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MATHEMATICAL MODELLING FOR PROTON EXCHANGE MEMBRANE FUEL CELL (PEMFC)

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ABSTRACT

Proton Exchange Membrane Fuel Cell (PEMFC) is one type of the renewable energy that are current increasingly popular in industry. The cost for the implementation of the PEMFC system is quite high in order to use in the experimental research field. Therefore, the simulation modelling is very useful to emulate the PEMFC system in real work. The objective of this paper is to develop the simple mathematical equation for steady-state and thermodynamic modelling based on the equivalent electrical circuit of the PEMFC. The Matlab/Simulink is used to simulate the modelling based on the practical parameters of the Horizon H-500 fuel cell stack. Comparison performance of parameters affects on the PEMFC model is investigated. The graph for I-P curve, I-V curve and the losses involve in the reaction are discussed.

Keywords: *Renewable Energy, Fuel cell, Proton Exchange Membrane Fuel Cell (PEMFC), Modelling, Matlab/Simulink*

1. INTRODUCTION

Referable to the insufficient of fossil fuels and the world environment crisis, the earth has forced into the searching for new energy sources as the substitute energy which could ensure the sustainability of natural resources for future generation [1]. Consequently, many renewable energy are brought in over the last decade such as wind energy, solar energy, and hydropower. Nevertheless, all the above-mentioned renewable energy are depending on the unpredictable nature and climate condition that can disrupt the performance output of the systems [2]. On the other hand, in order to solve the limitation, a device named fuel cell is introduced which used hydrogen (H_2) and oxygen (O_2) that are sustainable sources as a fuel for the system to create energy.

Apart from that, hydrogen has been named as one of the most workable and long term renewable alternatives to fossil fuel after solar [3]. Eventhough, fuel cell system is more preferred than the solar system because it does not need large field to implement the system, thus make the fuel cell system has no geographical limitation for the implementation. Fuel cell is one kind of renewable energy, which gives many advantages to the user. It is lightweight, mechanically ideal and quickly recharged when refueling [4].

Nowadays, half a dozen types of fuel cell presents which are Proton Exchange Membrane Fuel Cell (PEMFC), Direct Methanol Fuel Cell (DMFC), Alkaline Fuel Cell (AFC), Phosphoric Acid Fuel Cell (PAFC), Molten Carbonate Fuel Cell (MCFC), and Solid Oxide Fuel Cell (SOFC) [4-6]. PEMFC is the most preferable type of fuel

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cell as a power source due to its low operating temperature, high power density and high energy conversion efficiency that can achieved up to 50% - 60% conversion efficiency [7, 8].

Operation for fuel cell is simple, it is the device that converts chemical energy directly to electrical energy and the only waste from the system is water (H_2O). PEMFC gives zero emission when fueled with pure hydrogen, and gives near to zero emission when the fuel is coupled with reformers [7, 9]. The basic operation of the fuel cell can be illustrated in figure 1. Electrodes (carbon supported with platinum catalyst) [5] and electrolyte with the additional components for electrical connections are some of the basic element for the fuel cell stack [10].

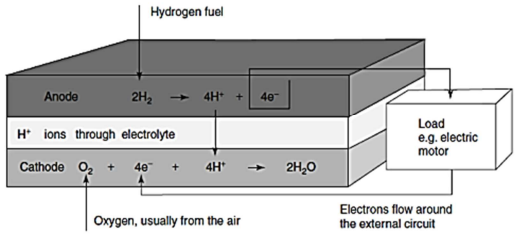

Figure 1: Basic operation of fuel cell [4].

Fuel cell consists of two electrodes which are called anode and cathode. At the anode side, proton (H^+) and electron (e^-) are released when the hydrogen gas is ionize (1) . Besides, at the cathode side, water and heat are the only product for the reaction when the oxygen react with electrons that accumulated at the electrode which flow through the external electrical circuit and H^+ that flow through the electrolyte (2). The electrolyte of the fuel cell only allows proton to pass through it, while the electrons produced at the anode side pass through the electrical circuit to the cathode side which represent as a current deliver for the system.

$$\text{Anode: } 2H_2 \rightarrow 4H^+ + 4e^- \quad (1)$$
$$\text{Cathode: } O_2 + 4H^+ + 4e^- \rightarrow 2H_2O + \text{heat} \quad (2)$$

Due to the complexity of the fuel cell system and the costly experimental implementation [11, 12], the actual simulation model of PEMFC plays a significant role in the research field. It is used to simulate the simulation model practically based on the real work. Besides, the simulation model could establish the parameter affecting the operation of the fuel cell in software, thus it can reduce the cost in the research development.

