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Development a new equation of polarization curve for a proton exchange membrane fuel cell at different channel geometry

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Abstract
The polarization curve of a proton exchange membrane fuel cell is an important parameter that is used to investigate the performance of it that is expressed with the Nernst equation with the equation of losses the voltage such as activation loss, ohmic loss and concentration loss that they are a function of temperature of the cell and the current density. In this study a new correlation for polarization curve is obtained that it is a function of temperature, current density and a new parameter of cross-section geometry of channels. For this purpose three PEM fuel cells with different channels geometry of rectangular, elliptical and triangular have constructed. The active area of each cell is $25cm^2$ that its weight is $1300gr$. The material of the gas diffusion layer is Carbon clothes, the membrane is nafion112 and the catalyst layer is a plane with 0.004 gr/cm^2 Platinum. Also a test bench designed and constructed for testing the cell and a series of experiments are carried out to investigate the influence of the geometry of the cell on performance of the cell. The results show that when the geometry of channel is rectangular the performance of the cell is better than the triangular and elliptical channel.

Keywords: Fuel cell; Curve fitting; Channel geometry; Performance.

1. Introduction

A fuel cell is an electro-chemical energy device that converts the chemical energy of fuel directly into electricity and heat, with water as a by-product of the reaction. Based on the types of electrolytes used, they are categorized into polymer electrolyte membrane fuel cells (PEMFCs), solid oxide fuel cells (SOFCs), phosphoric acid fuel cells (PAFCs), molten carbonate fuel cells (MCFCs), and direct methanol fuel cells (DMFCs). The polymer exchange membrane fuel cell (PEMFC) is considered to be the most promising candidate for electric vehicles by virtue of its high power density, zero pollution, low operating temperature, quick start-up capability and long lifetime.

Furthermore, the PEM fuel cell is being investigated as an alternate power generation system especially for distributed generation and transportation. The PEM fuel cell is providing reliable power at steady state; however, it is not able to respond promptly to a load step change. Since the fuel cell is an electrochemical energy conversion device that converts fuel into electricity, its dynamic behavior depends both on chemical and thermodynamic processes [1]. The polymer electrolytes work at low temperature, which brings this further advantage that a PEM fuel cell can start quickly. PEM fuel cells are being actively developed for use in cars and buses, as well as for a very wide range of portable

