# Performance Analysis of a Two phase Non-isothermal PEM Fuel Cell

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# ABSTRACT

A two-dimensional two-phase and non-isothermal model is presented to simulate a complete proton exchange membrane fuel cell (PEM FC). Water transport electrochemical and reactions are considered and all the governing equations for flow channels, catalysts, gas diffusion layers (GDL) and the membrane are solved. The model is nonisothermal and so the effects of temperature variation on cell performance are taken into account. Two phases of water which are liquid and gas are considered in the model. The dimensions are real values which are taken from Wang and Wang (2006). The flow fields are straight channels and the flows are taken in co-direction for the oxidizer and the fuel. To consider the effects of the flow direction, the calculations are done for a sample test of counter flow too. For the specified set of cell voltages, the cell's current densities are calculated and a polarization curve is developed for using air as oxidizer. The maximum power of the cell is also obtained. Some parametric studies are done to study the effect of the following parameters on the performance of the cell: porosity of the GDLs, porosity of the Catalysts, the channel width to length ratio, Anode Pressure, Cathode Pressure, and the oxidizer stoichiometric coefficient. The effect of each of the mentioned parameters on cell performance is obtained by keeping fixed all the others and varying only one, i.e. the partial derivative of the performance with respect to each parameter is numerically determined. The polarization curve is developed for each case. Depending on the obtained results, an optimized operating point for the whole cell is

attained. For each case the base case conditions are preserved for all the parameters that don't change.

# **1. INTRODUCTION**

Nowadays the demand for clean and renewable energy has accelerated the research activity for finding better sources. Fuel cells may be the answer to the increasing need of this kind of energy source. Fuel cells have applications in stationary, distributed, portable, mobile, and even biological power sources.[1]

Fuel cells convert chemical energy directly into electricity by separation of anodic oxidation of fuel and cathodic reduction of oxygen. Protons generated at the anode transport to the cathode, where they recombine with oxygen anions to form water. Fuel cells are consist of an anode part, a cathode part and a membrane. Anode and cathode parts contain flow channels, Gas diffusion layers (GDL) and catalysts. Two plates which are called bipolar plates, are placed on the outer surfaces of the cell to collect the electrical current.

One type of fuel cells are PEM (Proton Exchange Membrane) fuel cells which use Hydrogen as fuel and air as oxidizer. The electrochemical equation of Anode (1) shows that Hydrogen transforms into positive Hydrogen ions and electrons.

$$2H_2 \rightarrow 4H^+ + 4e^- \tag{1}$$

Cathode electrochemical equation (2) shows that atoms of Oxygen react with  $H^+$  ions (transferred via membrane) and electrons (transferred via outer wire) to form water.

$$O_2 + 4e^- + 4H^+ \rightarrow 2H_2O \tag{2}$$

Considering the equations (1) and (2), the governing equation of the cell can be written as in (3).

$$2H_2 + O_2 \rightarrow 2H_2O + Electrical Energy + Heat$$
 (3)

Equation (3) shows that the cell generates heat and electric current and water as products of the reaction. The generated electrons can perform work if they are transferred from anode to cathode via a wire.

One of the most important parts of the simulation is solving the energy equation that covers the water production heat, the loss due to resistance of the material and the latent heat of water evaporation.[9] All these effective terms are taken in to account.

In this report a two-dimensional two-phase and nonisothermal model is presented to simulate a complete proton exchange membrane fuel cell (PEM FC). The 3-D geometry of a PEM FC is shown in Fig. 1, with the computational domain shown as a planar vertical slice. This slice is shown in Fig.2. Two dimensional model with straight channels is fed with hydrogen as fuel and air/oxygen as oxidizer. Working current of the cell is calculated with constant voltages. Depending on the results, the pressure, the temperature and other parameters can be obtained all over the cell. Different effects of changing the direction of the flows and Hydrogen diffusion in anode GDL are studied and the polarization curves are drawn for different anode/cathode pressures. different catalyst/GDL porosities and different width to length ratios. The effects of oxygen stoichiometric coefficient on cell performance is also studied.

# 2. GOVERNING EQUATIONS

The governing equations in a fuel cell are continuity, momentum, energy, conservation of species, diffusion and electric field written in steady state form.

The equations are derived for steady state flow so we can neglect all the terms varying with time.

