 60, 300, and 1000 sec using 7 slices per layer.

4.4 Modeling the Temperature in the Interior Layer and Modeling the Gas Diffusion Layer

This section presents the derivations and modeling for the cathode GDL of the fuel cell created by Beuscher et al [8]. The models are derived from multiphase flow in porous media from the hydro geological literature. The differences between the GDL layer and the modeling of unsaturated soils are that the GDL is hydrophobic and soil is hydrophilic, the pore size distributions are different, and the GDL is a non homogeneous weave of carbon fibers. Despite these differences, the hydro geological models are quite useful for fuel cell GDL modeling. However, it sometimes may be difficult to use these models since many properties such as the temperatures, phases, pressure, and the velocity of the species in and surrounding the GDL are unknown parameters while the fuel cell is operating.

The simplified geometry is shown in Figure 4.5. The dashed lines at the top of Figure 4.5 illustrate the portion of the channel where the gas is flowing through. The bottom of the diagram is the catalyst side where heat and water are added to the system, and gas is absorbed. On the upper channel sides, gas is added, and heat and water are removed. Since half of the upper boundary is the solid cathode material, and half is open channel, the boundary conditions are mixed. The portion where there is no flux into the cathode has Neumann boundary conditions, and the portion where there is no liquid water in the channels has Dirichlet boundary conditions. The GDL in Figure 4.5 is $4d$ unit's long, and h units high. The aspect ratio is the perturbation parameter, and can be defined as $\epsilon = h/d \ll 1$. The lower surface abuts the cathode catalyst layer, and the upper surface is cathode. The channels can be at different pressures, and all quantities are assumed to be steady-state. The three-dimensional plot in MATLAB for the temperature of the interior layer using the equations derived in Appendix A and C-C-6 and the simulation result is shown in figure 4.6 and 4.7.

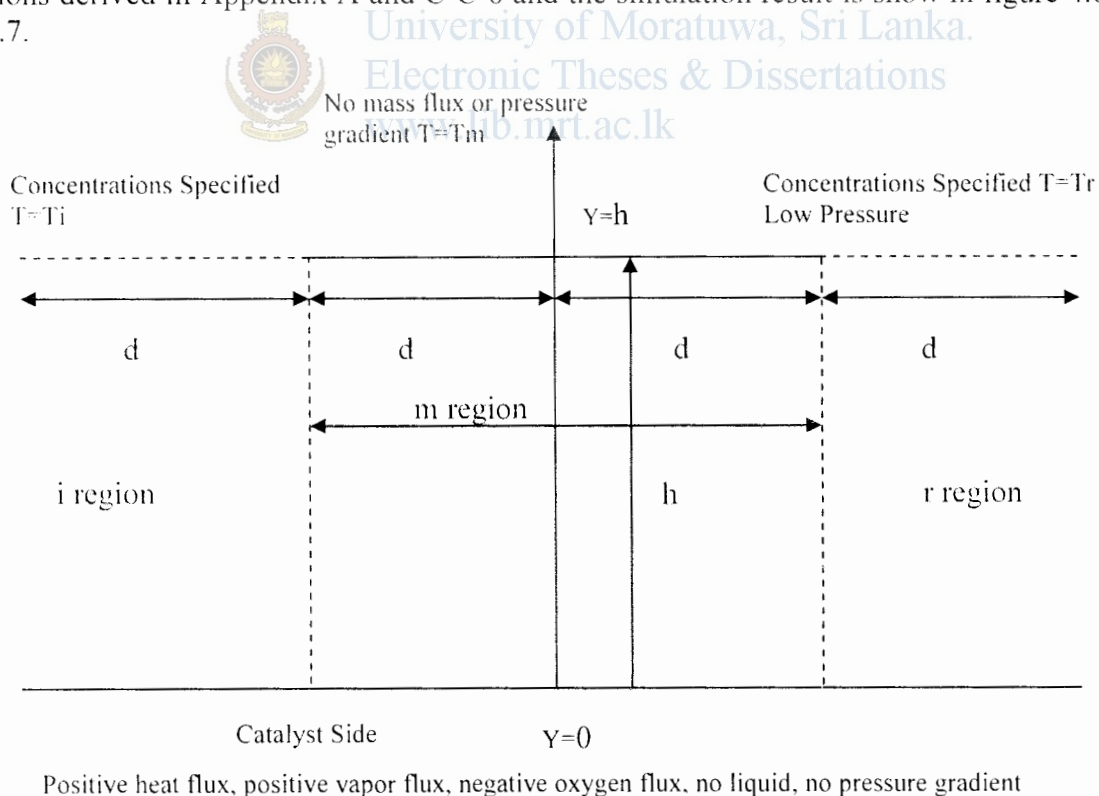


Figure 4.5-The simplified geometry of GDL.