applications, and also for combined heat and power systems. It could be argued that PEM fuel cells exceed all other electrical energy generating technologies in the breadth of scope of their possible applications. Scrivano et al. [2] presented the results of an experimental analysis performed on an Exchange miniaturized, 6W Proton Membrane Fuel Cell (PEMFC) system, integrated with on-site hydrogen production by electrolysis; in particular, they investigated the effects of environmental parameters such as the external temperature and the humidity on the performance of fuel cells. Also they proposed a simple semi-empirical mathematical model capable to perform rough prediction on the behavior of such systems when exposed at different ambient temperatures. The model threats the stacks as black boxes, not investigating singularly the inner phenomena which occur in the cell. Amphlett et al. [3, 4] investigated a theoretical model which was employed to provide the structure of the equations, and then, the parameters of these equations were found by using the regression techniques to fit the experimental results. Also they studied a semi-empirical model with a theoretical background that takes into account the main variables of the fuel cell operation such as the operating temperature, the partial pressures at the electrodes and the fuel cell current. Del Real et al. [5] investigated a simple empirical equation to model the fuel cell voltage with considering the variations of the main process variables. The model equation has 11 parameters: one parameter related to the mass of liquid water at the anode channel must be estimated due to technical constraints, and the other parameters are obtained from experimental data. Although the model proposed by them, fitted well with the experimental data, the equation of the fuel cell voltage does not have a theoretical basis, and, therefore, it is based on assumptions relating to the effects of temperature and partial pressures that are not proven to be general for fuel cells other than those used in [5]. Khazaee [6] investigated numerically the effect of using different obstacles on the performances, current density and gas concentration for different Aspect Ratios and compared the results with experimental results of a triangular channel geometry PEM fuel cell. He found that by increasing the hydrogen flow rate from 0.3 L/min to 0.7 L/min and the oxygen flow rate from 0.5 L/min to 0.9 L/min the cell performance enhances. Also he found that by increasing the number of the blocks in the channels and installation of rectangular block, the overall cell performance increases. Ferng et al. [7] performed analytical and experimental work to investigate a single PEM fuel cell. In their paper, they presented a study of the cell performance covering the effects of operating temperature and pressure on performance and the flow characteristics within the cell. Their paper shows the positive effects of temperature and pressure on the performance of a single PEM fuel cell. Hussain et al. [8] investigated a thermodynamic model of a polymer electrolyte membrane (PEM) fuel cell power system for transportation applications. Their analysis includes the operation of all the components in the system, which consists of two major modules: PEM fuel cell stack module and system module and a cooling pump. System module includes air compressor, heat exchanger, humidifier and a cooling loop. They found that with the increase of external load (current density), the difference between the gross stack power and net system power increases and the largest irreversibility rate occurs in the fuel cell stack. Park and Xianguo [9] investigated a numerical and experimental study to investigate the cross flow in a PEM fuel cell. Experimental measurements revealed that the pressure drop in a PEM fuel cell is significantly lower than that without cross flow and three-dimensional numerical simulation has been performed for wide ranges of flow rate, permeability and thickness of gas diffusion layer to analyze the effects of those parameters on the resultant cross flow and the pressure drop of the reactant streams. Xianguo et al. [10] investigated the characteristics of liquid water removal from GDL experimentally, through measuring unsteady pressure drop in a cell which has the GDL initially wet with liquid water. They controlled the thickness of GDL carefully by inserting various thicknesses of metal shims between the plates. They found that severe compression of GDL could result in excessive pressure drop from channel inlet to channel outlet. Xianguo et al. [11] developed a non-isothermal stack model to analyze the effects of flow variance and temperature distribution on the performance of a polymer electrolyte membrane fuel cell stack. Their stack model consists of the flow network solver for pressure and mass flow distributions for the reactant gas streams and cooling water, and the heat transfer solver for temperature distribution among the cells in the stack, as well as the fuel cell model for individual cell performance. They found that the effect of temperature is dominant on the cell voltage variance when the flow variance is small for sufficiently uniform distribution of reactant flow among the cells in the stack. In this study the effect of changing the cross-section geometry of channels has been investigated experimentally and a new equation for polarization curve obtained that is a function of temperature, current density and the geometry of channels. Therefore The main objective of this paper contrary to another works is to analyze the influence of different geometries of the channels or flow fields on the

voltage (and consequently the electric power) supplied to a PEM fuel cell at different levels of cell current.

2. Description of the experiments and method of the measurements

For experimental investigation of the performance of the fuel cell a setup has been fabricated. A schematic flow of the test bench is shown in Figure 1. It allows controlling several physical parameters, and the measurement of many output data. In fact, the polymeric membrane has permeability to hydrogen and oxygen; due to the high-pressure gradient from cathode to anode, this driving force could push hydrogen from cathode to anode across the membrane and a dangerous mix with oxygen could occur; this concentration must always be kept below a safety level. The test bench is made up of four main subsystems. First, the gases supply system, which sends the oxygen and hydrogen flow into the system for electrochemical reaction. Second, there is two humidifier that humidify the oxygen and hydrogen before going into the cell for complete transferring of proton from the membrane to the cathode side. Third, the nitrogen supply system is applied to inert any flammable mix inside the ducts and to purge the system before activation. Finally, there is the electrical power supply, regulated from an AC/DC voltage regulator driven from the control panel.

The specifications of the test system for this study are:

- The humidifier system is membranous.
- The test bench has the system of announcement the leakage of hydrogen.
- The system can control and show the temperature of the oxygen and hydrogen.
- The system can control and show the temperature of the cell.
- The system can control and show the flow rate of the oxygen and hydrogen.
- The system can control and show the inlet pressure of the oxygen and hydrogen.
- The system can show the voltage of the cell.
- The system can show the current of the cell.

Table 1 shows the environs of operation of the experimental setup in this study.