#### I – Continuity

$$\nabla . \rho \vec{u} = 0 \tag{4}$$

## **II- Momentum Equation**

$$\frac{1}{\varepsilon^2} \nabla .\rho \vec{u} \vec{u} = -\nabla p + \nabla .\rho \tau - \frac{\mu}{k} \vec{u}$$
(5)

where,  $\mathcal{E}$  is the porosity.

## **III- Energy Equation**

$$\nabla .(\rho \vec{u}h) = \nabla .(k \nabla T) + S_{ene} \tag{6}$$

$$S_{ene} = h_{phase} + h_{reaction} + I^2 R_{ohm}$$
<sup>(7)</sup>

where q is the conductive heat flux, and

h<sub>phase</sub>= water latent heat

h<sub>reaction</sub>= water production heat

 $I^2R_{ohm}$  = loss to current resistance

#### **IV** – Species conservation

$$\frac{\rho D_i}{\delta} (y_{i,surf} - y_{i,cent}) \eta = \frac{M_{\omega,i}}{nF} R_{an,cat}$$
(8)

where:

 $\begin{array}{ll} Di &= mass \ diffusion \ of \ i^{th} \ part(m^2/s) \\ \eta &= surface \ to \ volume \ ratio \ of \ catalysts(1/m) \\ y_{i,surf} &= mass \ fraction \ of \ i^{th} \ part \ on \ reaction \ surface \\ y_{i,cent} &= mass \ fraction \ of \ i^{th} \ part \ in \ element \ center \end{array}$ 

 $\delta$  = the average length between the surface and center of each element

## **3.** SIMULATION

The meshed model is developed with the geometrical characteristics of the cell which are shown in Table(1). There exist 58800 ( $700 \times 84$ ) cells in the meshed model that results in good aspect ratio and also in good convergence rate. The model is solved via the commercial CFD software package FLUENT. The continuity, momentum, energy, electrochemical, diffusion, electric field and other equations such as state equation are solved. The boundary conditions and dimensions for base case are shown in Table (1).

channel length (mm)	70	
Channel width (mm)	1	
GDL width (mm)	0.3	
Catalyst layer width (mm)	0.014	
Membrane width (mm)	0.1	
Current collector width (mm)	0.5	
GDL porosity	0.5	
Catalyst layer porosity	0.5	
Inlet temperature (K)	313	
Anode gauge pressure inlet(atm)	1	
Cathode gauge pressure inlet(atm)	2	

Table (1) – The base case parameters

The 2 dimensional fuel cell is in fact the central surface of a 3 dimensional cell which is shown schematically in Fig.1



Fig.1 The 3D schematic picture of the cell. The selected 2D slice is used for the present study.

The selected surface of Fig.1 is the 2-D model considered in present study. (Fig.2)

As shown in Fig.2 the MEA is consist of Membrane, and catalysts of both anode and cathode sides. The flow direction shown in the Fig.2 is co-flow. The dimensions shown on the fig (also in Table(1)) are the reasonable values taken from literature for example Wang and Wang. [2] and Berning and Djilali [3]



Fig.2 The 2D schematic picture of the cell.

#### 3.1 Porosity Study

The porosity of catalyst and GDL are changed and the effects are taken into account. The cell's polarization curve is developed for GDL porosity of 0.3, 0.4, 0.5, 0.6 and 0.7.

The polarization curve is acquired for catalyst porosities of 0.3 and 0.5.

### 3.2 Channel Width to Length Ratio Study

The cell's polarization curve is developed for channel widths of 1 mm and 2 mm while the length is considered to be equal to 70 mm.

#### **3.3 Anode Pressure Study**

The effects of pressure on cell performance are considered for anode pressures of 1atm and 2atm. (gauge pressures) The cathode pressure is taken equal to base case. The results are discussed considering the new polarization curve.

#### 3.4 Cathode Pressure Study

The effects of pressure on cell performance are considered for cathode pressures of 1atm and 2atm. (gauge pressures) The anode pressure is taken equal to base case. The results are discussed considering the new polarization curve.

#### **3.5 Cell Pressure Study**

The effects of changing anode and cathode pressure simultaneously are taken in to account and the importance of changing anode pressure is compared with cathode pressure changing.

#### 3.6 The Cathode Stoichiometric Coefficient

The cell's current is developed for Oxygen stoichiometric coefficients of  $0.2, 0.25, \ldots, 0.7$  in

cell voltage of 0.75v. The effects of increasing the stoichiometric coefficients of O2 are discussed.

