



ISSN 2278 – 0211 (Online)

Computational Modeling and Parametric Analysis of Pem Fuel Cell

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Abstract:

Fuel cells are devices for direct conversion of the chemical energy of fuels into electricity by electrochemical reactions. Among the various types of fuel cells, polymer electrolyte membrane fuel cells (PEMFC) are considered to be the most suitable system for portable and automobile applications because of their compactness, robustness and operational simplicity. A proton exchange membrane fuel cell stack forms the heart of such a system.

Understanding the mechanisms inside a fuel cell or a fuel cell stack and designing a typical system are highly involved tasks due to interdependent and complex phenomena involved. This includes electrochemical reactions, gas and water transport through specially designed channels, electrical potential. Nowadays, numerical modeling is used extensively to study these internal phenomena and their design level implications.

This thesis mainly aims at computational modeling and parametric analysis of a typical PEM Fuel Cell. MATLAB and COMSOL software are planned to be used for the purpose. Experimental results will be used to confirm the theoretical understanding.

Keywords: PEM fuel cell, Mathematical model, COMSOL Multiphysics

1. Introduction

Energy is essential for our daily lives and well-being. Energy is consumed or rather converted from one form to another as per the utility. Whereas the 19th Century was the century of the steam engine and the 20th Century was the century of the internal combustion engine, it is likely that the 21st Century will be the century of the fuel cell. Fuel cells are now on the verge of being introduced commercially, revolutionizing the way we presently produce power. Fuel cells can use hydrogen as a fuel, offering the prospect of supplying the world with clean, sustainable electrical power. Since the applications of proton exchange membrane fuel cell (PEMFC) systems were initially reported in the New Generation of Vehicles Program (PNGV) in the US in 1993, it has taken more than 10 years to reach the current test-phase or partial commercializing stage.

Over 85% of the current energy needs of our planet is met through the consumption of fossil fuels. Fossil fuels are consumed by combustion process which results in toxic emissions and thus damages the environment. Excessive use of fossil fuels for power generation has resulted in

1. Limitation of the fossil fuel resources.
2. Emission of large amount of pollutants.
3. Global warming

This calls for a switch over to a different energy technology which is reliable and environment friendly. Fuel cell technology has emerged as a potential solution to substitute the existing conventional energy conversion techniques based on fossil fuels, because, fuel cell involves sustainable energy conversion and is more efficient. PEMFCs have many advantages such as a low operating temperature, sustained operation at a high current density, low weight, compactness, the potential for low cost and volume, long stack life, fast start-ups and suitability for discontinuous operation. These features make PEMFCs the most promising and attractive candidate for a wide variety of power applications ranging from portable/micro power and transportation to large-scale stationary power systems for buildings and distributed generation.

1.1. Fuel Cell Basics

Fuel cells are energy convertors which transform chemical energy stored in a fuel and oxidant directly into DC electrical energy at high thermodynamic efficiencies. Schematic of a fuel cell system is shown in figure.1. The energy conversion is carried out using multi step electrochemical reactions with simultaneous mass, charge and energy transport. Since they are modular they can be built for

various power requirements, viz., milli watts to multi watt and even megawatt. They are used in variety of applications like portable power, transportation, and stationary power, etc.

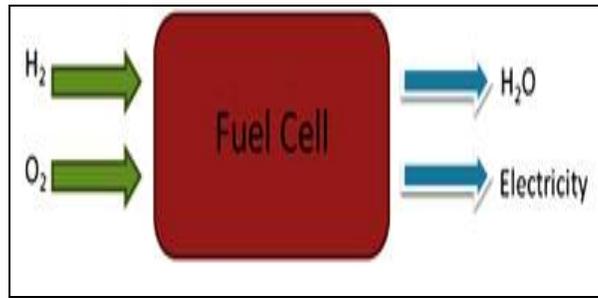


Figure 1: Schematic of a fuel cell system

2. Model

Figure 2 schematically shows a 3D single PEMFC and its various components, including membrane and the flow channel, GDL and catalyst layer on both anode and cathode sides.

GDL

2.1. Assumptions

The present model is established under the following assumptions

1. Flow is laminar everywhere due to small gas pressure gradient and low Reynolds number.
2. Reactant gases behave as the ideal gas mixture.
3. The temperature distribution across the cell is uniform and keeps constant.
4. Polymer electrolyte membrane is impermeable to reactant gas.
5. Proton can only transport through the electrolyte.
6. Three species including oxygen, water and nitrogen are considered on the cathode side while only hydrogen and water are considered on the anode side.

