# Fuel cell model based on proton exchange membrane (PEM)

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## ABSTRACT

This paper presents the development of the electrical and mathematical models which is able to simulate the static and dynamic phenomena of proton exchange membrane fuel cell (PEMFC). The models were validated against the current distribution data experimentally measured earlier. A parallel computational methodology was employed to substantially reduce the computational time and to make large-scale calculations involving millions of grid points. Simulation results were analyzed and validated against the available experimental data of current distribution under fully humidified conditions and cathode stoichiometric ratio equal to two. The comparisons of the simulations and experiments showed a lack of agreement in the current distribution, although the average polarization curves matched very closely.

**Keywords:** *Fuel cell model, Proton Exchange Membrane (PEM).*

## 1. INTRODUCTION

The dependence of the economy on depleting fossil fuels and the adverse environmental effects of conventional power generation systems created renewed interest in renewable energy sources towards building a sustainable energy economy in the next decade. The application of renewable energy system has become an important alternative as power provider in every area of the world when the price of oil is reaching its highest level. The fuel cell is one of the most promising converters devices in renewable energy technologies. It can be considered as green power because it is environmentally clean, has low emission of oxides of nitrogen and sulfur, and can operate with a very low level of noise. In addition, with efficient control system, fuel cells can provide energy with higher system efficiency than conventional power plants. The fuel cell converts hydrogen into DC power. There are different technologies of fuel cell. The fuel cell systems are under intensive development by several manufacturers and researchers around the world. Polymer Electrolyte Fuel Cells (PEFC), also known as Proton Exchange Membrane Fuel Cells (PEMFC), is currently considered to be in a relatively more developed stage for land transport applications. PEMFC has high power density, solid electrolyte and long cell/stack life time as well as low corrosion. Fuel cell systems have greater efficiency compared to other engines such as diesel engine, gasoline engine etc. and their use in modular electricity generation and propulsion of electric vehicles is promising [1]. Fuel cell efficiency is high at partial loads, which corresponds to the majority of urban and highway driving scenarios [2]. Hydrogen fuel can be generated by an infrastructure based on renewable energy such as solar, hydro, wind etc.

The structure of a PEMFC is shown in Fig. 1. The behavior of fuel cell is a key parameter for the usability of the fuel cell model. The fuel cell system power response is determined by the air and hydrogen supply, flow and pressure regulation, heat/ water management etc. In this research, a mathematical model is developed to simulate the static and dynamic phenomena of PEMFC and is validated against the experimentally measured current distribution data.

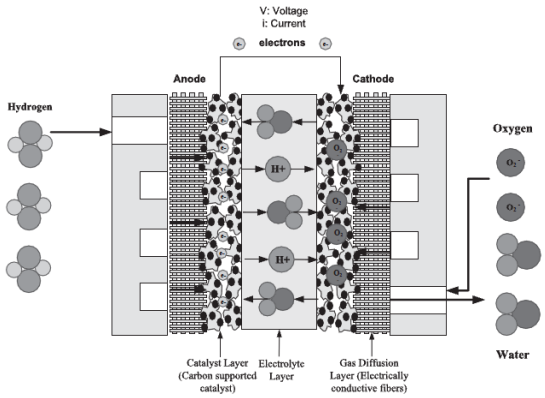


Fig. 1 The structure of a PEMFC [3, 4, 5]

## 2. FUNDAMENTALS OF PROTON EXCHANGE MENBREANE FUEL CELL (PEMFC)

The PEMFC uses a polymeric membrane as the electrolyte generally surfaced with platinum based catalysts. These cells operate at relatively low temperatures and can vary their output to meet shifting power demands. These cells are the best candidates for cars, (emergency) power supplies in buildings and smaller applications because of simple handling and small heat losses. A PEMFC consists of an electrolyte sandwiched between two electrodes. The electrolyte has a special property that allows positive ions (protons) to pass through while blocking electrons. Hydrogen gas passes through one electrode, called anode, and catalyst separates the gas into electrons and protons:

$$\text{Anode:} \qquad H_2\,(g) \rightarrow 2H^+\,(aq) + 2e^- \qquad (1)$$

The protons flow to the other electrode, called a cathode, through the electrolyte while the electrons flow through an external circuit, thus creating electricity. The protons and electrons combine with oxygen flow through the cathode and produce water:

$$\text{Cathode:} \qquad 1/2O_2\,(g) + 2H^+\,(aq) + 2e^- \rightarrow H_2O\,(g) \qquad (2)$$

$$\text{Overall:} \qquad H_2\,(g) + 1/2O_2\,(g) \rightarrow H_2O\,(g) + \text{elec. energy} + \text{heat} \qquad (3)$$

The basic PEMFC stack consists of a proton exchange membrane (PEM), catalyst and gas diffusion layers, flow field plates, gaskets and end plates. The actual fuel cell layers are the PEM, gas diffusion and catalyst layers. These layers are "sandwiched" together using various processes, and called the membrane electrode assembly (MEA). The outer surface of the backing layer is pressed against the flow field plates which serve as both reactant gas flow field and current collector. The plate is made of a light-weight, strong, gas impermeable, electron conducting material such as graphite or composite materials. The other side of the flow field plate is connected to the next cell. The number of cells stacked in one fuel cell stack depends on the power requirement of the stack, which varies across different applications. Depending on its operating conditions, a single fuel cell can provide a voltage from 0 to 1.0 volts with the nominal value of 0.7 volts. Typical characteristics of fuel cells are normally given in the form of a polarization curve, shown in Fig. 2, which is a plot of cell voltage versus cell current density (current per unit active area of the cell). The differences between actual voltage and the ideal voltage of the fuel cell represent the loss in the cell. A fuel cell stack consists of many MEAs, they are connected between bipolar flow field plates and only one set of end plates [3, 4].

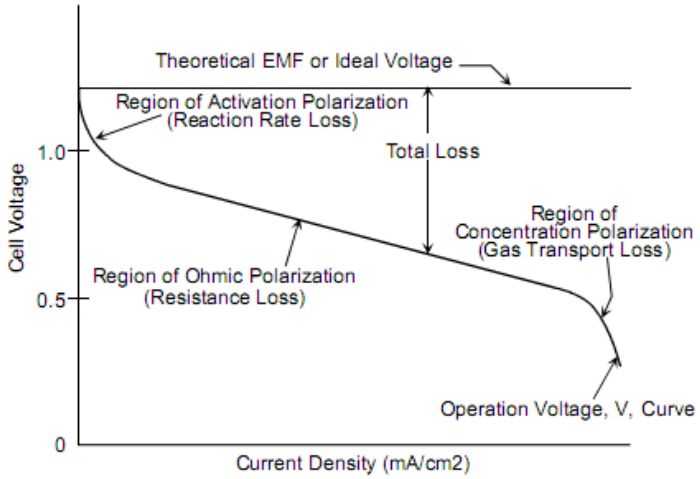


Fig. 2 Typical fuel cell polarization curve [3, 5]

## 3. FUEL CELL MODEL

The fuel cell model contains many interacting sub-models such as the stack voltage, the anode flow, the cathode flow, and the membrane hydration models. However, this paper focuses in stack voltage model. The fuel cell equivalent circuit is shown in Fig. 3 that shows the connection between $U_{fc}$ and the losses. The voltage is calculated as a function of stack current, cathode pressure, reactant partial pressure, fuel cell temperature and membrane humidity; the voltage loss can be represented by three main losses.