# 3.7 Counter Flow Study

To consider the effect of flow direction in cell performance, the base case is also studied in counterflow direction. The polarization curve is developed.

#### 3.8 Temperature Distribution

The contour of temperature is shown for all the layers in cell.

## 3.9 Balance of Oxygen and Water

The mass fraction of Oxygen in GDL and catalyst of Cathode also in membrane are shown. Mass fraction of water is developed for Anode and cathode GDLs and for membrane.

# 4. RESULTS AND DISCUSSION

With the boundary conditions listed in Table(1) the results are calculated for base case. Using the open circuit voltage of 1.18v the polarization curve is drawn. (Fig.3).



The results are compared with [5] and considering the tiny differences in the cases, a satisfactory equality is observed. It must be mentioned that the polarization curve differs largely while open circuit voltage and the inlet pressures change. Calculating the power and drawing the power vs. voltage for base case leads to Fig.4 that shows the maximum power can be obtained in voltage of 0.6v.



Fig.4 The power-voltage diagram

The water content (a factor expressing amount of water in membrane[1]) is an important factor in the current density. For all the points of polarization curve the water content is in a reasonable range. Based on the results it has a minimum of around 5 and maximum of around 15 and its average value is around 10.

The losses that affect the polarization curve can be categorized in 4 types:[4]

- 1- Open circuit loss due to fuel crossover
- 2- Rapid drop off due to activation losses
- 3- Linear drop off due to ohmic losses
- 4- Mass transport losses at high current densities

In Fig.5 the polarization curve for Anode/Cathode pressures of latm are drawn and these 4 parts are marked. By comparing this curve with the other curves the effects of different parameters on polarization curve can be seen. For instance by comparing Fig.3 ( $P_{ca}=2atm$  and  $P_{an}=1atm$ ) with Fig.5 ( $P_{ca}=P_{ca}=1atm$ ) the main difference can be found in part 4 which means that the effect of transport losses decreases when the pressure rises. Some other comparisons could be done in the same way to observe the effect of different parameters on polarization curve. The loss of open circuit reduces the maximum available voltage from 1.18v to about 1.1v, so the three other losses are more important which are explained more in part 4.1.



Fig.5 The power-voltage diagram

#### 4.1 Porosity Study

The polarization curve for GDL porosities of 0.3-0.7 is shown in fig.6.



Fig.6 The polarization curve for GDL porosities of 0.3-0.7

As explained before, the polarization curve can be divided into 3 parts: the high voltage region (above 1 v) in which the activation losses play the important role, medium voltage region (between 0.7 v and 1 v) in which the losses are linear, and low voltage region (below 0.7v) in which the Mass transport losses are more important. In high voltage region the current density is decreased as porosity is increased. In medium region the current density increases steadily as porosity is increased. In low voltage area mass transfer losses become so important that conceal the other losses...[4]

Since the thickness of catalyst is one order of magnitude smaller than GDL and more than 2 orders of magnitude smaller than channel width, changing catalyst porosity is not much sensible. The polarization curves for catalyst porosities of 0.3 and 0.5 are shown in fig.7 for instance.



Fig.7 The polarization curve for catalyst porosities of 0.3 and 0.5

### 4.2 Channel Width to Length Ratio Study

To consider the Channel width to length ratio effect the length is taken constant. (as in base case equal to 70mm) and the polarization curve is developed for channel widths of 1mm and 2mm. (Fig.8)



Fig.8 Channel width to length ratio effect

## 4.3 Anode Pressure Study

Upon the Darcy's law of diffusion[7] the transferred mass via porous media increases as the pressure gradient increases. So it is supposed to have higher current densities in higher pressures.[10] The results prove this to be correct. As we can see in Fig.9

# 4.4 Cathode Pressure Study

Like part 4.3 the cathode pressure study shows that increasing the pressure increases the current density. (Fig.9)

# 4.5 Cell Pressure Study

Changing both the anode and cathode pressures, we can compare the effect of anode pressure and cathode pressure. As can be seen in Fig.9 the current density increases while moving from anode/cathode pressure of 1at to anode/cathode pressure of 2at.

The interesting point is the fact that current density is higher with anode pressure of 2at and cathode pressure of 1at (green curve) comparing the case in which the cathode pressure is 2at and anode pressure is 1at.(red curve) It can be said that anode pressure plays a more important role in cell performance.



Fig.9 Anode/Cathode pressure effect on polarization curve

Considering the high voltage region (over 1v), we see that this effect is vice versa i.e. in high voltage region the cathode pressure is more important.