2.2. Governing Equations

Governing equations are assigned to each domain. By solving these equations we can determine the activation over potential (η_{act}), ohmic over potential (η_{act}), and concentration over potential (η_{act}) at different current density levels (j) and then finally be able to construct a j - V curve.

2.2.1. For Electrode

Gas transport in the electrodes can be explained using a diffusion model. At PEMFC cathode, however, three gas species are typically present (N_2 , O_2 , H_2O). Since there is no N_2 consumption or generation in the fuel cell (no nitrogen flux); we can ignore the nitrogen flux. This enables us to use a simple diffusion model based on Fick's law

$$N_i = -D_{ij}^{eff} \frac{dC_i}{dx} \quad (1)$$

In the case of gaseous reactants, the equation can be written as,

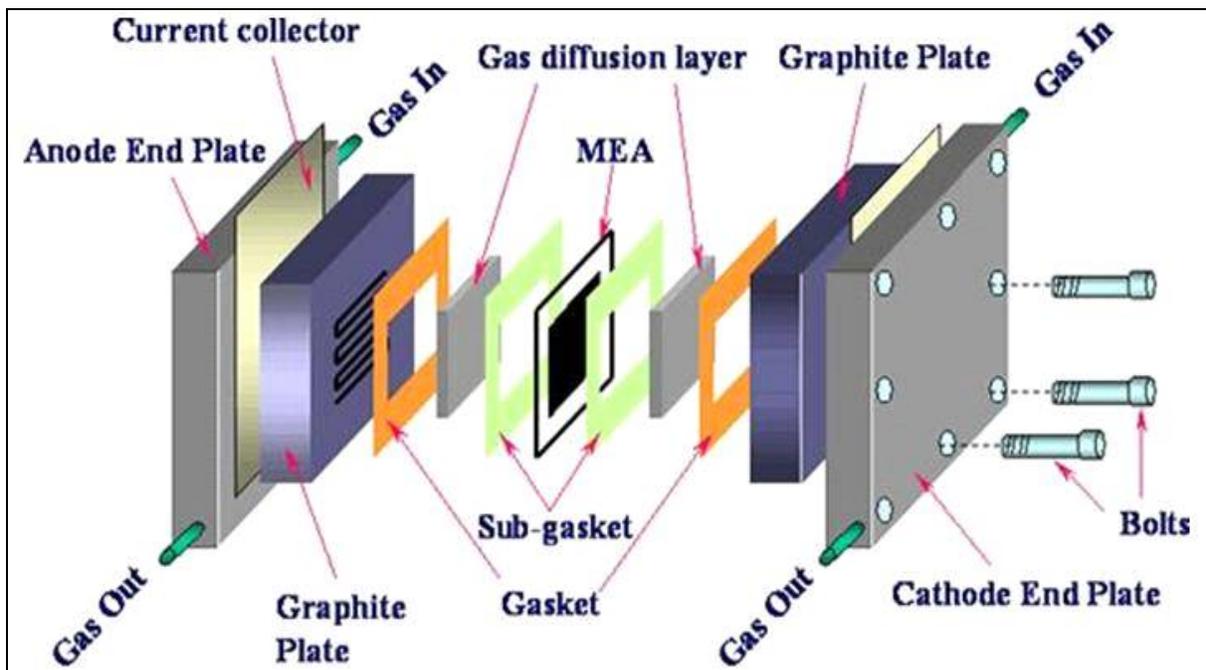


Figure 2: Three dimensional diagram of a PEMFC and its various components

$$N_i = -\frac{D_{ij}^{eff}}{RT} \frac{dp_i}{dx} = -\frac{p D_{ij}^{eff}}{RT} \frac{dx_i}{dx} \quad (2)$$

Ideal gas law ($C_i = P_i/RT$)

2.2.2. For Electrolyte

For PEMFC, water and proton (H^+) both transport through the membrane electrolyte. Proton flux is given and water flux through the membrane can be described as the combined effect of back diffusion and electro-osmotic drag.