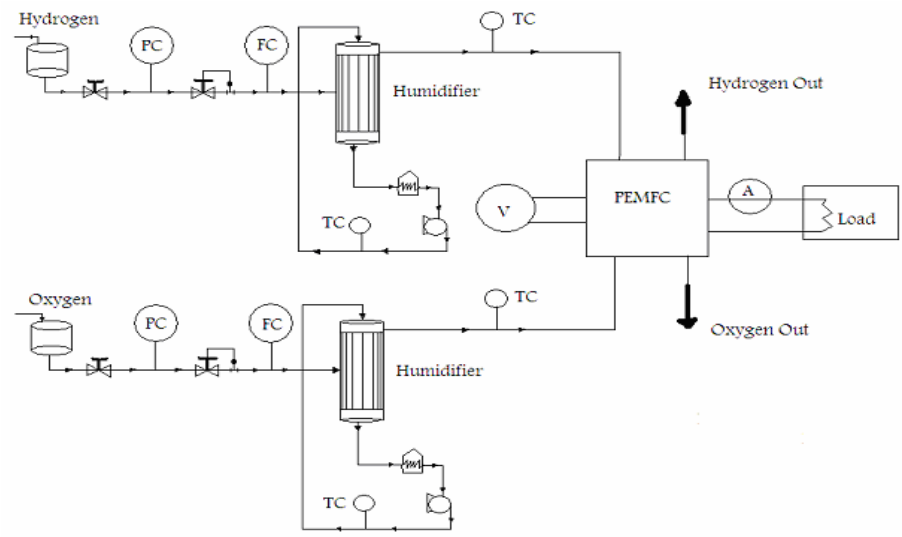

Figure 1. Schematic of the PEMFC system

Table 1. Operational characteristics of the test bench

Voltage	0-2 V
Current	0-20 A
Power	0-22 W
Moisture	100%
Flow rate	0-2 L/min
Gas temperature	Up to 75 ºC
Cell temperature	Up to 75 ºC

The PEM fuel cell considered in this study is a single cell with the size of 45x95x101 mm^2 and an active area of 25 cm^2 and serpentine and triangular flow field geometries of channels with the weight of 1300 gr. The width, land width and depth of the channel were selected to be 1, 0.8 and 2 mm respectively. For a bipolar plate, non-porous graphite is selected. A Nafion 117 membrane with 0.004 *gr/cm*^{2} Platinum for the anode and cathode was employed as a membrane electrode assembly. On both sides of the MEA, there were 0.33 mm thick carbon papers that acted as diffusion layers. The thickness of the catalyst layer and the proton exchange membrane is about 0.01 mm and 0.051 mm. The geometry of the channels of the cell in the experimental setup is shown in Figure 2. The examined prototype can operate at a maximum 5 bar absolute pressure; a pressure regulator valve is included, to make possible to vary the operating pressure of the FC system and the accuracy of monitoring the pressure is ±2%. Two flow meters is used to measure the flow rate of the oxygen and hydrogen that the accuracy of them is ±0.1L/min.