# 4.6 The Cathode stoichiometric coefficient Study

Increasing the cathode stoichiometric coefficient, the current density is obtained.(Fig.10) All the other parameters are taken constants. (equal to base case) the working voltage is 0.75v. since the voltage is constant, the increase in current density shows the

increase in power. So depending on economic limitations for feeding pure oxygen, higher powers can be attained.



Fig.10 Cathode stoichiometric coefficient effect on the current density

# 4.7 Counter flow study

Considering the base case with counter-direction results in Table(2), which shows that changing the direction of the flow has an insignificant effect on cell performance. The results of counter flow direction show that the maximum difference between the co and counter flow cases is around 0.007 A/cm<sup>2</sup>.

	co flow	counter flow	difference
V(v)	i(A/cm2)	i(A/cm2)	i(A/cm2)
0.35	2.304	2.297	0.007
0.45	2.04	2.035	0.005
0.55	1.782	1.778	0.004
0.65	1.509	1.508	0.001
0.75	1.207	1.207	0
0.85	0.873	0.873	0
0.95	0.521	0.521	0
1.05	0.1093	0.115	-0.0057
1.15	0.000666	0.000671	-0.000005

Table(2) co/counter flow currents

The obtained results show complete coherence with literature. For example compared to the results of Singh [8] and Rismanchi [6] the results are the same.

# 4.8 Temperature Distribution

Fig.11 shows that the temperature gradients are greater in depth of the cell comparing the gradients

along the flow channels. The temperature is higher in center of the cell due to the electrochemical reactions.



Fig.11 Temperature contour

4.9 Balance of Oxygen and water

The oxygen in cathode side diffuses through the GDL and catalyst layers to reach membrane. In Fig.12 the distribution of mass fraction of oxygen is shown. The mass fraction of cathode inlet for base case is 0.2 which is used for oxygen balance study. As can be seen the mass fraction of oxygen decreases as flow passes through GDL (bottom) and catalyst and membrane (top) i.e. there can be seen a decrease from the input mass fraction to zero.





Fig.12 Mass fraction of Oxygen in Membrane(top) and Cathode GDL (bottom)

The membrane can pass  $H^+$  only when there exists wetness. To moist the membrane the input Hydrogen flow must be humidified. The reactions as can be seen in equation (3) produce water too. And also the membrane must not get flooded. There exists a specific range for better performance of membrane. [1] So water balance of cell is of high importance.



Fig.13 Mass fraction of H<sub>2</sub>O in Anode GDL(top), Membrane (middle) and Cathode GDL (bottom)

Fig.13 shows water balance in cell. As can be seen, water transfer direction is from GDL to membrane. Fig.14 shows the contour of mass fraction of  $H_2O$  in membrane.



Fig.14 Contour of Mass fraction of H<sub>2</sub>O in Membrane

# **5.** CONCLUSION

A parametric study has been done for a PEM fuel cell of the configuration shown in Fig.2. the study includes the test cases for:

 $\varepsilon_{\text{GDL}} = \{0.3, 0.4, 0.5, 0.6, 0.7\},\$ 

 $\epsilon_{catalyst} {=} \{0.3,\,0.5\}$  ,

Anode Pressure=  $\{1atm, 2atm\}$ ,

Cathode Pressure={1atm, 2atm},

Channel width= $\{1mm, 2mm\},\$ 

Oxygen stoichiometric coef =  $\{1, 1.5, 2.0, 2.5, 3, 3.5\}$ 

and counter flow direction of base case.

In a Fuel cell the most important goal is to produce maximum power, and to achieve this goal it is necessary to know that in which voltage the maximum power is obtained As can be seen we can now find the optimum working point of the cell. Using Fig.4 it can be said that the maximum power occurs at open circuit voltage of around V = 0.6v. The maximum power is around 1 watt in this case. cell studied in this report, the optimal For the values are as follows:  $\varepsilon_{GDL}=0.6$ ,  $\varepsilon_{catalyst}=0.5$ , Channel width=1 mm, Pan=Pca=2 atm, Oxygen coefficient=3.5 (depending on stoichiometric economic and also design limitations the more the pressure and the stoichiometric coefficient are increased the higher power can be obtained.) as mentioned in part 4.4 the importance of anode pressure increase is more than cathode. So in case of having any limitations in supplying higher pressure, it is more economical to increase anode side pressure.

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