We can account for both these fluxes, in the combined equation for water flux balance within the membrane as

$$J_{H_2O}^M = 2n_{drag} \frac{j}{2F} \frac{\lambda}{22} - \frac{\rho_{dry}}{M_m} D_m \frac{d\lambda}{dz} \quad (3)$$

2.2.3. For Catalyst Layer

The oxygen partial pressure is the dominant factor in determining the cathodic overvoltage. Simplified Butler Volmer equation,

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \frac{j C_{O_2}^0}{j_0 C_{O_2}} \quad (4)$$

For an ideal gas, ($P=CRT$) and the above equation becomes,

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \left(\frac{j p^0}{j_0 p^C x_{O_2}} \right) \quad (5)$$

Where,

P^0 is the reference pressure = 1atm

In the PEMFC Modeling the H_2 and H_2O transport at the anode is expressed as,

$$N_{H_2}^A = \frac{-p^A D_{H_2, H_2O}^{eff}}{RT} \frac{dx_{H_2}}{dz} \quad (6)$$

$$N_{H_2O}^A = \frac{-p^A D_{H_2, H_2O}^{eff}}{RT} \frac{dx_{H_2O}}{dz} \quad (7)$$

On applying the master flux balance equation to the above equations (6) and (7), we obtain

$$x_{H_2}(z) = x_{H_2}|_a - z \frac{jRT}{2F p^A D_{H_2, H_2O}^{eff}} \quad (8)$$

$$x_{H_2O}(z) = x_{H_2O}|_a - z \frac{\zeta jRT}{2F p^A D_{H_2, H_2O}^{eff}} \quad (9)$$

At the anode and membrane interface, b we calculate the hydrogen and water concentration profile

$$x_{H_2}|_b = x_{H_2}|_a - t^A \frac{jRT}{2Fp^A D_{H_2, H_2O}^{eff}} \quad (10)$$

$$x_{H_2O}|_b = x_{H_2O}|_a - t^A \frac{\zeta jRT}{2Fp^A D_{H_2, H_2O}^{eff}} \quad (11)$$

Where, t^A is the thickness of the anode.

In a similar manner we can obtain the oxygen and water concentration profile at the membrane and cathode interface (c) as,

$$x_{O_2}|_c = x_{O_2}|_d - t^C \frac{jRT}{4Fp^C D_{O_2, H_2O}^{eff}} \quad (12)$$

$$x_{H_2O}|_c = x_{H_2O}|_d + t^C \frac{(1+\zeta)jRT}{2Fp^C D_{O_2, H_2O}^{eff}} \quad (13)$$

Where, t^C is the thickness of the cathode.

Having determined the oxygen concentration at the cathode catalyst layer,

On combining equations (4) and (11), the cathodic overpotential is given by the equation,

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \left[\frac{J}{j_0 p^C \left\{ x_{O_2}|_d - \frac{t^C jRT}{4Fp^C D_{O_2, N_2}^{eff}} \right\}} \right] \quad (14)$$

The ohmic overpotential calculation is most crucial in the case of PEMFC as at first we need to calculate the water profile which will let us calculate the membrane resistance.

$$\eta_{ohmic} = j * AR_m \quad (15)$$

The membrane conductivity of the Nafion membrane K_M is given by

$$K_M(T, \lambda) = K_{M,303K}(\lambda) \exp \left[1268 \left(\frac{1}{303} - \frac{1}{T} \right) \right] \quad (16)$$

Where,

$$K_{M,303K} = 0.005193 \lambda - 0.00326 \quad (17)$$

To obtain the water profile, substitute equation (13) in (17) and integrate

$$\lambda(z) = \frac{11 \zeta}{n_{drag}^{SAT}} + B \exp \left(\frac{j M_m n_{drag}^{SAT}}{22 F \rho_{dry} D_\lambda} z \right) \quad (18)$$

Water content (λ) at anode – membrane interface-b

$$\lambda|_b = \lambda(0) = \frac{11 \zeta}{n_{drag}^{SAT}} \quad (19)$$

Water content (λ) at cathode – membrane interface -c

$$\lambda|_b = \lambda(L^M) = \frac{11 \zeta}{n_{drag}^{SAT}} + B \exp \left(\frac{j M_m n_{drag}^{SAT}}{22 F \rho_{dry} D_\lambda} L^M \right)$$

(20)