Preliminary, fuel cell models had been categorized as analytical, semi-empirical or mechanistic by some researchers [13-16]. However, these model are complicated to develop. Besides, some work has been described in the literature on steady-state fuel cell modelling, and also for the dynamic modelling [17-22]. In recent years, many researchers attempted to study the dynamic modelling of the fuel cells [23]. A detailed explanation of the fuel cell electrochemical properties and the equivalent electrical circuit including a capacitor due to the effect of charge double-layer inside the fuel cell are discussed in [5].

In this paper, electrical circuit are used to present the dynamic model of the PEMFC. MATLAB/SIMULINK tools are used in order to simulate the simple steady-state, dynamic and thermodynamic model. Firstly, the development of steady-state model is to observe the activation losses, concentration losses and ohmic losses for each cell of the PEMFC. Besides, a dynamic model is constructed by considering the double-layer charging effect which represents as capacitor in the circuit to observe the dynamic power and dynamic voltage performance of the PEMFC. Thermodynamic characteristic inside the PEMFC is modelled as well into the modelling in order to take account the temperature inside the fuel cell. All of the mathematical equation for these models are discussed in section 2 while the simulation result are explained in section 3.

2. PEMFC MATHEMATICAL EQUATION EXPLAINED BASED ON FUEL CELL EQUIVALENT CIRCUIT IMPLEMENTED IN MATLAB/SIMULINK ENVIRONMENT.

This section explained on the mathematical equation of the PEMFC based on the equivalent electrical circuit figure 2. The simulation model developed in the Matlab/Simulink environment are presented in this section.

2.1 PEMFC Single Cell Mathematical Equation

The fuel cell voltage is thermodynamically predicted by the reversible voltage denotes as E in figure 2. Generally, the voltage deliver at the fuel cell terminal (Vcell) is lower than the voltage created inside the fuel cell (E) that can be obtained in (5). This is due to the voltage drop at the three losses occurred inside the fuel cell reaction, that are activation loss (13), concentration loss (15), and ohmic loss (16) that are labelled as R_{act}, R_{conc}, and R_{ohmic} respectively in figure 2.

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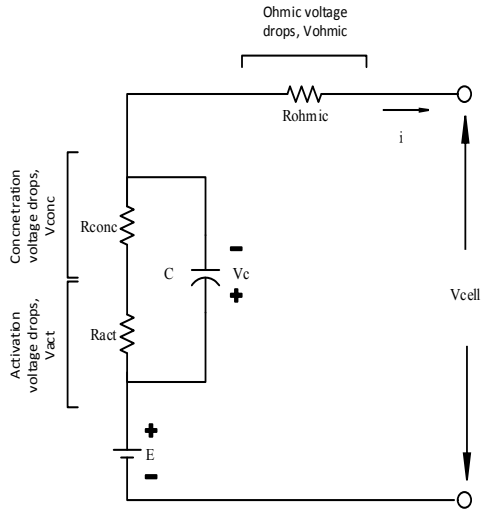

Figure 2: Fuel Cell equivalent circuit.

2.1.1 Steady-state model

Steady-state model (3-17) is the first criteria should be consider on the modelling of the actual PEMFC model. Activation losses, concentration losses and ohmic losses are three main losses that deliver practically from the fuel cell and can be observe through this steady-state model.

V_{cell} in (3) is the voltage output of the fuel cell and it can be illustrated from the fuel cell equivalent circuit (Figure 2) which does not include the behavior of the double layer charging effect, Vc. The voltage is represent in the form of voltage drop as shown in (3):

$$V_{cell} = E - V_{act} - V_{conc} - V_{ohmic} \quad (3)$$

Where:

E = Reversible voltage.
V_{act} = Activation voltage.
V_{conc} = Concentration voltage.
V_{ohmic} = Ohmic voltage.