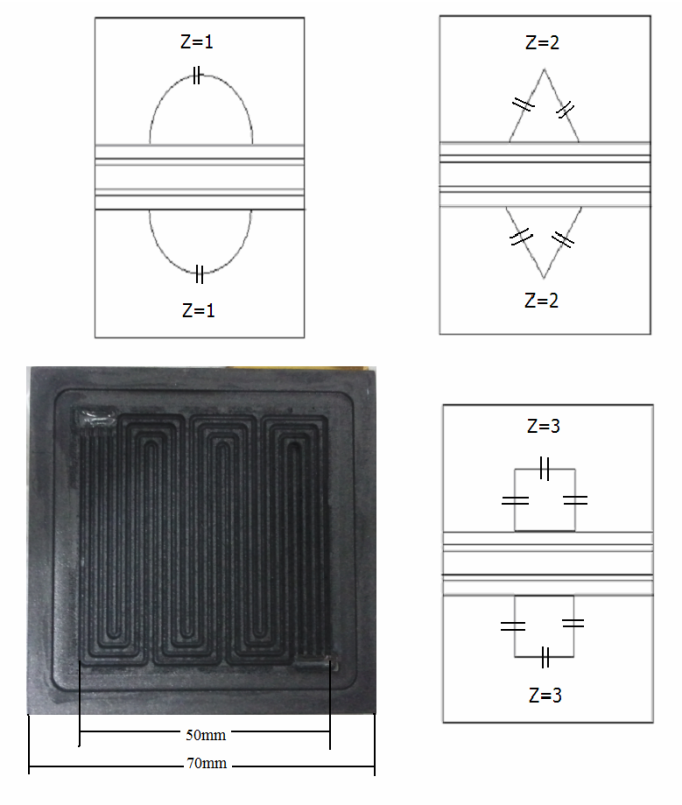

Figure 2. The channels of the PEM fuel cell

In order to plot the polarization curve and simulate a variable load, a resistors box was used that the accuracy of monitoring the voltage and ampere is ±1%. The resistors box, located outside the test chamber, is manually operated; the box and the cables do not introduce relevant errors because they are shielded from external magnetic fields (due to the very low current values). In order to operate in equilibrium conditions, current and voltage values corresponding to each particular value of the total resistance were measured after a sufficient time period to ensure stationary conditions to have been reached as concerns both fuel cell performance and the values of humidity and temperature in the test chamber. The temperature of the inlet gases was measured by digital thermometer with ±0.1ºC accuracy.
The changed parameters are: input oxygen temperature (To_2), input hydrogen temperature (T_{H2}), cell temperature (T_{cell}), input pressure (P), oxygen flow rate ($\dot{Q}_{O2}$) and hydrogen flow rate ($\dot{Q}_{H2}$) and the measured parameters are voltage and current of the cell. The Range of changing the parameters in this study is shown in Table 2.
At first, we perform the experiments by humidifying the membrane of the fuel cell by saturation water vapor and then change the input oxygen temperature, input hydrogen temperature, cell temperature, input pressure, oxygen flow rate and hydrogen flow rate and measure the pointed parameters and the voltage and the current of the cell after steady state condition. Figure 3 shows the experimental setup.

Table 2. Range of changing the parameters in this study

($\dot{m}_{H2}$) Hydrogen flow rate	0.3-0.9 L/min
($\dot{m}_{O2}$) Oxygen flow rate	0.5-1.3 L/min
(Po_2) Oxygen pressure	2-5 bar
(P_{H2}) Hydrogen pressure	2-5 bar
(T_{H2}) Hydrogen temperature	40-60 ºC
(To_2) Oxygen temperature	45-65 ºC
(T_{cell}) Cell temperature	40-60 ºC

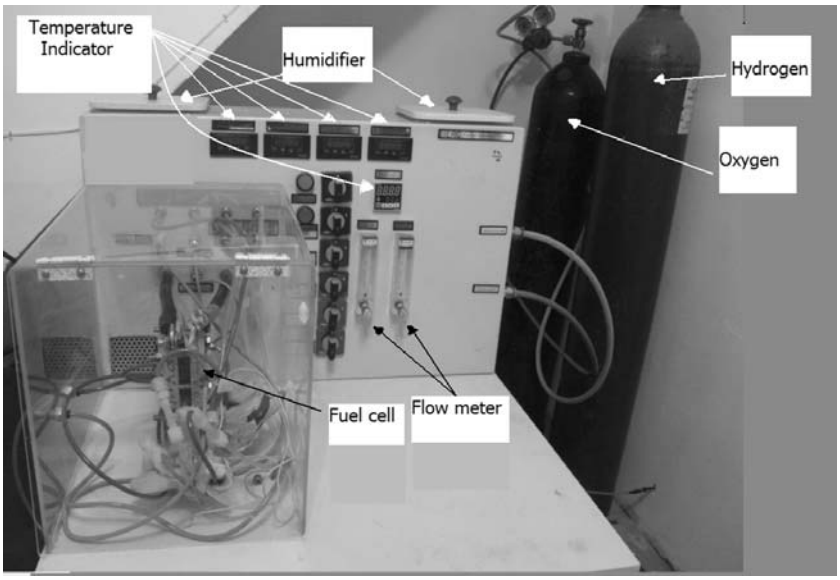

Figure 3. A photo of the experimental setup

3. Results and discussion

The main goal of this study is to investigate the effects of some parameters on the polarization curve of a PEM fuel cell and the performance of it. The Range of changing the parameters in this study is shown in Table 2 and the experiments for each of the parameters done and repeated while the steady condition occurred. Figures 4-6 show the effect of cell temperature on the performance of the fuel cell at P=2.905 bar, To_2=55 ºC, T_{H2}=55 ºC, $\dot{Q}_{O2}$=0.5 L/min and $\dot{Q}_{H2}$=0.3 L/min for elliptical, rectangular and triangular channel geometry. It is clear that increasing in the cell temperature leads to the increase in the performance of the cell which is due to the decreasing of activation overpotential and increase in the electrochemical reaction. This is because of the exchange current density of the oxygen reduction reaction increases rapidly with temperature due to the enhanced reaction kinetics, which reduces activation losses. A higher temperature leads also to a higher diffusivity of the hydrogen protons in the electrolyte membrane, thereby reducing the membrane resistance and this leads to reducing the potential loss in the membrane. Also they indicate that at the conditions of the higher operating voltage (lower over- potential), the influence of the internal flow modification on the overall fuel cell performance is negligibly small. At lower operating voltage conditions, on the other hand, the effect of the internal flow modification on the polarization curves becomes important.

