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Simulation of pem fuel cell activation losses with different electrolyte material based on tafel equation

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ABSTRACT

This paper focuses on the charge transfer in fuel cell which is the electrons that created or consumed are depending on the quickness of the electrochemical reaction that proceed based on the suitable parameter. In Proton Exchange Membrane (PEM) fuel cells, the hydrogen oxidation are very high than the oxygen reduction. In this paper, the main purpose is to identify the relationships between the constant current density and constant temperature. To stimulate the activation polarization in fuel cell using software MATLAB or Simulink coding are presented and discussed in order to prove the increasing of temperature lead to the decreasing of the activation polarization. The temperature of operation is a key parameter in determining the performance and durability of a polymer electrolyte membrane fuel cell (PEMFC). Controlling temperature and choosing the electrolyte material will response for effective operation and design of better systems. The sensitivity to temperature means that the uncertainty in this parameter leads to variable response and can identify the factors affecting the performance. It is important to be able to determine the impact of temperature uncertainty and quantify how much PEMFC operation is influenced under different operating conditions utilising the value of exchange current density. Results show that temperature variation has the greatest effect at higher currents and lower nominal operating temperatures.

Keywords - Fuel cell, MATLAB Software, polarization, PEMFC, charge transfer.

INTRODUCTION

The renewable energy is generally defined as energy that collected considered to be one of the growing energy demands in depletion of fossil fuels and global

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warming issues [1]. Hydrogen fuel cells produce electricity without any pollution, clean and reduce on fossil fuels of dependency. Most of the nation think of the renewable energy such as solar, wind, hydroelectric, biomass and geothermal because of increasing demand and also the higher price of fossil fuels that makes the nation thinks of RE and they want to used it because of the price is not too high.

Fuel Cell

Fuel cell electrochemistry is a device that converts fuel such as hydrogen or chemical energy into electric energy. These sources are important nowadays because of

their low temperature operation, low maintenance, high power density, reliability and also higher efficiency. Therefore, there are five main type of technologies in fuel cell such as Alkali Fuel Cell, Solid Oxide Fuel Cell (SOFC), Polymer Electrolyte Membrane Fuel Cell (PEMFC), Phosphoric Acid (PAFC) and Molten Carbonate Fuel Cell (MCFC). PEM are the most popular and attract the nation at first their start up time because of PEM has low operating temperature range (50-100^0 C), high power density and a long life than the other(1).

PEM Operational System

Polymer electrolyte membrane (PEM) fuel cell (PEMFC) as shown in Figure 1 is one of the electrochemical sources that generates electricity continuously. It consists of anode and cathode which is separated by the electrolyte membrane. The working principle of PEM fuel cell is once the hydrogen gas is supplied to the anode,the cathode is supplied by the oxygen. Hydrogen ions pass through to the membrane and the electrons will flow to the circuit and produce the current flow. Later, electrons were in the external circuit which is in the part of cathode and supply oxygen to form water (1). The reaction for overall reaction is follows as;

At the anode:

$$2H_2 \rightarrow 4H^+ + 4e^- \quad (1)$$

At the cathode:

$$O_2 + 4H^+ + e^- \rightarrow 2H_2O \quad (2)$$

Overall cell reaction:

$$2H_2 + O_2 \rightarrow 2H_2O + \text{Electricity} + \text{Heat} \quad (3)$$

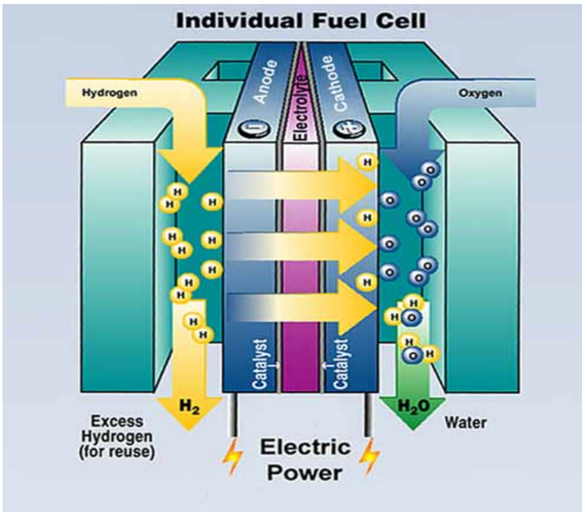

Figure 1: Polymer electrolyte membrane (PEM) fuel cell (PEMFC)

