Operating Parameters Optimization of a Mono Cell Proton Exchange Membrane Fuel Cell

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Abstract

Large numbers of experiments are often needed to find the effects of the parameters on performance of PEMFC, but it is well known that pressure and temperature were the effective parameters in Performance of fuel cell. In this study, the genetic algorithm was applied to determine working conditions that obtaining maximum power density of a PEMFC. A quasi two dimensional, isothermal model was used for the Proton exchange membrane (PEM) fuel cell as fitness function of genetic algorithm and experimental setup was developed to validation of that modeling. At last the best values of parameters were determined.

Keyword: PEM Fuel Cell, Genetic algorithm, Analytical Model, Optimization

1 Introduction

Polymer electrolyte membrane fuel cell is considered as being one of the most promising technologies able to produce efficient and environmentally friendly energy [1]. The performance of PEMFC, is known to be influenced by many parameters such as operating temperatures both fuel cell and humidifiers, pressure, flow rates and relative humidity of fuel and etc. Other variables which are out of the operating parameters such as different membrane thickness and type, different catalyst load, path of the reactants flow and etc, although very important, but they are not operating variables and. they can not be modified during the cell utilization [2]. Large numbers of studies discuss the parameters affecting the performance of PEMFC. Wang et al. [3] studied experimentally the effects of different operating parameters on the performance of PEMFC. Ticianelli et al. [4] studied experimentally to improve the performance of PEMFC. The most of past research was focused in discrete and certain value of parameters because that research was done by experimental approach. Temperature and pressure optimization
of fuel cell in cathode and anode side affecting the performance of PEMFC as some of the main important parameters, so we optimize these parameters using Genetic Algorithm that is one of the most suitable optimization tool. This paper considers these parameters in low discrete step domain by analytic model and genetic algorithm.

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2 Genetic algorithm descriptions

Genetic algorithms method combines mathematical analysis with random search to build artificial systems having properties similar to natural systems. GAs is a highly parallel mathematical algorithm that transforms a set of individual mathematical objects (chains of chromosomes); each of them associated to a fitness criterion, into a new population using genetic operations. These operations are modeled based on the Darwin theory of reproduction and survival of the fittest, as a result of the execution of a series of them [5]. There are some operator eq. crossover and mutation that they are applied for searching of best solution in determined domain. More information about description of genetic algorithm exists in literature. A modify GA with elitist concept was applied to keeping the best part in each population and no missing the best chromosomes. We wrote this program by manuscript file of MATLAB software that is very simple and user friendly. The parameters values of genetic algorithms used are given in Table 1. Table 2 gives the upper and lower limits of the optimized parameters.

Table 1.Values of genetic algorithm parameters.

Number of generations	150
Population size	25
Number of parameters	3
Crossover rate	90%
Mutation rate	10%

Table 2. Upper and lower values of the parameters to be optimized (search space).

parameter	Lower limit	Upper limit
Cathode pressure	1 bar	5 bar
Anode pressure	1 bar	5 bar
Cell temperature	$50^{o}C$	$80^{o}C$

3 GA Fitness Function

The serious part of Genetic algorithm is fitness function as gauge of chromosomes. Our fitness is maximum power density, in other word, goal is to find the best value of anode and cathode pressure and temperature that have highest output power. For fitness calculation, maybe more than thousand cases must be calculated. Unfortunately experimental method need to large numbers of experiments, that this manner is very time-consuming and costly, to overcome this challenge we modeled the PEMFC using analytical method and used as fitness function.

4 PEMFC Analytical Modeling

Two-one dimensional models were used to simulate flow behavior in channels and PEM. These models solve the governing equations in the direction of channels to calculate concentration, velocity and pressure distribution and also, the equations in the direction normal to the channel to find fuel cell polarization curve. Governing equations in each section are as following.