In Figure 7 the effect of channel geometry on the overall cell performance of three PEM fuel cells for T_{cell}=60 ºC, To_2=55 ºC, T_{H2}=55 ºC, $\dot{m}_{O2}$=0.5 L/min, $\dot{m}_{H2}$=0.3 L/min and P=2.905 bar is shown. It is clear that when the geometry of the cell is rectangular, the overall cell performance is better than the elliptical geometry and triangular geometry that this is due to decrease in penetration of the gases into the gas diffusion layer and decreasing the chemical reaction at the surface of catalyst layers. At these conditions the maximum difference between the performance of rectangular and elliptical geometry is about 12% and between the rectangular and triangular geometry is about 18%.

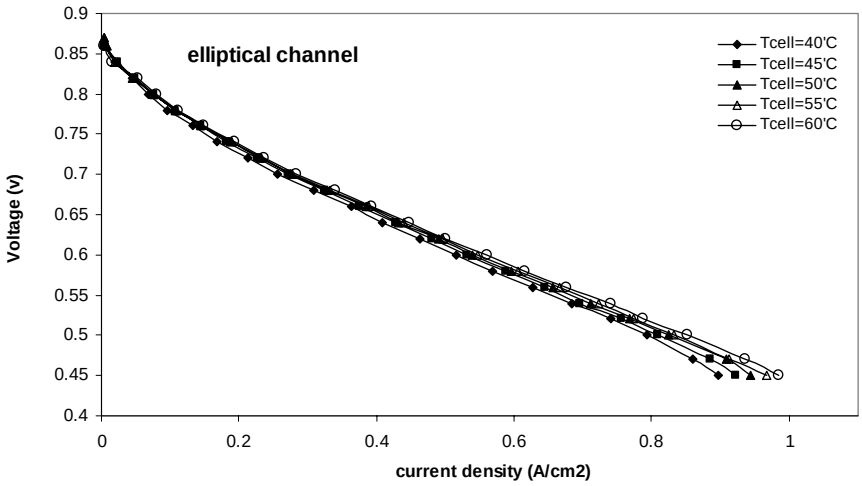

Figure 4. Variation of cell performance of elliptical channel geometry at different cell temperatures for P=2.905 bar, $\dot{m}_{H2}$=0.3 L/min, $\dot{m}_{O2}$=0.5 L/min, To_2=55 ºC, T_{H2}=55 ºC

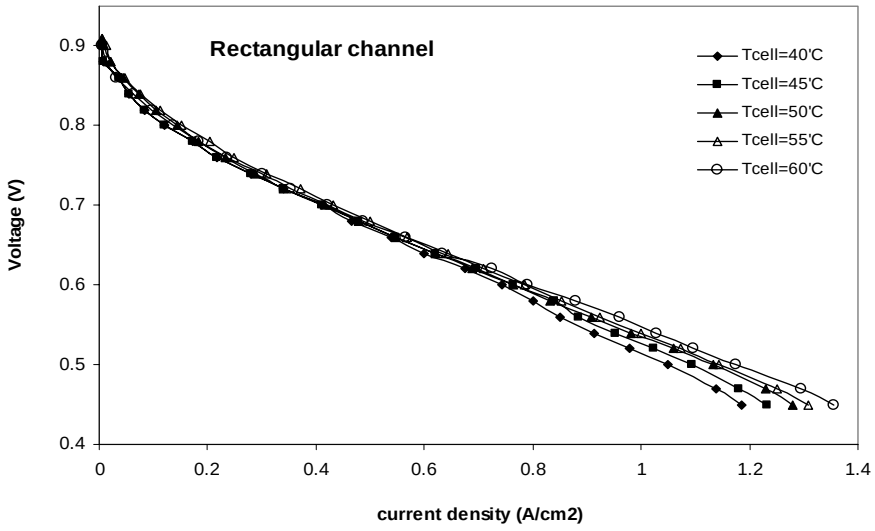

Figure 5. Variation of cell performance of rectangular channel geometry at different cell temperatures for P=2.905 bar, $\dot{m}_{H2}$=0.3 L/min, $\dot{m}_{O2}$=0.5 L/min, To_2=55 ºC, T_{H2}=55 ºC