Heat and temperature are from a branch of thermodynamics and show their relation to energy and work. In thermodynamics there have two laws which are the first law is energy cannot be created or destroyed and the second law is heat energy flows only from warmer things toward cooler things [2]. In this theory explained why the heat engine was not efficient and the reasons is gives off some of its heat [2]. In chemical reaction, when the energy released it is called exothermic and when the energy added then it is called endothermic. As long as the process released it should be in exothermic and when it still added the energy, the process of reaction still remains as endothermic [2].

Effect of Activation Losses

The general curve effect explanations show that when the exchange of current density is low, the kinetics becomes lethargic. Therefore, the over potential activation will be larger for any specific net current. When the system supply large current, the over potential will be negligible because of the exchange current is very large. If the exchange current density small it will have no significant current flows to the system unless the over potential is applied with large amount of activation.

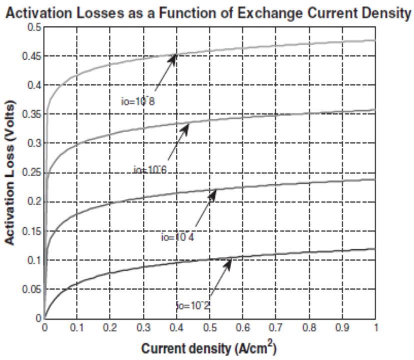

Figure 2: Activation losses as function of exchange current density

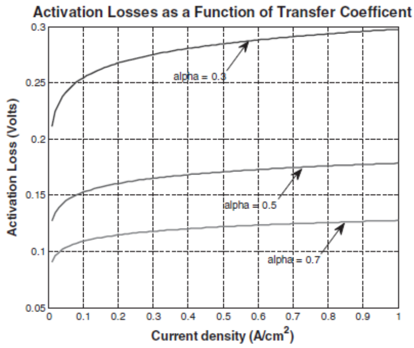

Figure 3: Activation losses as function of transfer coefficient

For the charge exchange that across interface, the exchanged current can be viewed as an "*idle*" current. When the small net current is drawn from the fuel cell, the over potential will be small that required to be obtained. If a net current exceeds the exchange current, it will be delivered to the system at some required rate and only can be achieved by applying the significant over potential. Therefore, this system will able to deliver a net current with significant energy loss when it occurs in this situation. These curve using a Butler-Volmer equation to show the curve between current density (A/cm^2) versus activation loss (Volts). The effect of transfer coefficient is the change a polarization. Therefore, it will leads to the change in reactions rate for the fuel cell [3].

RESEARCH METHODOLOGY

PEM Fuel Cell Performance Based on Tafel Equation

The Tafel equation is an equation in electrochemical kinetics relating the rate of an electrochemical reaction to over potential. The Tafel equation was first deduced experimentally and was later shown to have a theoretical justification. The equation is named after Swiss chemist Julius Tafel. The expression for this equation as shown below [4]:

$$\Delta Vact = a + b\ln(i) \tag{4}$$

Where;

$$a = \frac{RT}{\alpha F}\ln(i_0) \tag{5}$$

$$b = -\frac{RT}{\alpha F} \tag{6}$$

R is ideal gas constan (8.314 J/[mol*K]), *F* is Faraday's constant (96485 C mol^{-1}), α is charge transfer coefficient, *i* is current density per unit catalyst surface area (A/cm^2), i_0 is exchange current density, *T* is temperature in Kelvin and *Vact* is activation polarization in volt.