4.1 Channel

Variations of velocity and concentration through the channel were assumed one dimensional and so for single phase flow, we have:

$$\frac{d}{dx}[\rho U] = -\frac{M\,N}{H} \tag{1}$$

where U is average velocity in the channel and N is molar flux between the channel and MEA. Also, H and ρ are channel's height and gas mixture's density, respectively. By the conservation of species, equation of single phase flow for each component is:

$$\frac{d}{dx}[U_i\,C_i^{\,k}] = -\frac{h_m^k(C_i^{\,k} - C_i^{\,k}\big|_{y=H_{ch}})}{H} \tag{2}$$

where C is molar concentration and k is an identifier for the type of species in each side (i.e, Hydrogen at anode and oxygen and water vapor at cathode side). The right hand side of equation 2 shows the effect of diffusion at channel/backing layer interface. Coefficient h_m can be estimated by:

$$h_m^k = Sh\,\frac{D_{eff}^k}{H} \tag{3}$$

Where H is channel's height and Sh is Sherwood number. Also, D_{eff}^k is effective diffusion coefficient of fluid from channel to backing layer.

4.2 PEM modeling

1-D model was used to simulate gases flow and concentration variations through PEM. So, assuming single phase flow, the continuity equation leads to:

$$d(\rho u) = S \tag{4}$$

S is rate of consumption or production in catalyst layers and equal to:

$$S_a = S_{H_2} + S_{H_2O} \quad \text{at the anode side} \tag{5}$$

$$S_c = S_{O_2} + S_{H_2O} \quad \text{at the cathode side} \tag{6}$$

Where rate of consumption of each species is

$$S_{H_2} = -\frac{I}{2F} \tag{7}$$

$$S_{O_2} = -\frac{I}{4F} \tag{8}$$

$$S_{H_2O} = -\frac{\alpha I}{2F} \quad \text{at the anode side} \tag{9}$$

$$S_{H_2O} = -\frac{(1+\alpha)I}{2F} \quad \text{at the cathode side} \tag{10}$$

α is net water transport coefficient across the membrane.

And so, the mass flow rate per unit area is

$$\rho u = cte \tag{11}$$

Also, from Darcy's equation we have:

$$\nabla p = -\frac{\mu}{k}u \tag{12}$$

3

Which k and μ are permeability of cathode baking layer and viscosity of gas, respectively. Distribution of spices at cathode side (oxygen, water vapor and carbon dioxide) can be estimated

by Maxwell's equation of distribution as:

$$\nabla x_i = \sum_j \frac{x_i N_j - x_j N_i}{C_T D_{ij}^{eff}} \tag{13}$$

which x and N are the mole fraction and molar flow rate of each species, respectively, and D_{ij} is the diffusion coefficient.

In catalyst layers, transports of species in each side are given by:

$$\nabla(\rho v x_i) = -\nabla N_i + S_i \tag{14}$$

i is H$_2$ or H$_2$O vapor at anode side and O$_2$ or H$_2$O vapor at cathode side

Current density, j, is related to H$_2$ and O$_2$ concentrations by simplified Butler-Volmer equation:

$$j_a = A_{av} j_{0,a}^{ref} \left(\frac{C_{H_2}}{C_{H_2,ref}}\right)^{1/2} \left(\frac{\alpha_a + \alpha_c}{RT} F \eta_a\right) \qquad \text{at the anode side} \tag{15}$$

$$j_c = A_{av} j_{0,c}^{ref} \left(\frac{C_{O_2}}{C_{O_2,ref}}\right) \exp\left(-\frac{\alpha_c}{RT} F \eta_c\right) \qquad \text{at the cathode side} \tag{16}$$

Where η and α are respectively, overpotential and charge transfer coefficient. A_{av} and j_o are active area and reference current density at each side. Cell voltage can be obtained as follows:

$$V = E_0 - \eta_a - \eta_c - E_{ohm} \tag{17}$$

where E_0 is open circuit voltage and E_{ohm} is ohmic voltage losses, η_a and η_c are anode and cathode overpotential, respectively.