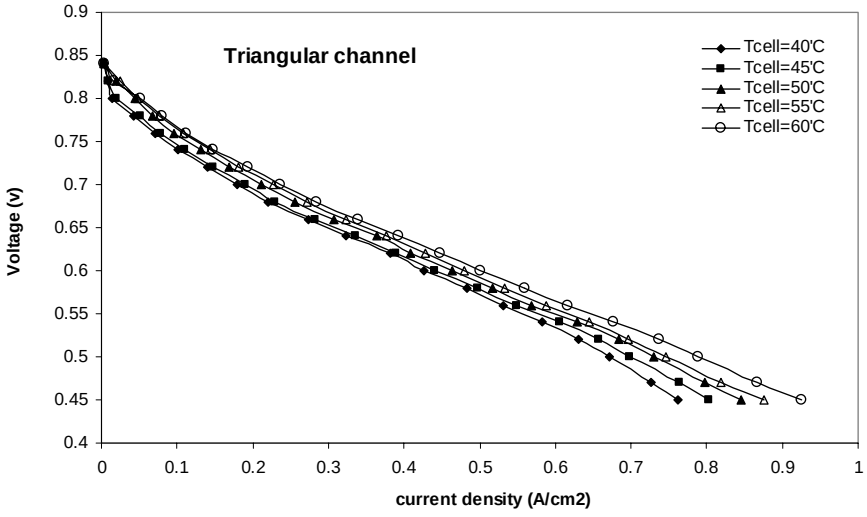

Figure 6. Variation of cell performance of triangular channel geometry at different cell temperatures for P=2.905 bar, $\dot{m}_{H2}$=0.3 L/min, $\dot{m}_{O2}$=0.5 L/min, To_2=55 ºC, T_{H2}=55 ºC

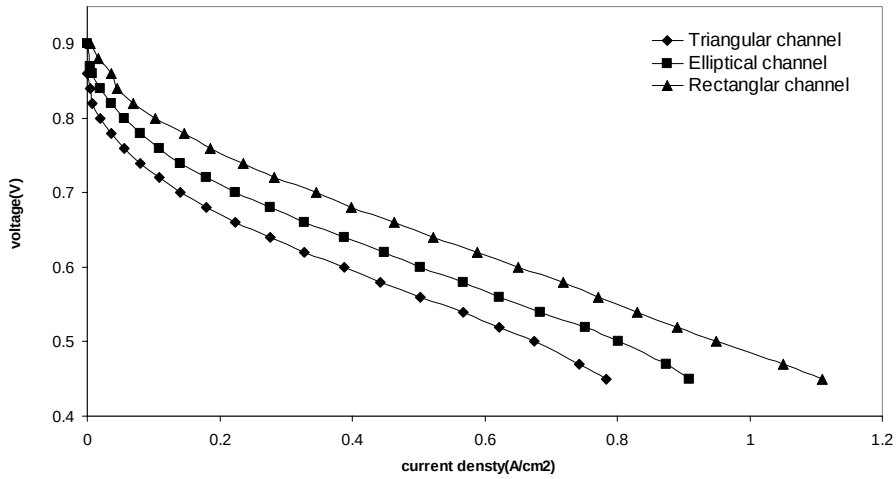

Figure 7. Variation of cell performance at different channel geometry for T_{cell}=60 ºC, $\dot{m}_{O2}$=0.5 L/min, $\dot{m}_{H2}$=0.3 L/min, P=2.905 bar, To_2=55 ºC, T_{H2}=55 ºC

3.1 A new equation for polarization of the PEM fuel cell

By doing the experiments, it is clear that some parameters such as cell temperature (T_{cell}) and channel geometry specification (Z) affect the performance of the cell. The main reason of changing the polarization curve by changing these parameters is the electrochemical reaction at the catalyst surfaces but the more details described in previous sections. Therefore the main goal of this paper is to obtain a semi-empirical equation for polarization curve that the method of fitting used in this paper is the least square method. This method fits a set of data points (x_i, y_i) to a function that is a combination of any number of functions of the independent variable x. The goal of nonlinear regression is to determine the best-fit parameters for a model by minimizing a chosen merit function. Where nonlinear regression differs is that the model has a nonlinear dependence on the unknown parameters, and the process of merit function minimization is an iterative approach. The process is to start with some initial estimates and incorporates algorithms to improve the estimates iteratively. The new estimates then become a starting point for the next iteration. These iterations continue until the merit function effectively stops decreasing. The nonlinear model to be fitted can be represented by:

$$y = y(x;a) \tag{1}$$

The merit function minimized in performing nonlinear regression the following:

$$\chi^2(a) = \sum_{i=1}^{N} \left\{ \frac{y_i - y(x_i;a)}{\sigma_i} \right\}^2 \tag{2}$$

where σ_i is the measurement error, or standard deviation of the *i*th data point. For understanding how the results calculated we have:

The *ith* predicted, or fitted value of the dependent variable Y, is denoted by $\hat{Y}_i$. This value is obtained by evaluating the regression model $\hat{Y} = f(X, \hat{\beta}_j)$, where $\hat{\beta}_j$ are the regression parameters, or variables. Then the residuals $(Y_i - \hat{Y}_i)$ and sum of the residuals $\sum_{i=1}^{n} (Y_i - \hat{Y}_i)$ calculated and then, the average of residuals and residual of sum of squares calculated.

SSE = Residual or Error Sum of Squares (Absolute) = $\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$

SSE_R = Residual or Error Sum of Squares (Relative) $=\sum_{i=1}^{n}[(Y_i-\hat{Y}_i)^2 * W_i]$ where $W_i = 1/\sigma_i^2$ normalized so that $\sum_{i=1}^{n} W_i = n$, σ_i = the standard deviation of the i_{th} data point Y_i and n is the number of data points, or observations.

The principle behind nonlinear regression is to minimize the residual sum of squares by adjusting the parameters $\hat{\beta}_j$ in the regression model to bring the curve close to the data points. This parameter is also referred to as the error sum of squares, or *SSE*. If the residual sum of squares is equal to 0.0, the curve passes through every data point.

Thus, the model that is used in this paper is an equation that is similar to Nernst equation [1]:

$$V = E_{rev}(T) - \eta_{act} - \eta_{ohm} - \eta_{conc} \tag{3}$$

The $E_{rev}(T)$ is a function of temperature of the cell that is:

$$E_{rev}(T) = 1.229 + aT + bT^2 \tag{4}$$

η_{act} ,η_{ohm} *and* η_{conc} are the activation loss, ohmic loss and the concentration loss that in this paper they have selected similar to equations that have described in reference [1] as:

$$\eta_{act} = T[c + dLn(i)] \tag{5}$$

$$\eta_{ohm} = (e + fT + gT^2)i \tag{6}$$

$$\eta_{conc} = (h + jT + kT^2)(l + mZ + nZ^2)Ln\left[1 - \frac{i}{o + pT + qT^2}\right] \tag{7}$$

that in this equation current density is in A/cm^2, temperatures are in ºC and Z=1 for elliptical channel and Z=2 for triangular channel and Z=3 for rectangular channel that this parameter is only in concentration loss that it can be seen in Figure 2.

In equations (4), (5), (6) and (7) the constants a, b, c, d, e, f, g, h, j, k, l, m, n, o, p and q are undefined and by using a software as Datafit which fits the results of experiment from one to more independent variables that in Table 3 the value of these constants was shown.

Figure 8 shows the comparison between the experimental results of Miansari et al. [12] at Z=3 and the 1mm depth of the channels and the correlated equation at To_2=70 ºC, T_{H2}=70 ºC, T_{cell}=70 ºC, and P=1.905 bar. It is clear that there are significant agreements with them. Figure 9 shows the comparison between the experimental results and the correlated equation of the polarization curve for To_2=55 ºC, T_{H2}=55 ºC, T_{cell}=60 ºC, P=3.905 bar, $\dot{m}_{O2}$=0.5 L/min, $\dot{m}_{H2}$=0.3 L/min and three different channels geometry. It is clear that there are significant agreements with them.