Simulation of PEM Fuel Cell Performance Using MATLAB

Matrix Laboratory is also known as MATLAB which is built the software those include the vectors. Other than that, this software manage to produce the output of 2D and 3D graphics because this software one of the easier programming languages.

The simulation procedure of PEM fuel cell performance is stated below;

a. The suitable data or parameters of PEM fuel cell with different electrolyte material is used in this paper.
b. After data of PEM fuel cell received which is the parameter that will be used, the calculation will begin by using the Tafel equation.
c. The simulation of coding, the output will appear as V-I curves in 2D.
d. 3D curve is developed. The first step is to change the value of current, exchange current density and temperature for each parameter. After that, the equation will calculate and produce two graph which is one for function as temperature and another one is function as current density. Collect the data activation loss from the graph function as current density by change all the value of temperature and current but remains the value of exchange current density, io. Lastly, repeat all the steps for another parameter. This data are collected to produce the 3D graphical.

RESULTS AND DISCUSSION

Four types of electrolyte material have been used in this simulation. They are platinum, gold, iron and mercury. These types of electrolyte have different exchange current density and there has a coding to represent for each type material. The high temperature over than 80 ^{0}C or 353 K is applied in this simulation. This temperature is considered as low operation temperature [5], it can be operated on the temperature of over than 100 ^{0}C or 373 K [6]. The curve of activation loss as function of temperature and activation loss as function of current density are shown in Figure 4 and Figure 5.

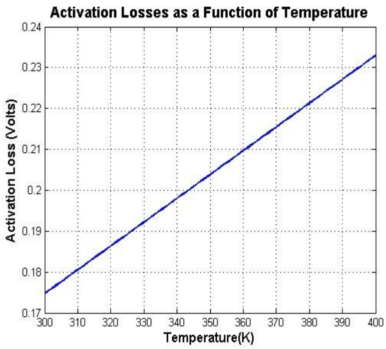

Figure 4: Activation losses as function of temperature

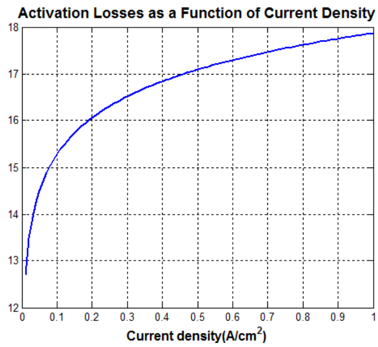

Figure 5: Activation losses as function of current density

Figure 4 show that the fuel cell temperature of fuel cell affects the activation loss. It is also affect the current density as shown in Figure 5. Increasing the fuel cell temperature would cause a voltage drop, therefore the terminal voltage would decrease. It decreases linearly with fuel cell temperature in the range of voltage and temperature. The reason for the linear decrease in activation loss is due to the decrease in thermodynamic reversible potential which decrease with fuel cell temperature, thus causing the terminal voltage of fuel cell to decrease[(7)].