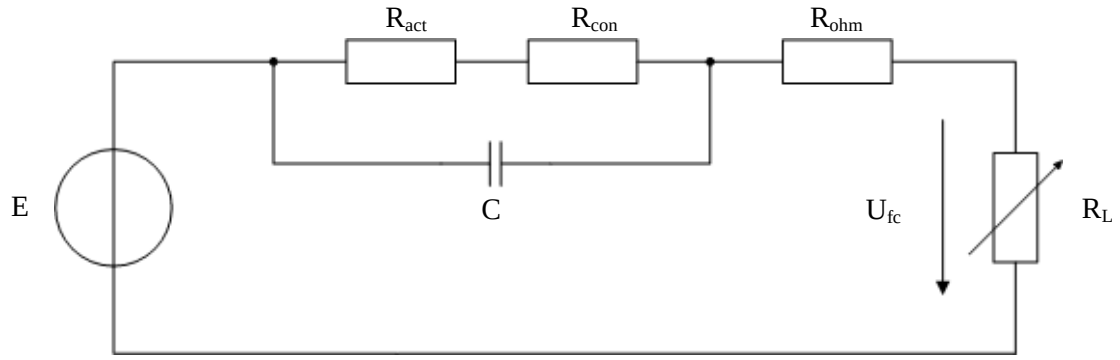


Fig. 3 Fuel cell equivalent circuit

A fuel cell directly converts chemical energy into electrical energy. The chemical energy released from the fuel cell can be calculated from the change in Gibbs free energy ($\Delta g_f$), which is the difference between the Gibbs free energy of the product and the Gibbs free energy of the reactants. In a fuel cell, the external work involves moving electrons round an external circuit [3, 4]. For a hydrogen/oxygen fuel cell, the change in the Gibbs free energy is:

$$\Delta g_f = g_f \textit{ of products - } g_f \textit{ of reactants} = \left(g_f\right)_{H_2O} - \left(g_f\right)_{H_2} - \left(g_f\right)_{O_2} \tag{4}$$

The change in Gibbs free energy varies with both temperature and pressure.

$$\Delta g_f = \Delta g_f^0 - \overline{R}T_{fc} \ln\left[\frac{p_{H_2} p_{O_2}^{\frac{1}{2}}}{p_{H_2O}}\right] \tag{5}$$

Where, $\Delta g_f^0$ is the change of Gibbs free energy at standard pressure (1 bar) which varies with the temperature of the fuel cell ($T_{fc}$) in Kelvin; $p_{H2}$, $p_{O2}$ and $p_{H2O}$ represent the partial pressures of hydrogen, oxygen and water (in bar); $\overline{R}$ is the universal gas constant. If the fuel cell process is considered reversible, all of the Gibbs free energy would be converted to electrical energy, which is the electrical work used to move an electrical charge around a circuit. For each mole of hydrogen, two moles of electrons pass around the external circuit and the electrical work done is:

$$\textit{Electrical work done} = -2FE \tag{6}$$

Where, F is the Faraday's constant which represents the electric charge of one mole of electrons and E is the voltage of the fuel cell. If the system were reversible, this electrical work done would be equal to the change of Gibbs free energy.

$$\Delta g_f = -2FE \tag{7}$$

By substituting equation (7) in equation (5) and solving this for E results:

$$E = \frac{-\Delta g_f}{2F} = \frac{-\Delta g_f^0}{2F} + \frac{RT_{fc}}{2F} \ln\left[\frac{p_{H_2} p_{O_2}^{\frac{1}{2}}}{p_{H_2O}}\right] \tag{8}$$

In practice, the fuel cell process is irreversible. The equation (8) also reveals that some of the chemical energy is converted into heat. The change of Gibbs free energy in equation (8) varies from standard state (25 °C and 1 atm) reference potential (1.229 V) in accordance with the temperature in:

$$-\frac{\Delta g_f^0}{2F} = 1{,}229 + \left(T_{fc} - T_0\right)\left(\frac{\Delta S^0}{2F}\right) \tag{9}$$

As the variation in specific heat with the expected changes in temperature is minimal, the entropy change ($\Delta S^0$) of a given reaction is approximately constant and can be set to the standard value:

$$-\frac{\Delta g_f^0}{2F} = 1{,}229 - \frac{298{,}15 * \Delta S_0^0}{2F} + \left(\frac{\Delta S_0^0}{2F}\right) T_{fc} \tag{10}$$