4.3   Methodology of solution

For solving governing equations, first, channel must be divided into small parts and then by coupling PEM and channels equations for each element, polarization curve of fuel cell can be calculated. By following this process, current density and cell voltage can be estimated. Figure 1, gives an overview of the solution procedure.
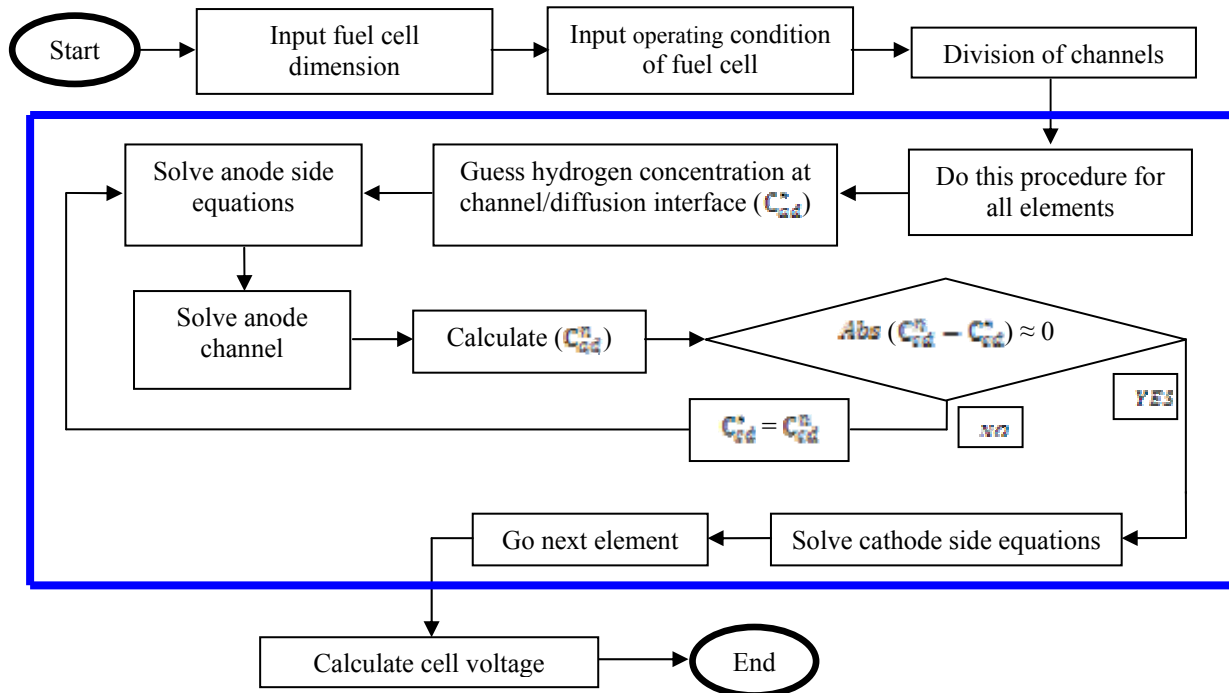
Figure 1: Solution algorithm.

5 Validation of modelling

For this purpose, an experimental set up was developed. Mono cell Proton exchange membrane fuel cell with 5cm*5cm active area was used to experimental validation of our analytic model. A standard MEA consists of a Nafion N112 membrane in combination with platinum and gas diffusion layers made of carbon cloth was purchased from E-TEK and used. Total specifications of MEA are given in Table 3.

Table 3. MEA properties.

MEA thickness	2 mills
Electrode active area	5cm*5cm
MEA total area	8cm*8cm
Amount of catalyst in cathode side	0.4 mg Pt/cm^2
Amount of catalyst in anode side	0.4 mg Pt/cm^2
Type of gas diffusion layer	Carbon cloth