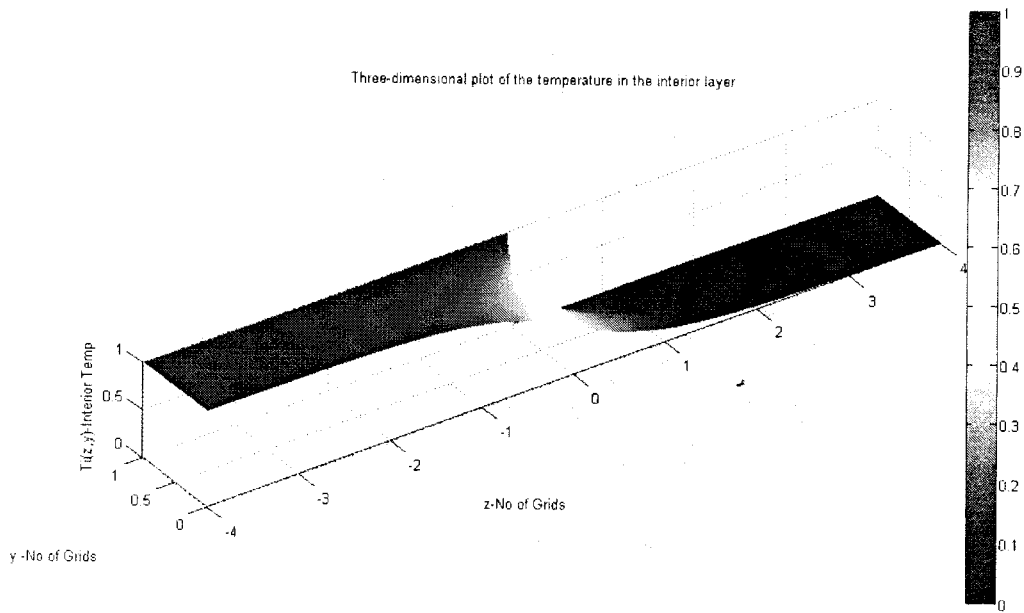


Figure 4.6-3D plot of Temperature variance in Interior Layer

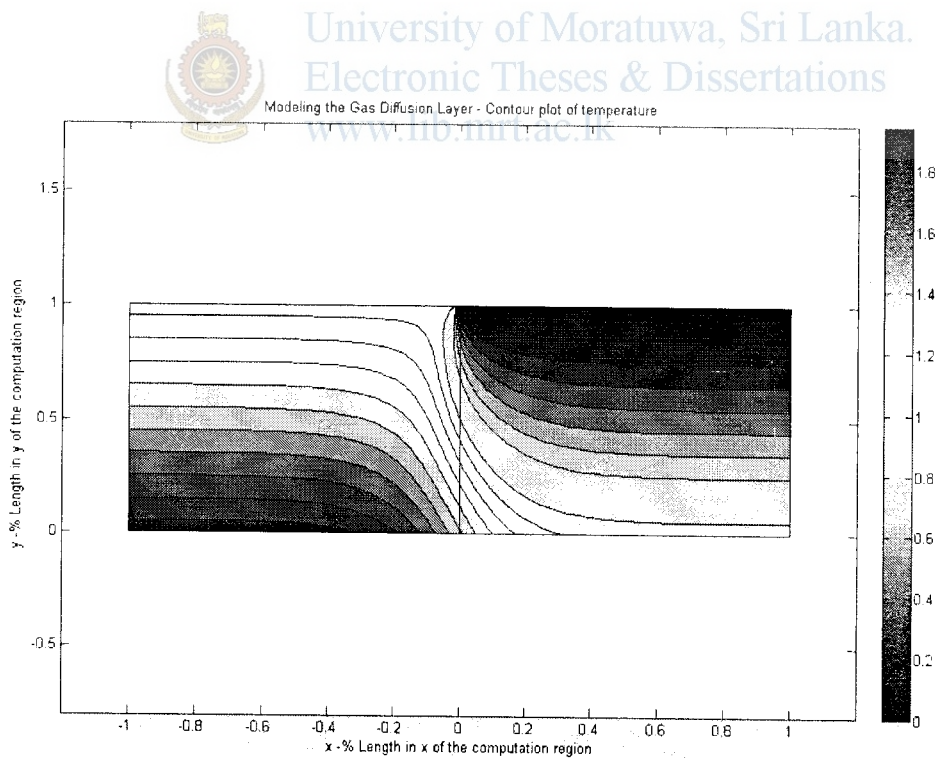


Figure 4.7- Temperature variance in Gas Diffusion Layer

4.5 Pressure Drop in Flow Channels

In many fuel cell types, the flow fields are usually arranged as a number of parallel flow channels; therefore, the pressure drop along a channel is also the pressure drop in the entire flow field. In a typical flow channel, the gas moves from one end to the other at a certain mean velocity. The pressure difference between the inlet and outlet drives the fluid flow. By increasing the pressure drop between the outlet and inlet, the velocity is increased. The flow through bipolar plate channels is typically laminar, and proportional to the flow rate. The pressure drop can be approximated using the equations for incompressible flow in pipes

$$\Delta P = f \frac{L_{chan}}{D_H} \rho \frac{\bar{V}^2}{2} + \sum K_L \rho \frac{\bar{V}^2}{2} \quad (4.14)$$