Table 3. Value and limits of constants of correlated equation

constant	value	constant	value
a	9921.0	j	37177.-586
b	00013478.0	k	73922.9
c	00789.1	l	56617.647
d	00033137.0	m	75213.0
e	25095.-139	n	21267.-0
f	78474.-17	o	72615.36237
g	25433.0	p	55053.-210
h	60255.-12736	q	39646.1

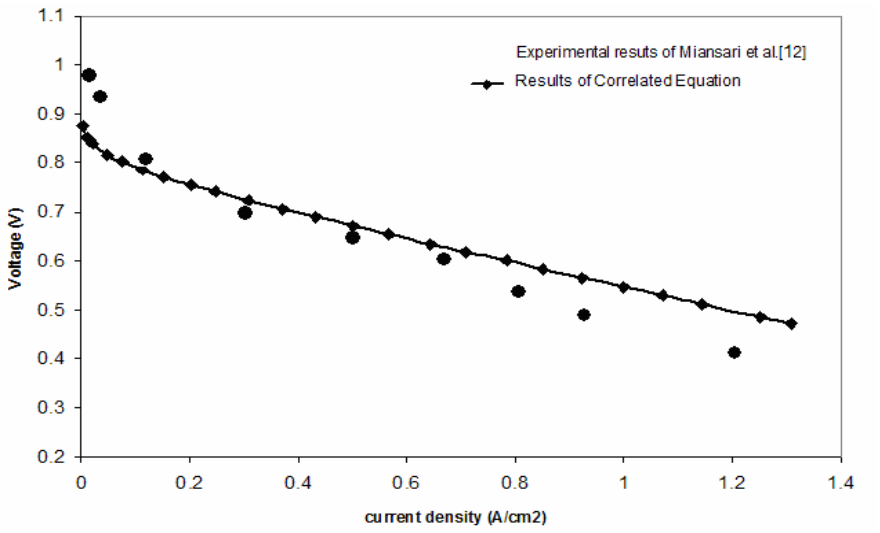

Figure 8. Comparison between the experimental results of Miansari et al. [12] at Z=3 and the correlated equation at To_2=70 ºC, T_{H2}=70 ºC, T_{cell}=70 ºC, P=1.905 bar

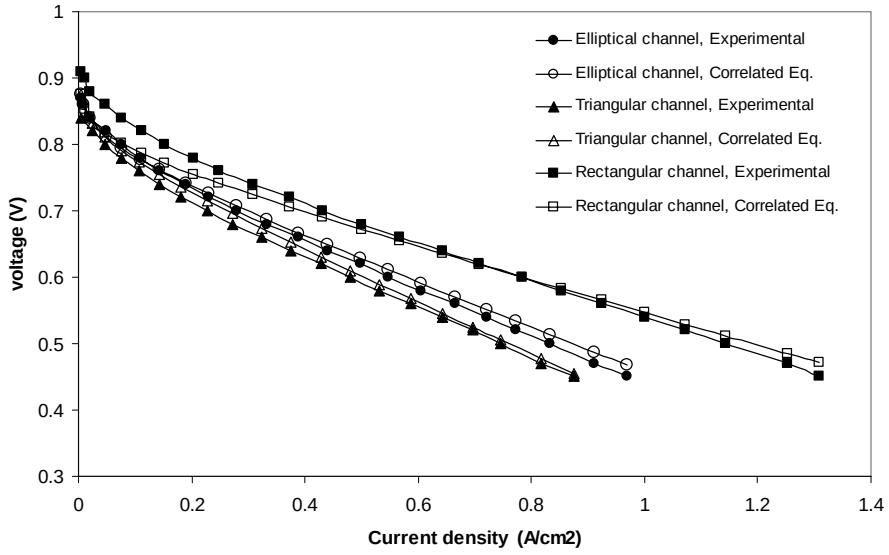

Figure 9. Comparison between the experimental results and the correlated equation of the polarization curve for To_2=55 ºC, T_{H2}=55 ºC, T_{cell}=60 ºC, P=3.905 bar, $\dot{m}_{O2}$=0.5 L/min, $\dot{m}_{H2}$=0.3 L/min and three different channels geometry

4. Conclusion

In this study a new correlation for polarization curve is obtained that it is a function of temperature, current density and a new parameter of cross-section geometry of channels. We have found out that:

● Increasing in the cell temperature from 40 ºC to 60 ºC leads to the increase in the performance of the cell about 17%, 11% and 9% for triangular, rectangular and elliptical channel which is due to the decreasing of activation overpotential and increase in the electrochemical reaction.

● When the geometry of the cell is rectangular, the overall cell performance is better than the elliptical geometry and triangular geometry that this is due to decrease in penetration of the gases into the gas diffusion layer and decreasing the chemical reaction at the surface of catalyst layers.

● A new correlation for predicting the polarization curve of a PEM fuel cell according to cell temperature and the parameter of cross-section channel geometry was proposed and there was a good agreement between its results and the experimental results of Miansari et al. [12].

Acknowledgment
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