By further expanding equation (10) using thermodynamic values of the standard state entropy, it results into:

$$E = 1{,}229 - 8{,}5 * 10^{-4}\left(T_{fc} - 298{,}15\right) + 4{,}308 * 10^{-5} T_{fc}\left(\ln\left(p_{H_2}\right) + 0{,}5\ln\left(p_{O_2}\right)\right) \tag{11}$$

In practice the actual fuel cell voltage ($U_{fc}$) is less than calculated in equation (11). The difference is a result of losses associated by the resistances $R_{act}$, $R_{conc}$ and $R_{ohm}$, where $R_{act}$ represents the activation losses, $R_{conc}$ the concentration losses and $R_{ohm}$ the ohmic losses. By combining all voltage drops, the fuel cell voltage can be written as:

$$U_{fc} = E - U_{act} - U_{ohm} - U_{conc} \tag{12}$$

***The activation loss:***

The activation loss or activation overvoltage ($U_{act}$) arises from the need to move electrons and to break and form chemical bonds in the anode and cathode. A part of the available energy is lost in driving the chemical reaction that transfers the electrons to and from the electrodes. The relation between $U_{act}$ and the current density (i) is described by the Tafel Equation (13).

$$U_{act} = a \ln\left(\frac{i}{i_0}\right) \tag{13}$$

The Tafel equation is only valid for $i > i_0$ for the low temperature PEMFC, the typical value of $i_0$ is about 0.1 mA/cm$^2$ [3, 4]. Another similar function that is valid for the entire range of *i* is preferred in the fuel cell simulation. Therefore, the function in equation (13) is approximated by

$$U_{act} = u_0 + u_a\left(1 - e^{-c_1 i}\right) \tag{14}$$

Where, $u_0$ is the voltage drop at zero current density and $u_a$ and $c_1$ are constants [2].

***The ohmic loss:***

The ohmic loss is caused by the electrical resistance of the electrodes and the resistance to the flow of protons in the electrolyte. The voltage drop is proportional to the current density [3]:

$$U_{ohm} = i \times R_{ohm} \tag{15}$$

The area related ohmic resistance is a function of the membrane conductivity ($\sigma_m$) and the thickness of the membrane ($t_m$) [4]:

$$R_{ohm} = \frac{t_m}{\sigma_m} \tag{16}$$

The membrane conductivity ($\sigma_m$) is a function of the membrane water content ($\lambda_m$) and the fuel cell temperature as shown in Equation 17. The value of $\lambda_m$ is expressed between 0 and 14 corresponding to the relative humidity of 0% and 100% [4]:

$$\sigma_m = \left(b_{11}\lambda_m - b_{12}\right) * e^{\left(b_2\left(\frac{1}{303} - \frac{1}{T_{fc}}\right)\right)} \tag{17}$$

The constants $b_{11}$, $b_{12}$ and $b_2$ are determined empirically [4].

***The Concentration losses:***

The concentration loss or concentration overvoltage ($U_{conc}$) results from a slight reduction in the concentration of the oxygen at the anode while the operation of the fuel cell. These changes in concentration will cause a reduction in the partial pressures of the oxygen and hydrogen. In both cases, the reduction in the gas pressure is the reason for rapid voltage drop at high current density [1]. An equation that approximates the voltage drop is given by [4]:

$$U_{conc} = i\left(c_2 \frac{i}{i_{\max}}\right)^{c_3} \tag{18}$$

Where $c_2$ and $c_3$ are constant values which can be determined empirically and $i_{max}$ is the maximum current density of the fuel cell. The values of $c_2$, $c_3$ and $i_{max}$ depend on the temperature and the partial pressure of the reactant.