Active area was obtained by grooving gas channels having 1*1mm^2 channel's cross section and with 1mm for channel rib. A schematic of PEMFC experimental setup for the experimental validation is shown in Figure 2. In Figure 3, the results of modeling at various input pressure was compared by experimental result.
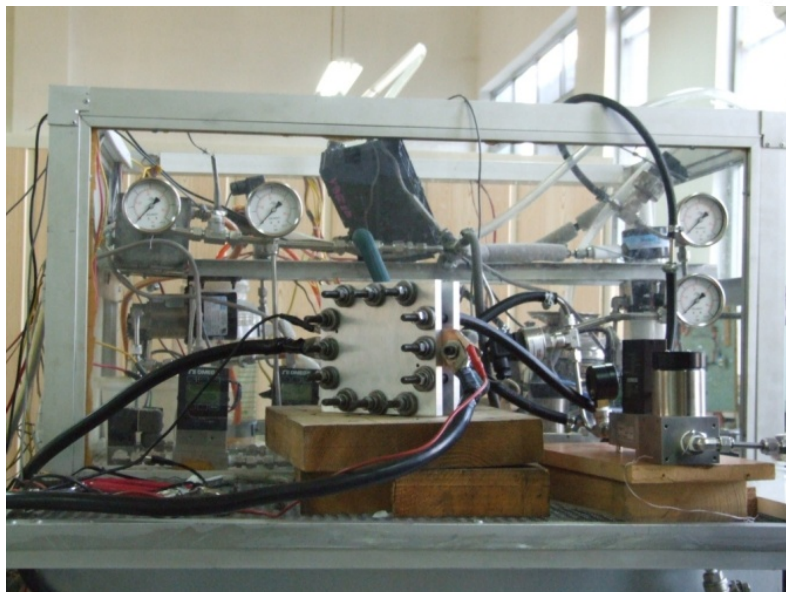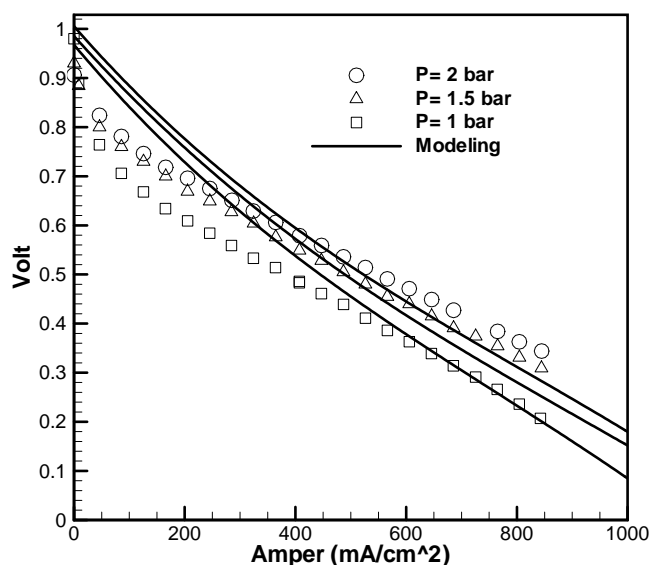
Figure 2: PEMFC experimental set up.

Figure 3: Polarization curves at different anode and cathode equal pressure. Fuel cell temperature is 60°C.

6 Constant primitive process parameters

The initial constant values for fuel cell modeling are different in research papers. Our fuel cell characterization and the constant values for simulation and optimization are shown in Table 4. It is used parallel geometrical for process optimization, because this type of channels for modeling have better agreement with experimental results. Input flow rate on both side and the constant of geometrical parameters are shown in Table 5.

Table 4. Parameters.

6

Condition and parameters in use	value	Ref
Anode and Cathode relative humidity (%)	100	Assumed
Anode and cathode diffusion layer thickness(cm)	0.02	[6]
Anode and cathode catalyst layer thickness(cm)	0.00287	[7]
Anode and cathode diffusion layer porosity	0.4	[7,8,9]
Anode and cathode catalyst layer porosity	0.4	[7,10]
Anodic transfer coefficient (α_a)	0.5	[6,7]
Cathodic transfer coefficient (α_c)	0.5	[6]
Anode and cathode specific area(1/cm)	6	Assumed
Anode and cathode hydraulic permeability	1	Assumed
MEA thickness(cm)	0.023	[7]
MEA Ionic conductivity (s/cm)	4.25	[9]
MEA porosity	0.1	[6]