The voltage output in a cell also can be represented in the form of voltage gain (n) as shown as equation (4) below:

$$V_{cell} = E + n_{act} + n_{conc} + n_{ohmic} \quad (4)$$

The reversible voltage of the cell is represented as E, can be calculated by (5):

$$E = 1.229 - 8.5 \times 10^{-4}(T_{cell} - 298.15) + 4.308 \times 10^{-5}\left(\ln P_{H_2} + \frac{1}{2}\ln P_{O_2}\right) \quad (5)$$

Figure 3 below shows the subsystem of E that implement in the Matlab/Simulink. Partial pressure of the two input which are hydrogen and oxygen are important parameter to take into account in E.

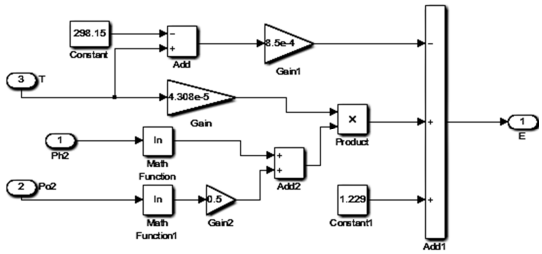

Figure 3: Predicted thermodynamic voltage.

Where partial pressure of hydrogen, P_{H_2} is expressed in (6):

$$P_{H_2} = 0.5 P_{H_2O}{}^{sat}\left[\exp\left(-\frac{1.635J}{T_{cell}{}^{1.334}}\right)\frac{P_a}{P_{H_2O}{}^{sat}} - 1\right] \quad (6)$$

Partial pressure of oxygen, P_{O_2} is defined in (7):

$$P_{O_2} = P_{H_2O}{}^{sat}\left[\exp\left(-\frac{4.192J}{T_{cell}{}^{1.334}}\right)\frac{P_c}{P_{H_2O}{}^{sat}} - 1\right] \quad (7)$$

Where:

P_a = Partial pressure for anode
J = Current density (A/cm^2)
P_c = Partial pressure for cathode
$P_{H_2O^{sat}}$ = Saturation pressure for water (8)

$$\log_{10} P_{H_2O}{}^{sat} = -2.18 + 2.95 \times 10^{-2} T_c - 9.18 \times 10^{-5} T_c{}^2 + 1.44 \times 10^{-7} T_c{}^3 \quad (8)$$

$$T_c = T_{cell} - 273.15 \quad (9)$$

Figure 4 shows that the input pressure from the hydrogen tank and input pressure of the oxygen from surroundings are important to get the partial pressure of the hydrogen and partial pressure of oxygen in the PEMFC. The saturation pressure of water also calculated in this subsystem.

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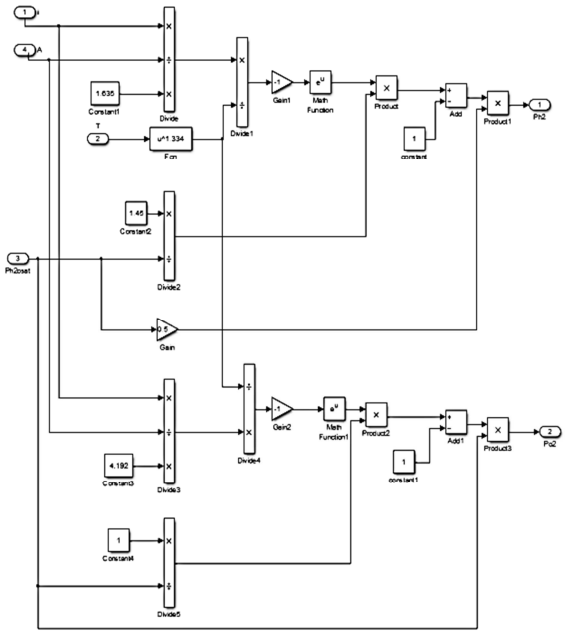

Figure 4:Partial pressure.