**Behavior of PEMFC at different operating conditions:**

A fuel cell behavior of PEMFC is influenced by many parameters including different pressure values, temperature and partial pressure of reactants and membrane humidity. These values have a direct influence on the polarization curve of PEMFC. The operating temperature of PEMFC is in the range of 30°C to 50°C, which allows a safe operation. The pressure varies between 1 to 4 bars, and the humidity at the cathode outlet should be above 80% but must be less than 100%. If the humidity is 100% or more, liquid water would flood the gas diffusion layer and block the air supply. The influence of pressure on the polarization curve is shown in Fig. 4.

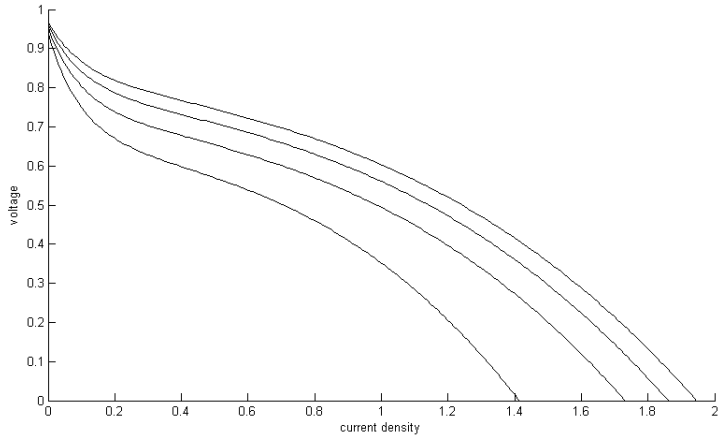


Fig. 4 Fuel cell polarization for different operating pressures

## 4. MATLAB/SIMULINK SIMULATION PROCEDURE

A block diagram of the stack model is shown in Fig 5. In the voltage model, an equation is used to calculate stack voltage for a set of operating conditions at different pressure, temperature, reactant gas partial pressure, and membrane humidity. Although the heat generated due to the reaction is calculated, the stack temperature is assumed to be constant for simulation.

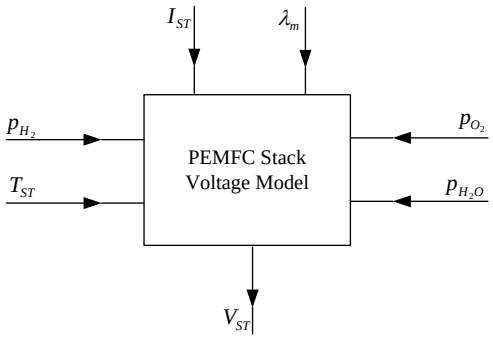


Fig. 5 Block diagram simulation of fuel cell

This model is built using the relationship between output voltage and partial pressure of hydrogen, oxygen and water. Fig 6 shows the detailed model of the PEMFC, which is then embedded into the Simulink of Matlab. The FC system model parameters used in this model are as follows: current (I), activation area (A), number of cells (n), stack temperature (T_FC), are input parameters

while output parameters consist of stack power ($P_{el}$), stack voltage ($U_{bz}$), efficiency (eta_el1), hydrogen usage (V_H2), air usage (V_O2), water production (V_H2O) and polarization curve.