Where,

$$n_{\text{drag}}^{\text{SAT}} = 2.5$$

 M_m = Nafion equivalent weight = 1.0kg/mol

 D_λ = Diffusivity of water in nafion membrane

 ρ_{dry} = Dry density of nafion = 0.00197 kg/cm³

3. 3D Modeling of PEM fuel cell using COMSOL Multiphysics

More rigorous and accurate modeling of a 3D PEM fuel cell is necessary to make realistic and deeper understanding of the system performance. But, this is a highly involved task because of the enormity of scaling issues and nonlinearity as well as coupling of various mechanisms. Dedicated modeling and simulation platforms are often resorted to under such situations and COMSOL Multiphysics is the one used here.

COMSOL Multiphysics is one of the widely used modeling and simulation software. It is an integrated software application for solving systems of time dependent or stationary second order in space partial differential equations in one, two and three dimensions. Sophisticated and convenient tools for geometric modeling are also available with COMSOL Multiphysics. The model we are about to consider is a PEM unit cell where the transport of reactants and products (H₂ and O₂) of both anode and cathode, mass and momentum transport in flow channels, GDL, electrode, as well as electrochemical currents in GDL, Electrode and membrane, are in steady state.

For modeling multiple parallel channel configurations, symmetry conditions are applied along the longitudinal direction of GDLs and porous electrodes. Parameters such as cell dimensions, individual species diffusion coefficient, GDL conductivity and permeability are considered based on the real values in practice as well as that values commonly considered for general modeling and simulations, in literature.

Two interfaces are used in this model. They are discussed below

3.1. Secondary Current Distribution Interface

The secondary current distribution interface is used to model the electrochemical currents using Ohms Law.

 Φ_S = Electric potential

 Φ_L = Ionic potential

In porous electrodes the current density depends on both electric and ionic potential as well as on the reactant concentration and this effect is captured for the anodic reaction using the linear zed Butler- Volmer equation and for the cathodic reaction using Tafel equation. The GDL boundaries facing flow at anode is set at zero potential and the GDL boundaries facing flow at cathode is set to cell potential. The remaining boundaries are insulated.

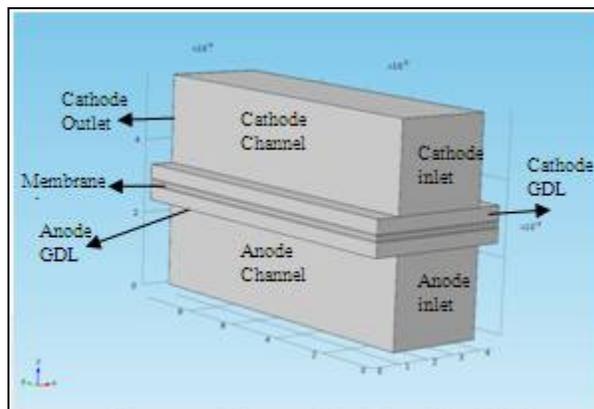


Figure 3: 3D PEMFC model comprising anodic and cathodic compartments

3.2. Reacting Flow in Porous Media

The reacting flow in Porous media interface is introduced for the anode and cathode separately. This interface can be used to model

- The mass transport
- The momentum transport

For mass transport the weight fractions of the species are modeled using Maxwell Stefan Equation separately for anode as well as cathode.

Except for the inlets and outlets all other boundaries are at no flux condition.

The anode and cathode inlet velocities at the flow channels are given as input and they are modeled using Navier stokes equation.