Table5. Geometrical and flow rate parameters.

parameter	value
number of channel	10
Number of cells in stack	1
Anode and cathode width of channel (cm)	0.1
Anode and cathode height of channel (cm)	0.1
Anode and cathode length of channel (cm)	5
Input flow rate in cathode side (kg/s)	1.5e -5
Input flow rate in anode side (kg/s)	1e -4

7 Results and Discussion

By executing this MATLAB optimization code, solutions were generated in maximum power densities that are shown in Table 6. Figure 4 illustrates the convergence of the genetic code towards the best solution.

Table 6. Parameters value that produce maximum power.

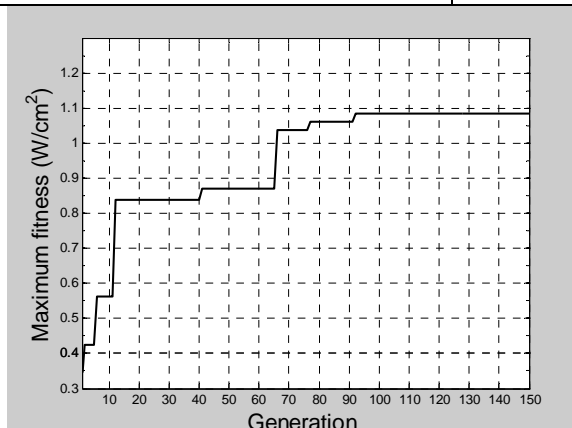| Cell temperature(^{o}C)	74
Anode pressure(bar)	5
Cathode pressure(bar)	5

Figure 4: Maximum fitness during the generations.

7

When the temperature goes above 50°C, the fuel cell performance gets better, but when it goes above 74°C, it drops due to the reason that at temperatures higher than the humidifier tank, MEA loses its moisture dramatically as a result of cell body warmth, therefore, the proton's conductivity in MEA would be decreased. This results in the enhancement of the cell internal resistance and the drop in cell performance. Maximum power density for different cathode and anode pressure at optimum temperature are shown in Figure 5, another pressure side is constant and equal to 5 bar. It is obvious that Anode pressure is more sensitive than cathode pressure.
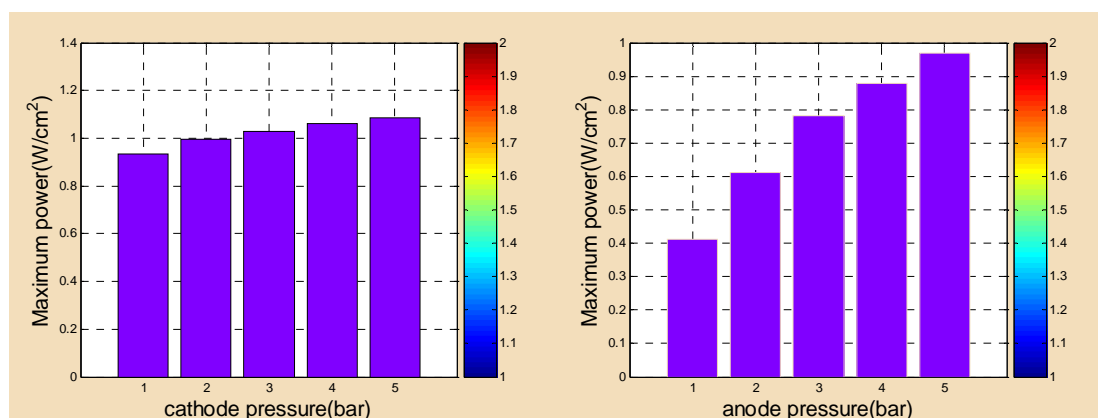

Figure 5: Maximum power at different cathode and anode pressure.