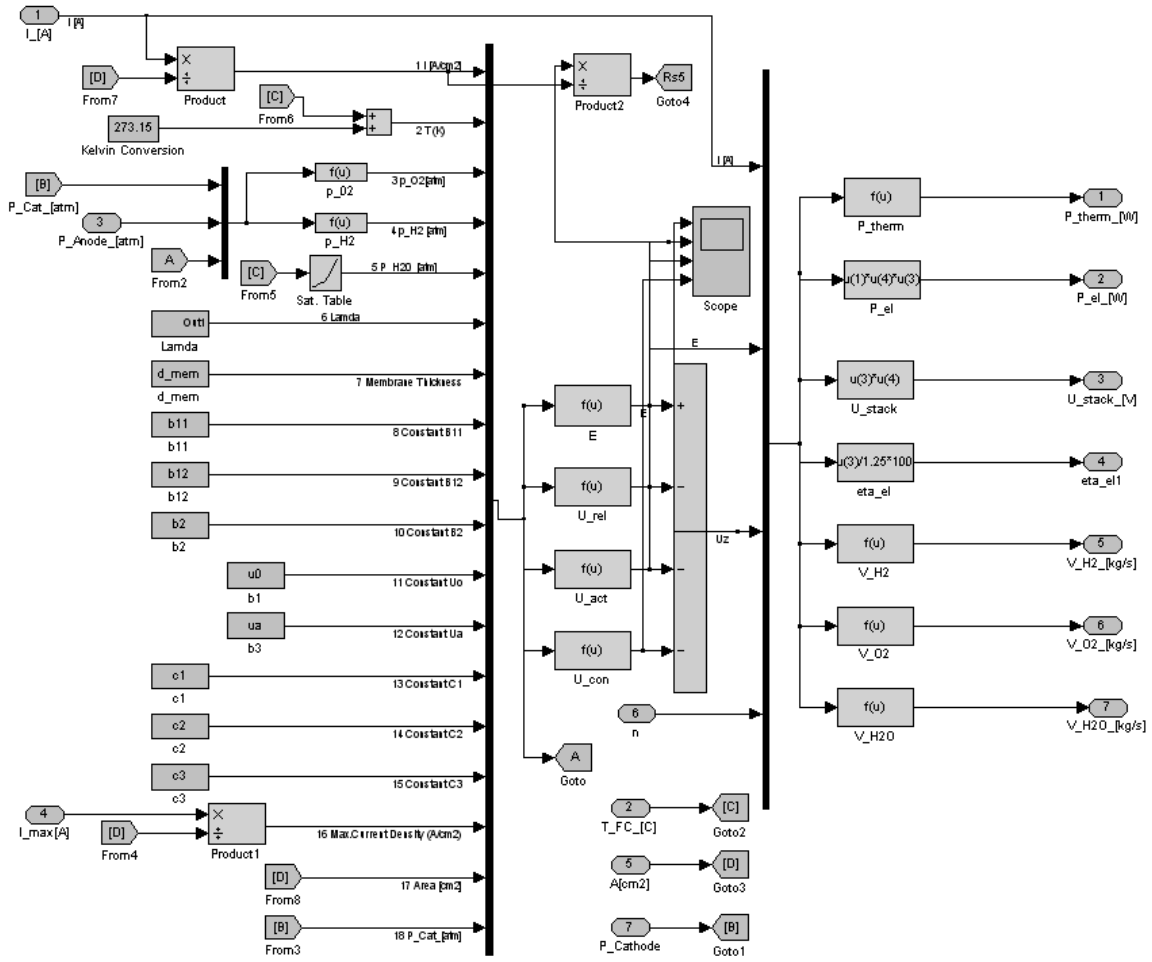


Fig. 6 The model of the PEMFC.

## 5. SIMULATION RESULT AND DISCUSSION

The simulation results show all significant parameters as follows: the polarization curve, P-I characteristic curve, the fuel cell power losses, and polarization curve for different membrane water content. Fig. 7 shows the polarization and P-I characteristic curves of PEMFC at the operating condition of 50$^{o}$C stack temperature and fully humidified conditions and cathode stoichiometric ratio equal to two. It was found that the maximum power of fuel cell stack was 438.19 W at stack voltage of 26.08 V and stack current of 16.80 A.

The plots of voltage drop caused by each of the losses are shown in Fig. 8. The fuel cell losses are attributed to three categories: the activation loss, the ohmic loss, and the concentration loss or the transportation loss. Each of this loss is considered and modeled separately.

The effect of membrane water content on the cell voltage is shown in Fig. 9, which shows the fuel cell polarization curve for membrane water content of 14 (100%) and 7 (50%). The figure also shows the highest value of voltage at membrane water content of 14 (100%) because of the low ohmic loss.