Equations (10-12) shows the relationship between the voltage gain (n) and the voltage drop of the three losses.

$$n_{act} = -V_{act} \quad (10)$$

$$n_{conc} = -V_{conc} \quad (11)$$

$$n_{ohmic} = -V_{ohmic} \quad (12)$$

Firstly, activation losses are the losses that occur due to resistance at the surface of the electrode. Besides, mass transport losses and the resistance for the concentration on the electrode surface in the cell are represents as the concentration losses in the mathematical model. Lastly, ohmic losses occurs when the transfer of proton and electron happen in the reaction. These equation are mostly referred from [24, 25].

The activation polarization losses is defined in (13):

$$n_{act} = -0.9514 + 3.12 \times 10^{-3} T_{cell} - 1.87 \times 10^{-4} T_{cell} \ln i + 7.4 \times 10^{-5} T_{cell} \ln C_{O_2} \quad (13)$$

Where the concentration of the oxygen mathematical equation is based on the equation (14).

$$C_{O_2} = \frac{P_{O_2}}{5.08 \times 10^6 \times e^{\left(-\frac{498}{T_{cell}}\right)}} \quad (14)$$

The concentration polarization loss and ohmic polarization loss are defined in (15) and (16) repectively:

$$n_{conc} = B \ln\left(1 - \frac{i}{i_{lim}}\right) \quad (15)$$

$$n_{ohmic} = -iR_{int} \quad (16)$$

The internal resistance of the fuel cell is represent in equation (17):

$$R_{int} = 1.605 \times 10^{-2} - 3.5 \times 10^{-5} T_{cell} + 8 \times 10^{-5} \quad (17)$$

Figure 5 – figure 7 shows the subsystem of the activation, concentration, and ohmic polarization of the PEMFC developed in Matlab/Simulink.

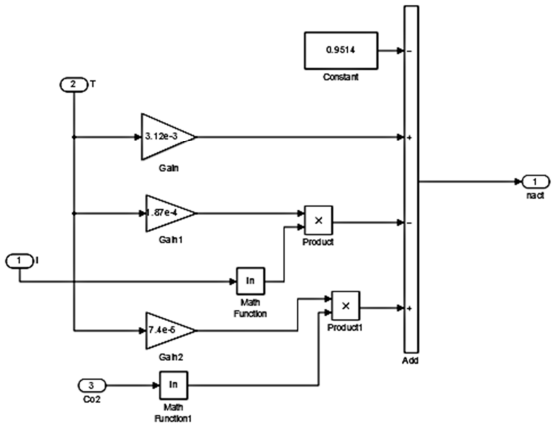

Figure 5: Steady-state activation losses.

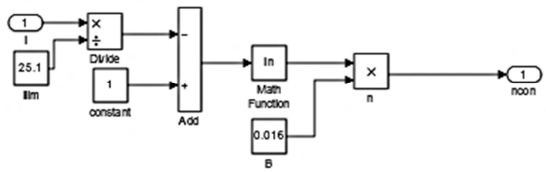

Figure 6: Concentration losses.

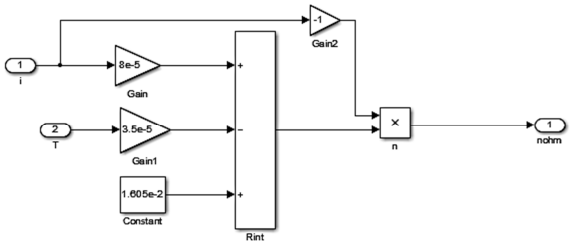

Figure 7: Ohmic losses.

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2.1.2 Thermodynamic model

Dynamic modeling approach for fuel cell is a coupled of some complex system which are fluid–solid–heat–electrochemistry that consider the process of the electrochemical reaction to occur [26]. To understand the dynamic electrical behaviour of the fuel cell, the effect of the Charge Double-Layer (CDL) capacitance labelled as V_c in figure 2 is need to consider in the model.

CDL occurs when two material are in contact, that form a charge on the surface or the charge is transferred from one to the other. In practical the CDL occurs due to the reaction between the electrode and the ions in the electrolyte [5]. The (18-20) shows the differential equation for CDL referred to the fuel cell equivalent circuit (Figure 2).

$$V_c = V_{act_0} + V_{conc} \quad (18)$$

$$R_c = \frac{V_{act_0}+V_{conc}}{i} \quad (19)$$

$$\frac{dV_{act}}{dt} = \frac{i}{C} - \frac{V_{act}}{R_c C} \quad (20)$$

Figure 8 shows the dynamic activation losses of the PEMFC. V_{act_0} is taken from the steady-state model.