Figure 6 shows Maximum power according to the temperature and one pressure side that another pressure side is 5 bar. Unfortunately our experimental set up cannot suffer this loading condition test because that sealing system has not ability to pass this pressure condition and heater has not ability to create this loading temperature, but Our optimal result for maximum power density are agree with Süleyman et al. [11] closely, so reported 75°C temperature and 5 bar for anode and cathode pressure.
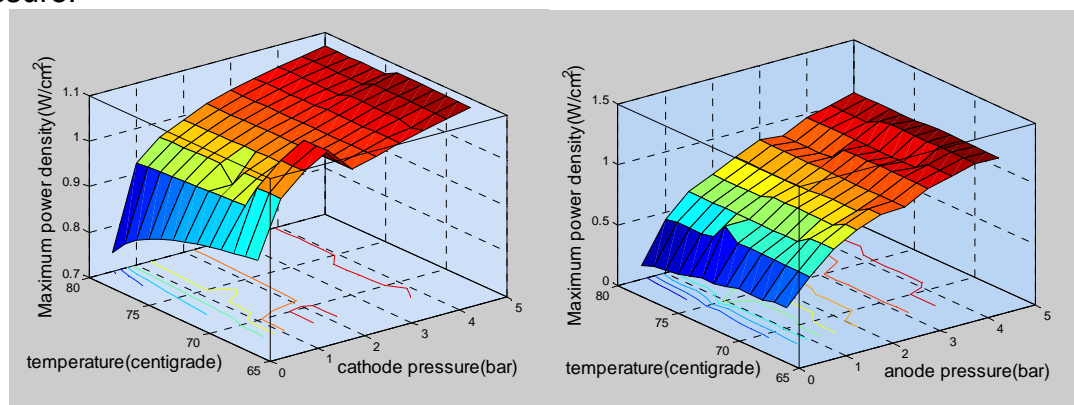

Figure 6: Maximum power value according to temperature and cathode/ anode pressure.

8 Conclusions

In this study, the genetic algorithm was applied to determine the Parameters of Process for Maximum Power of a mono cell PEMFC. A quasi two dimensional (1D-1D), isothermal model was presented for the PEM fuel cell. The model solves

governing equations of PMFC in the direction of the channel and a direction normal to it. We used this model as fitness function for GA. A genetic code was developed using MATLAB. Optimum working conditions obtained in maximum power density of a PEMFC.

Nomenclature

x	Channel's direction coordinate (cm) or mole fraction	R	Universal gas constant (8.314 J mol^{-1} K^{-1})	eff	Effective value
U	Channel's Velocity (cm s^{-1})	T	Temperature (K)	a	Anode side
N	Molar flow rate (kg cm^{-2} s^{-1})	V	Cell voltage (V)	c	Cathode side
H	Channel height (cm)	E	Electromotive force (V)	H_2	Hydrogen
M	Molecular weight (kg mol^{-1})			H_2O	Water
C	Molar concentration (mol cm^{-3})	***Greek symbols***		O_2	Oxygen
y	MEA normal direction coordinate (cm)	α	Net water transport coefficient or charge transfer coefficient	av	Active
D	Diffusion coefficient (cm^2 s^{-1})	μ	Viscosity of gas (kg m^{-1}s^{-1})	ref	Reference state
S	Rate of consumption (mol s^{-1} cm^{-2})	η	Overpotential (v)	ohm	Ohmic losses
j	Current density (A cm^{-2})	ρ	Density (kg m^{-3})	T	Total
j_o	Reference current density (A cm^{-2})	v	Kinetic viscosity (cm^2 s^{-1})	ad	Anode diffusion
u	Velocity in y direction (cm s^{-1})			cd	Cathode diffusion
F	Faraday's constant (96,487 C mol^{-1})	***Superscript***		***Acronym***	
I	Current density (A cm^{-2})	k	Identifier	PEMFC	Polymer electrolyte membrane fuel cell
p	Pressure (Pa)	ref	Reference value	GA	Genetic algorithm
k	Permeability	eff	Effective value		
A	Area (cm^2)	***Subscript***			
		ch	Channel		

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