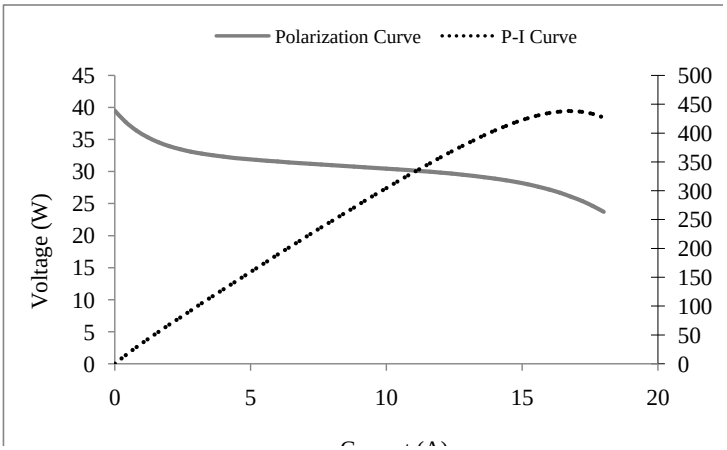


Fig. 7 Polarization curve and P-I curve of PEMFC

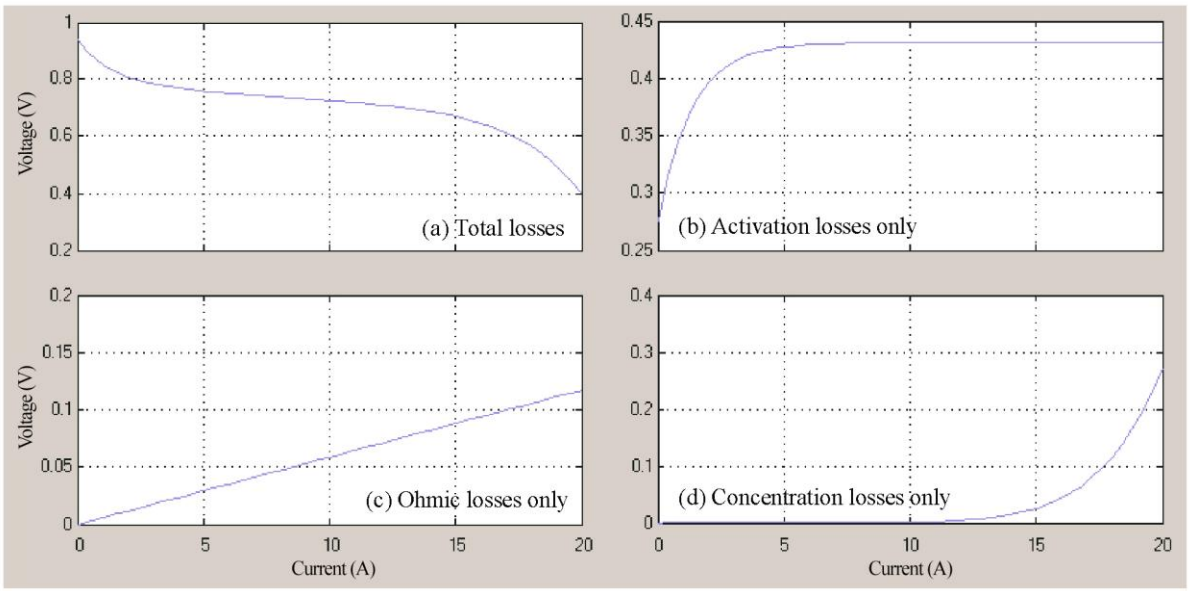


Fig. 8 Voltage drops caused by different types of losses in fuel cell

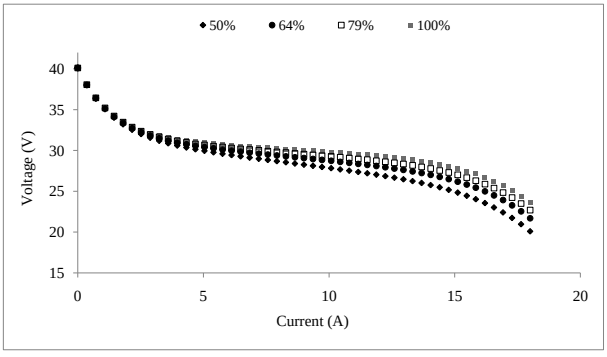


Fig. 9 Fuel cell polarization curve for differences membrane water content values from 50% to 100%

Model validation is an important step in the model-building process; however, it is often neglected. Validating a mathematical model usually consists of quoting the $R^2$ statistic from the fit. Unfortunately, a high $R^2$ value does not mean that the data actually fit well. If the model does not fit the data well, this negates the purpose of building the model in the first place. There are many statistical tools that can be used for model validation, which include residuals, normal distribution of random errors, and missing terms in the functional part of the model. The graphical residual analysis is used in this paper. The P-I curve of PEMFC by simulation and experiment in Fig.10 shows that the relative difference is less than 1% in range from 0 to 10 A whereas the relative increase up to 7% in starting from 10 A.