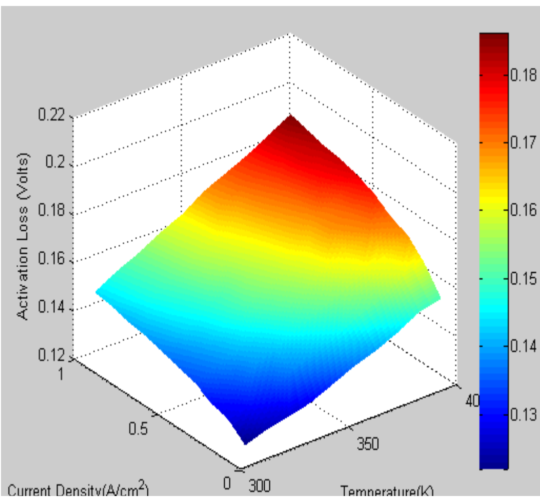

Figure 6: 3D activation losses for gold as electrolyte material

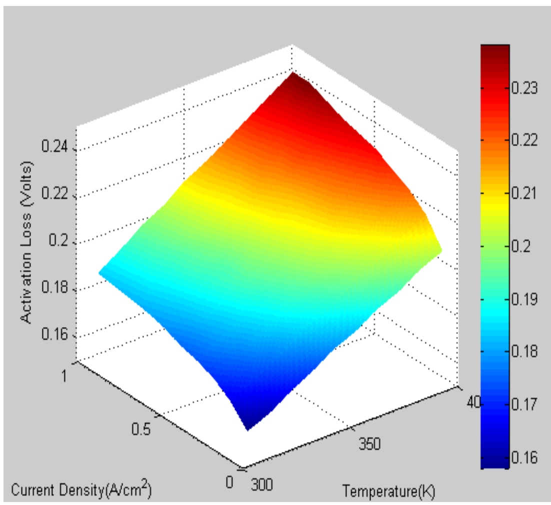

Figure 7: 3D activation losses for iron as electrolyte material

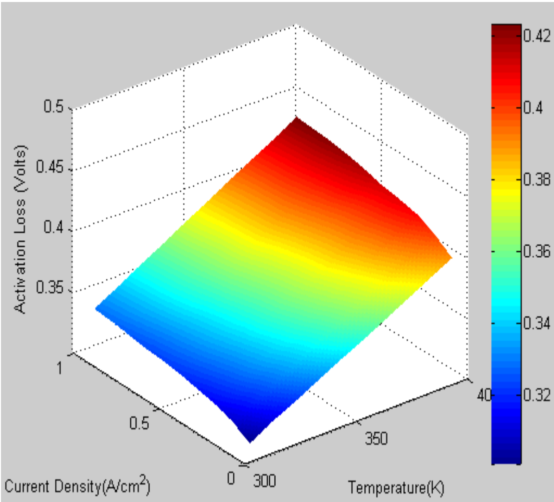

Figure 8: 3D activation losses for mercury as electrolyte material

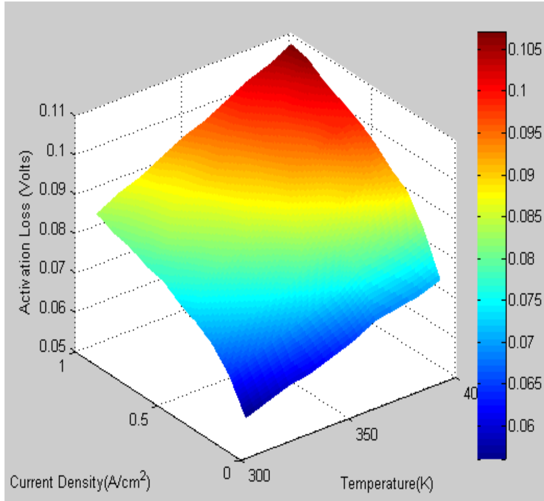

Figure 9: 3D activation losses for platinum as electrolyte material

Figure 6 to Figure 9 show 3D activation loss as function of both of current density and temperature for several of electrolyte material (gold, iron, mercury and platinum). They show that the fuel cell temperature affects the activation loss. The higher fuel cell temperature causes the higher activation loss. It means the voltage drop would be higher and causes the fuel cell terminal voltage would decrease.

The study of simulation and modelling show a relationship between the temperature (K) and activation polarization. It shows the curve when the temperature increases and how it decreases the activation polarization. In this paper also derived the Tafel equation to calculate and plot the activation losses for the fuel cell at the current density.

CONCLUSIONS

The comparison between all of the parameter, it shows the reduction of hydrogen in fuel cell based on the electrolyte material. From the data that has been collected, the observation has made up that the factors affect the exchange current density is a temperature, redox reduction of hydrogen, concentration and electrode composition.

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