3.3. List of Parameters to Be Used in the Model

L	0.01[m]	Cell length
H_ch	0.0008[m]	Channel height
W_ch	0.001[m]	Channel width
W_rib	0.0001[m]	Rib width
H_gdl	380e-6[m]	GDL width
H_electrode	50e-6[m]	Porous electrode thickness
H_membrane	125e-6[m]	Membrane thickness
eps_gdl	0.4	GDL porosity
kappa_gdl	1.18e-11[m ²]	GDL permeability
sigma_gdl	222[S/m]	GDL electric conductivity
wH ₂ _in	0.743	Inlet H ₂ mass fraction (anode)
wH ₂ O_in	0.023	Inlet H ₂ O mass fraction (cathode)
wO ₂ _in	0.228	Inlet oxygen mass fraction (cathode)
U_in_anode	0.2[m/s]	Anode inlet flow velocity
U_in_cathode	0.5[m/s]	Cathode inlet flow velocity
mu_anode	1.19e-5[Pa*s]	Anode viscosity
mu_cathode	2.46e-5[Pa*s]	Cathode viscosity
MH ₂	0.002[kg/mol]	Hydrogen molar mass
MN ₂	0.028[kg/mol]	Nitrogen molar mass
MH ₂ O	0.018[kg/mol]	Water molar mass
MO ₂	0.032[kg/mol]	Oxygen molar mass
D_H ₂ _H ₂ O	9.15e-5*(T/307.1[K]) ^{1.75} [m ² /s]	H ₂ -H ₂ O Binary diffusion coefficient
D_N ₂ _H ₂ O	2.56e-5*(T/307.15[K]) ^{1.75} [m ² /s]	N ₂ -H ₂ O Binary diffusion coefficient
D_O ₂ _N ₂	2.2e-5*(T/293.2[K]) ^{1.75} [m ² /s]	O ₂ -N ₂ binary diffusion coefficient
D_O ₂ _H ₂ O	2.82e-5*(T/308.1[K]) ^{1.75} [m ² /s]	O ₂ -H ₂ O binary diffusion coefficient
T	55+273.15[K]	Cell temperature
p_ref	100000 [Pa]	Reference pressure
V_cell	1.012	Cell voltage
cO ₂ _ref	40.88[mol/m ³]	Oxygen reference concentration
cH ₂ _ref	40.88[mol/m ³]	Hydrogen reference concentration
eps_l	0.3	Electrolyte phase volume fraction
eps_cl	1-eps_l-eps_gdl	Open volume fraction for gas
kappa_cl	kappa_gdl/5	Permeability (porous electrode)
sigma_m	9.825[S/m]	Membrane conductivity

Table 1: Modeling parameters for 3D Model

4. Result and Discussion

The polarization curve for the above model is drawn and various plots are generated to study the variation of current density and concentration of Oxygen at different inlet velocities for various voltage values. The concentration profile of oxygen at 0.8 and 0.6V is generated for two different inlet velocities (u=0.6m/s and 0.06m/s) is plotted and compared.

The electrode current density for cathode is plotted at 0.8V and 0.6V for two different inlet velocities (u=0.6m/s and u= 0.06m/s) of oxygen is plotted and compared.

Current density variation within the cells at the operating voltage of 0.8 V at different air velocities is obtained shown in Figure 7.2 & 7.3. We can see that the reaction sites are concentrated under the ribs and these are the areas where current is being generated. Large areas underneath the open channels do not contribute to the reactions at all.

- Voltage 0.8V
- Cathode inlet velocity =0.6m/s

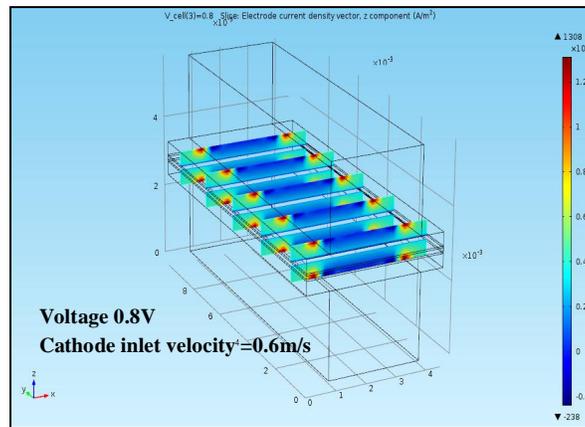


Figure 4: Slice graph representation of Current density plots for 0.8 V & air velocity 0.6 m/s

In computational analysis the operating voltage of PEMFC is 1.012V. This slice graph representing the current density variation in cathode electrode region. The scale is provided on the right side of the figure. The current density is depending on the parameters such as channel length, channel height, width etc