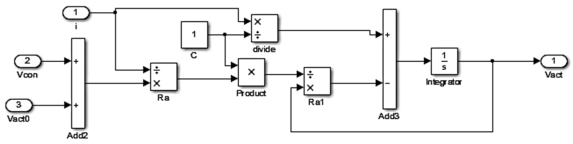

Figure 8: Dynamic activation losses.

A part from that, several factors such as heat from the electrochemical reaction, heat evacuate to the surrounding, heat transfer between the fuel cell electrode could change the temperature of the fuel cell. Equation (21) represents as the differential equation of the thermodynamic model of PEMFC.

$$C_t \frac{dT}{dt} = i(E - V_{cell}) - H(T_{cell} - T_f) \quad (21)$$

Where:
Ct = 10 J/K (Total thermal capacitance for all the volume or mass of fuel cell).
H = 10 W/K (Total heat transfer coefficient for all the surface of fuel cell).
Tf = 303.15K (Reference temperature of environment).
T_{cell} is lumped temperature of fuel cell (K).

Figure 9 is the lumped temperature subsystem of the fuel cell. Overall subsystem of the PEMFC model is shown in figure 10.

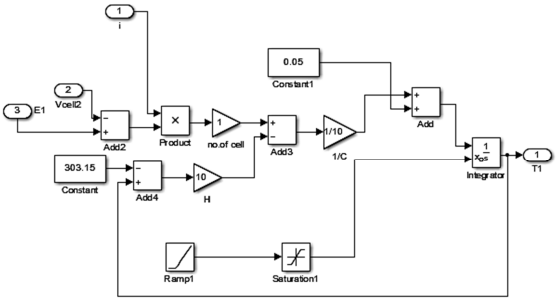

Figure 9: Thermodynamic.

2.2 PEMFC Stack Mathematical Equation

This section shows how to get the voltage and power deliver performance in a stack of PEMFC system.

V_{stack} (22) is the total voltage produce by a group of cells which are combined in series to increase the voltage deliver from the system.

$$V_{stack} = nV_{cell} \quad (22)$$

Where:
n = number of cell.

P_{stack} (23) is the total dynamic power deliver from the system where i is a current deliver. The maximum power deliver of fuel cell system is operate with maximum power point (MPP) which is tracked with maximum power point tracking (MPPT) algorithm [27].

$$P_{stack} = iVstack \quad (23)$$

Figure 11 is the overall stack system of the PEMFC implemented in Matlab/Simulink environment.