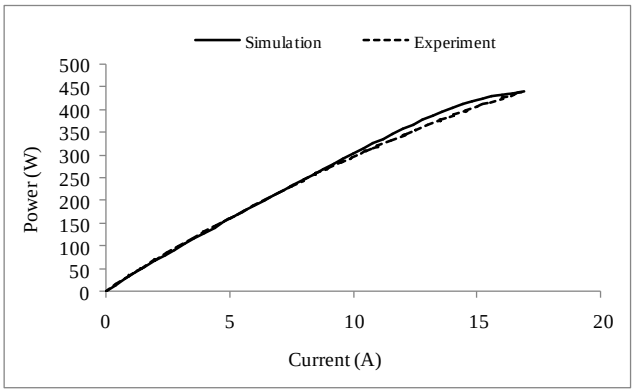


Fig. 10 P-I curve of PEMFC between simulation and experiment

Fig. 11 shows the scatter plot of current versus the residuals. It shows that the maximum of residuals is 3.8 % at current of 13 A, i.e., less than 5 %. Therefore, the developed model fits well with experimental data.

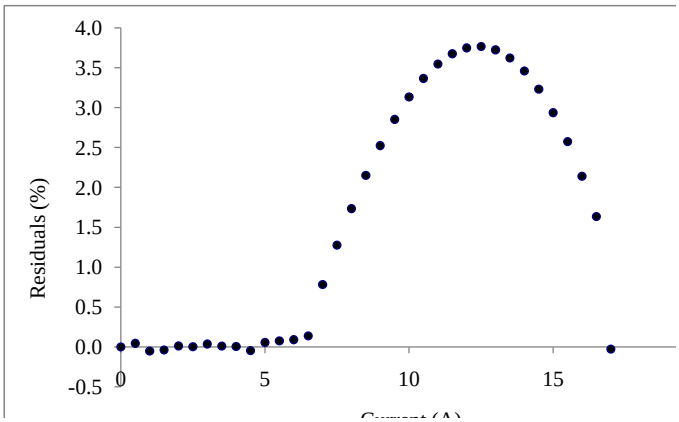


Fig. 11 Scatter plot of current versus residuals

## 6. CONCLUSION

The realized PEMFC model can be used as a tool for simulating the performance of fuel cell operated with fully humidified gas feed and was validated against the current distribution data measured earlier. It leads to the conclusion that experimental validation of PEMFC models must be done against data at the distribution level. There is excellent agreement in the global polarization curve between the simulations and experiments for both cases of cathode stoichiometry, and also the agreement on the current distribution level is

satisfactory. The development of Matlab/Simulink models for PEMFC to study the dynamic response proved to be successful.

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