- Voltage = 0.8V
- Cathode inlet velocity = 0.06m/s

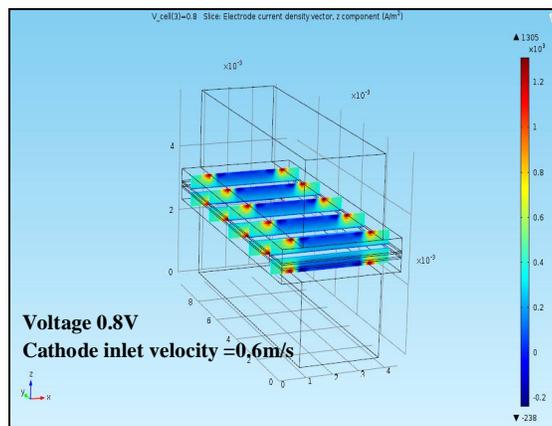


Figure 5: Slice graph representation of Current density plots at 0.8 V & air velocity of 0.06 m/s

Current density variation within the cells at the operating voltage of 0.8 V at different air velocities are obtained specifically for the surface of the electrode.

- Voltage = 0.8V
- Cathode inlet velocity = 0.6m/s

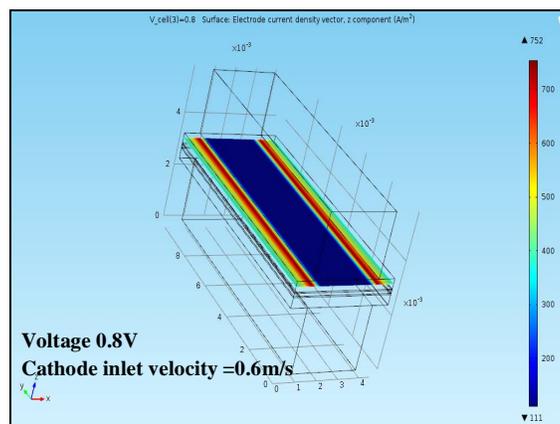


Figure 6: Surface plot representation of current density for 0.8 V at 0.6 m/s air velocity

To obtain more clarity in understanding the current generation, it would be necessary to increase the length of the channel. For the given geometry, the change in gas velocity does not bring in any significant variation in current density distribution.

- Voltage = 0.8V
- Cathode inlet velocity =0.06m/s

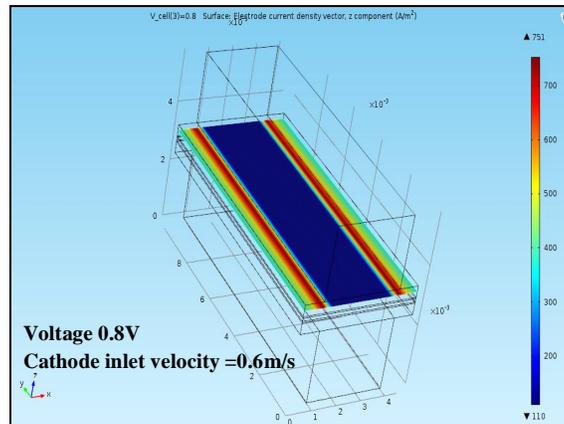


Figure 7: Surface plot representation of current density for 0.8 V at 0.06 m/s air velocity

Current density variations within the cells at the operating voltage of 0.8 V at different Air velocities are obtained. Similar plots are generated for a lower voltage value. There is a significant increase in the current density levels. Still, the geometrical design is found to be holding good, even with flow velocity reduction.

- Voltage = 0.6V
- Cathode inlet velocity =0.6m/s

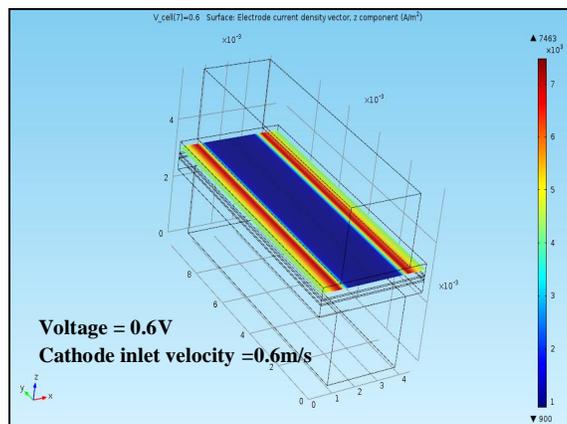


Figure 8: Surface plot representation of current density for 0.6 V at 0.6 m/s air velocity