Where f is the friction factor, L_{chan} is the channel length, m, D_H is the hydraulic diameter, m, ρ is the fluid density, kg/m³, \bar{V} is the average velocity, m/s, and K_L is the local resistance. The hydraulic diameter for a circular flow field can be defined by:

$$D_H = \frac{4 \times A_c}{P_{cs}} \quad (4.15)$$

Where A_c is the cross-sectional area, and P_{cs} is the perimeter. For the typical rectangular flow field, the hydraulic diameter can be defined as:

$$D_H = \frac{2 w_c d_c}{w_c + d_c} \quad (4.16)$$

Where w_c is the channel width, and d_c is the depth. The channel length can be defined as:

$$L_{chan} = \frac{A_{cell}}{N_{ch}(W_c + W_L)} \quad (4.17)$$

where A_{cell} is the cell active area, N_{ch} is the number of parallel channels, w_c is the channel width, m, and W_L is the space between channels, m. The friction factor can be defined by:

$$f = \frac{56}{Re} \quad (4.18)$$

The velocity at the fuel cell entrance is:

$$v = \frac{Q_{stack}}{N_{cell} N_{ch} A_{ch}} \quad (4.19)$$

where v is the velocity in the channel (m/s), Q_{stack} is the air flow rate at the stack entrance, m³/s, N_{cell} is the number of cells in the stack, N_{ch} is the number of parallel channels in each cell, and A_{ch} is the cross-sectional area of the channel.

The total flow rate at the stack entrance is:

$$Q_{stack} = \frac{1}{4F} \frac{S_{O_2}}{r_{O_2}} \frac{RT_{in}}{P_{in} - \Phi P_{sat}(T_{in})} N_{cell} \quad (4.20)$$

where Q is the volumetric flow rate (m³/s), I is the stack current, F is the Faraday's constant, S_{O_2} is the oxygen stoichiometric ratio, r_{O_2} is the oxygen content in the air, R is the universal gas constant, T_{in} is the stack inlet temperature, P_{in} is the pressure at the stack inlet, Φ is the relative humidity, P_{sat} is the saturation pressure at the given inlet temperature, and N_{cell} is the number of cells in the stack. By combining the previous equations, the velocity at the stack inlet is:

$$v = \frac{1}{4F} \frac{S_{O_2} (W_c + W_L) l_{chan}}{r_{O_2} W_c d_c} \frac{RT}{P - \phi P_{sat}} \quad (4.21)$$

Liquid or gas flow confined in channels can be laminar, turbulent, or transitional and is characterized by an important dimensionless number known as the Reynold's number (Re). This number is the ratio of the inertial forces to viscous forces and is given by:

$$Re = \frac{\rho v_m D_{ch}}{\mu} = \frac{v_m D_{ch}}{\nu} \quad (4.22)$$

Where V_m is the characteristic velocity of the flow (m/s), D_{ch} is the flow channel diameter or characteristic length (m), r is the fluid density (kg/m³), μ is the fluid viscosity [kg/(m * s or N * s/m²)], and ν is the kinematic viscosity (m²/s). When Re is small (<2300), the flow is laminar.

The flow rate at the stack outlet is usually different than the inlet. If it is assumed that the outlet flow is saturated with water vapor, the flow rate is:

$$Q_{stack} = \frac{1}{4F} \left(\frac{S_{O_2}}{r_{O_2}} - 1 \right) \frac{RT_{out}}{P_{in} - \Delta P - \phi P_{sat}(T_{out})} N_{cell} \quad (4.23)$$

Fuel cell gas streams are rarely composed of a single species. Usually, they are gas mixtures, such as oxygen and nitrogen from the air. The following expression provides a good estimate for the viscosity of a gas mixture:

$$\mu_{max} = \sum_{i=1}^N \frac{X_i \mu_i}{\sum_{j=1}^N X_j \phi_{ij}} \quad (4.24)$$

Where ϕ_{ij} is a dimensionless number obtained from

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_i}{M_j} \right)^{1/4} \right]^2 \quad (4.25)$$

Where N is the total number of species in the mixture, x_i and x_j are the mole fractions of species i and j, and M_i and M_j are the molecular weight (kg/mol) of species i and j. For porous flow fields, the pressure drop is determined by Darcy's law:

$$\Delta P = \mu \frac{Q_{cell}}{k A_c} L_{chan} \quad (4.26)$$

Where μ is the viscosity of the fluid, Q_{cell} is the geometric flow rate through the cell, m³/s, K is the permeability, m², A_c is the cross-sectional area of the flow field, m², and L_{chan} is the length of the flow field.

The modeling of pressure drop through a PEM fuel cell cathode flow field of a single graphite plate with 100-cm² cell area. The stack operates at 3 atm at 60 °C with 100% saturated air. The flow field consists of 24 parallel serpentine channels 1 mm wide, 1 mm deep, and 1 mm apart. The cell operates at 0.7 A/cm² at 0.65 V. the result output is given as shown in Appendix C-C-7.