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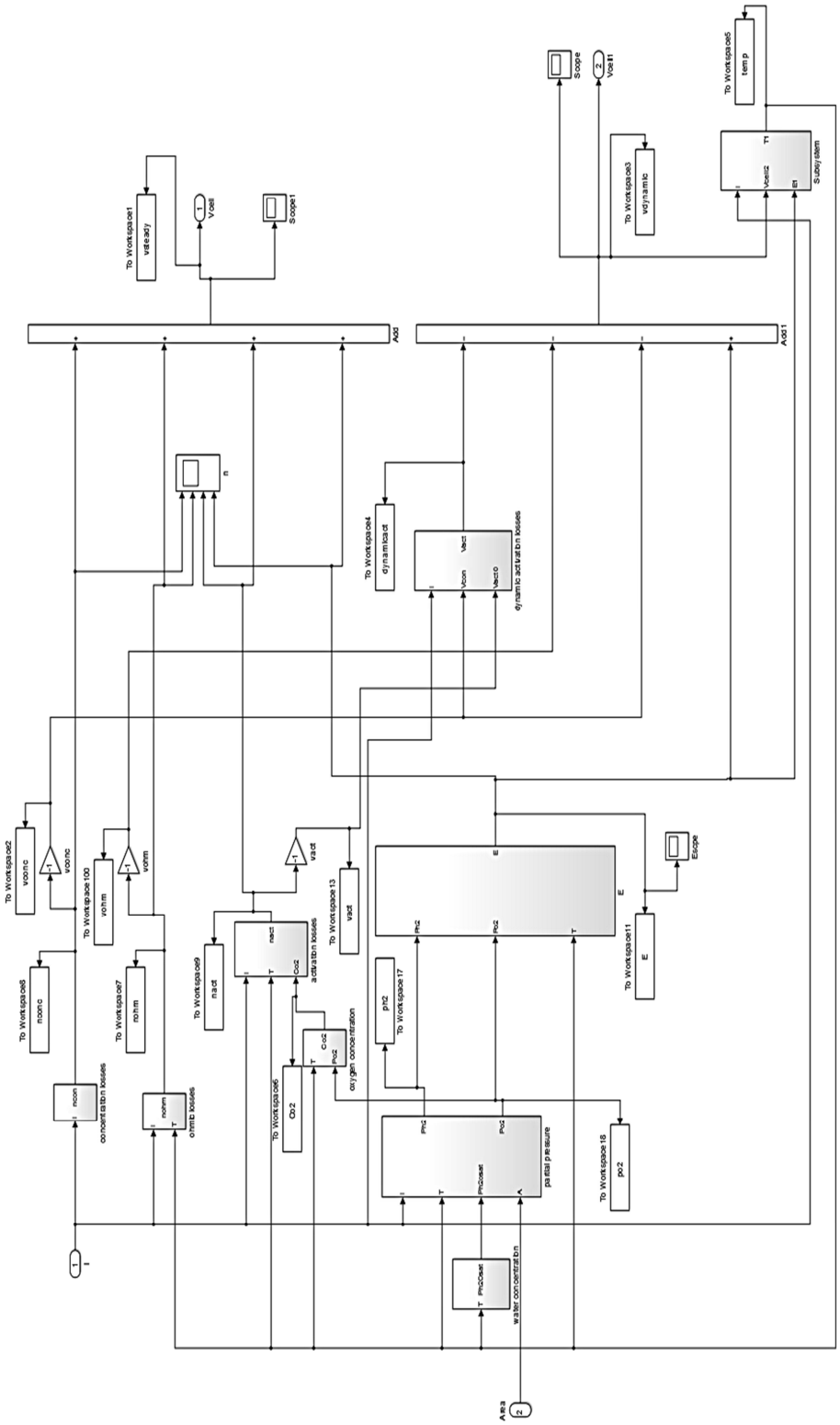

Figure 10:Overall subsystem for dynamic model.

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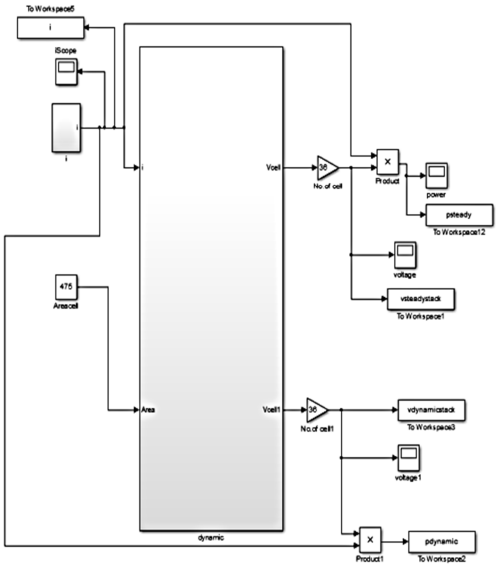

Figure 11: Stack PEMFC model in Matlab/Simulink.

3. SIMULATION RESULTS AND DISCUSSION

This section briefly explained the simulation result for the PEMFC modelling. The input parameter for the simulation (Table 1) is based on the Horizon H-500 fuel cell stack specification [28].

Table 1: Horizon H-500 Fuel Cell parameter.

Parameter	Value
No.of cell	36
Area of the cell	475 cm^2
Rated current performance	24 A
External Temperature	278.15K – 303.15K

The steady-state model for the PEMFC is developed by using equations (3-17), while in the addition of equations (18-21) the thermodynamic performance of the PEMFC are obtained. Other than that, equations (22) and (23) are used to calculate the stack performance of the PEMFC model.