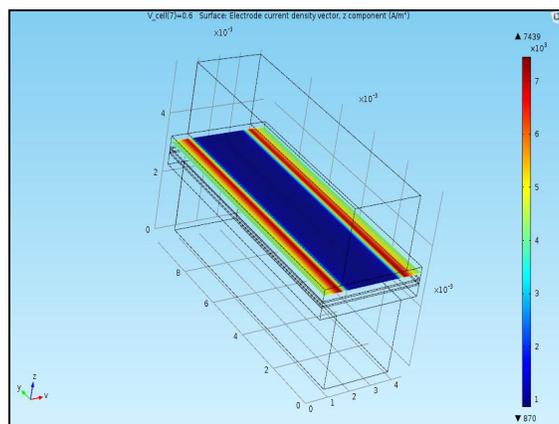


Figure 9: Surface plot representation of current density for 0.6 V at 0.06 m/s air velocity

For the computational analysis at different pressure conditions the polarization graphs shows some differences in current densities. The maximum operating pressure is 3 bar and the cell voltage is 0.8V. Only the electrode thickness is different (50 micron). At 0.6 bar and 1 bar the polarization curve lies on same current densitie

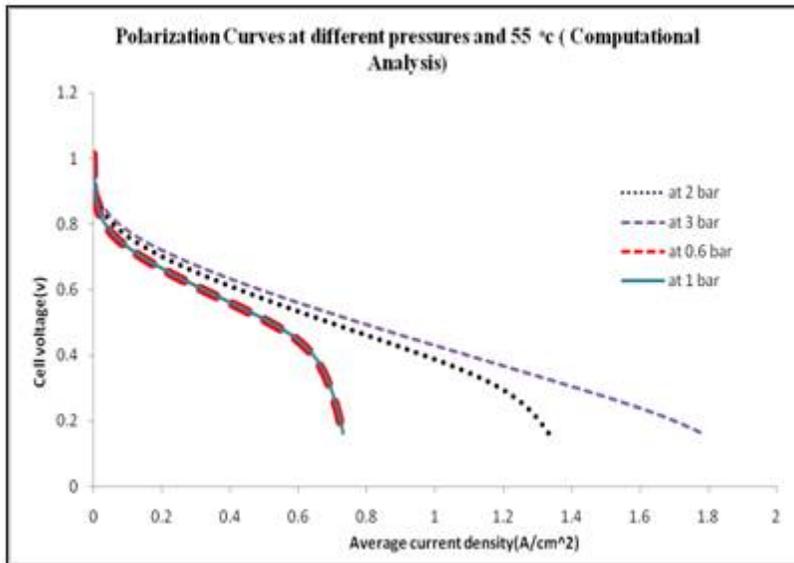


Figure 10: Polarization curve at different pressure conditions (computational analysis)

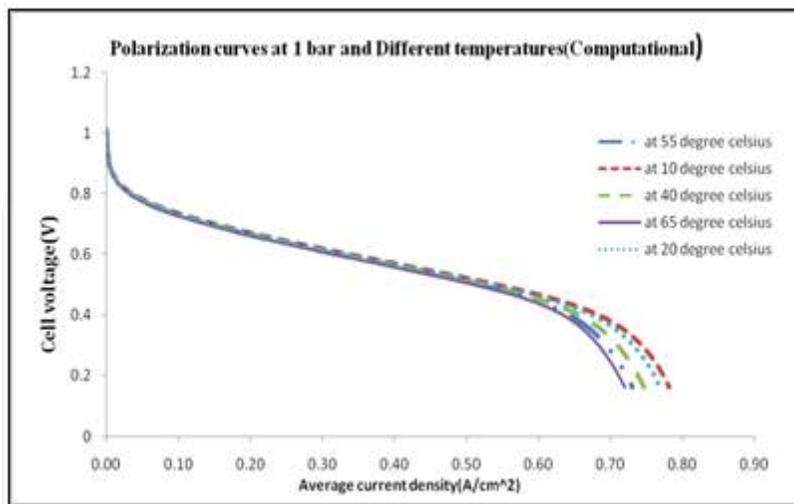


Figure 11: Polarization curve at different temperature condition (computational)

The polarization curve of experimental analysis is plotted and it shows the same effect that at we have seen at computational analysis. At different pressures and temperature condition current densities varying continuously.

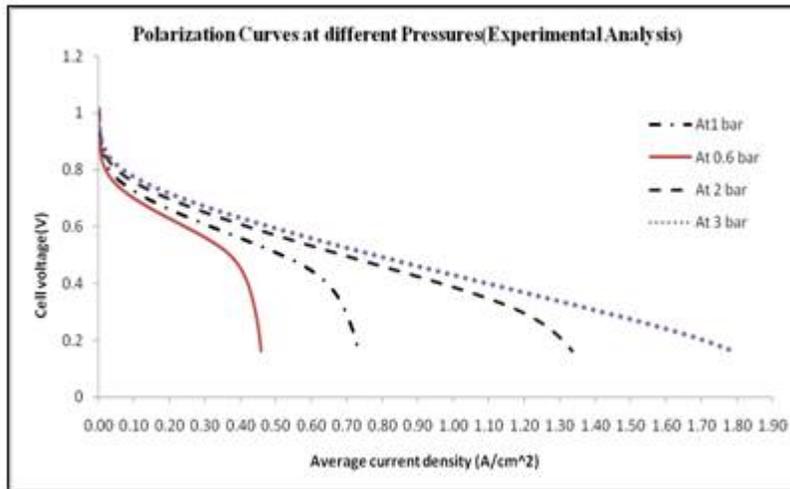


Figure 12: Polarization curve at different pressures (Experimental Analysis)

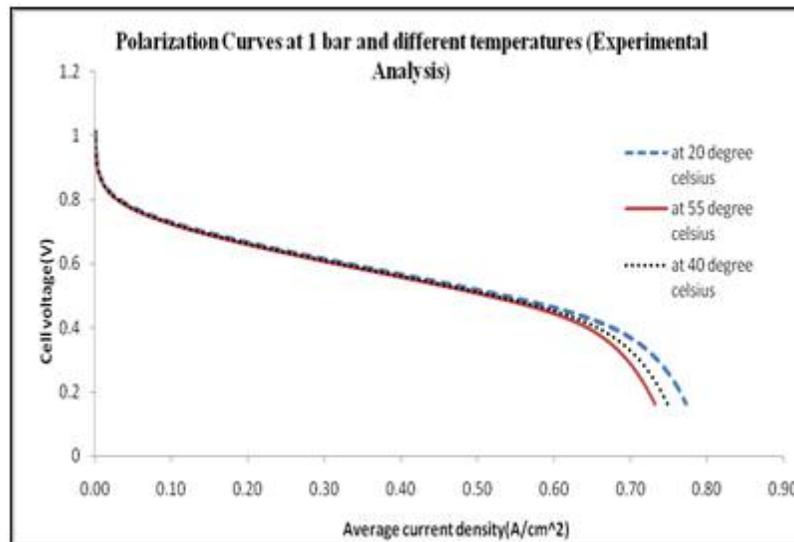


Figure 13: Polarization curve at different temperature (Experimental analysis)

5. Conclusions

In this study, a 3D PEMFC cathode model is developed and the kinetic phenomena in the catalyst layer are examined, specifically the reaction order of the Oxygen reaction rate. The main objectives of this thesis were to simulate PEMFC cathode behavior with experimental and computational data's. It was shown that there was little impact on the predicted polarization curve or the current density plots, and there was a very small drop of about 0.01 V in the predicted performance when the influence of the concentration overpotential was included in the model.

The influence of oxygen concentration on the fuel cell performance was examined in both the experimental as well as computational models. The oxygen concentration at the channel boundary was varied to simulate the effect of decreasing oxygen concentration at points downstream along the serpentine channel of a bipolar plate. The largest relative decreases in the predicted current density, at the membrane boundary, were observed at low and high cell potentials where activation and mass transport losses are dominant.

The power of a PEM fuel cell also depends on operating conditions such as flow rates, relative humidity and temperature of the gases. Mathematical modeling is very important for understanding this complexity. The models and results of other researchers is compared and evaluated. Results for the V-I characteristic of a fuel cell shows the expected output voltage is dependent on the load current. Dynamic interaction effects within a PEM fuel cell are significant, and detailed modeling for such transient effects is necessary. Using a simple procedure and data obtained from the literature, it is possible to obtain a model for a fuel cell stack. The fuel cells are modeled by using various mathematical equations.

6. Acknowledgement

Our sincere thanks to Nehru College of Engineering And Research Center, Pampady and Vikram Sarabhai Space Centre/ISRO, Thiruvananthapuram for providing the technical support.

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