3.1. PEMFC Single Cell Performance

Based on the equation (3), a single cell of the PEMFC voltage performance (Figure 12) can be calculated by minus the predicted thermodynamic potential (Figure 13) with all of the three losses (Figure 14 – figure 16). From figure 12, it is clearly shown that the voltage of the PEMFC decreases in the three stages which are first stage (activation losses), second stage (ohmic losses), and third stage (concentration losses) [4].

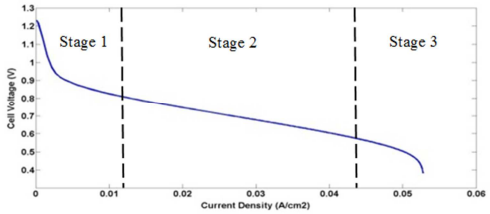

Figure 12: Dynamic Cell Voltage.

Figure 13 is the graph which thermodynamically predicted the voltage deliver in a cell, E. Theoretically, it gives 1.2V for a single cell [5]. Figure 14, figure 15 and figure 16 shows the voltage losses involved in the reaction of the fuel cell.

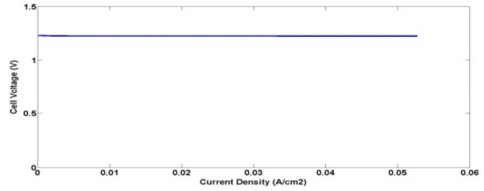

Figure 13: Reversible voltage.

At the first stage of the fuel cell output is dominated by the activation behaviour. The voltage rapidly decreases at low current density (Figure 14) due to the overpotential occurred at the surface of the electrode. Based on the equation (13), the activation losses is related to the concentration of the oxygen at the cathode side.

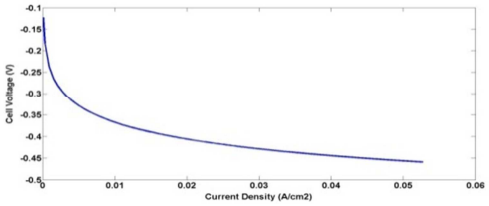

Figure 14: Activation Voltage.

Ohmic losses are dominating at the second stage of the fuel cell voltage performance. As stated in the equation (16), the ohmic losses is directly proportional to the negative current and the electrical resistance (Figure 15). The ohmic losses is caused by the electrical and ionic conduction losses through the connections and all related part.

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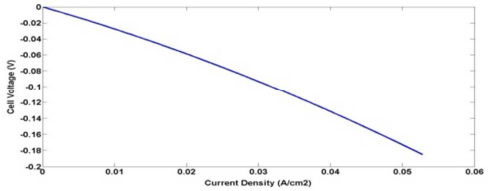

Figure 15: Ohmic Voltage.

The losses at the third stage is dominated by the concentration polarization (Figure 16). This is due to the mass transport limitations of the reactants to the electrode.

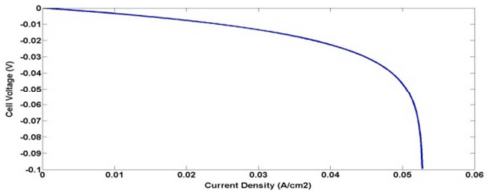

Figure 16: Concentration Voltage.

3.2. PEMFC Stack Performance

These results are generated using equations (3-23) by implementing the specifications of the Horizon H-500 of the PEMFC system into the thermodynamic model. Figure 17 and figure 18 shows the power and the voltage deliver for the PEMFC dynamic model. Based on (23), the power deliver from the PEMFC should be linear in increasing of the current demand. However, due to the i_{lim} in the equation (15), the power slowly drops caused by maximum rate of the concentration at the electrode that can be seen in the dynamic power graph below (Figure 17).

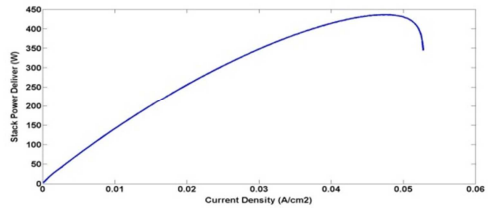

Figure 17: Dynamic Power.

Figure 18 shows the dynamic stack voltage versus current density of the PEMFC deliver from the simulation model.

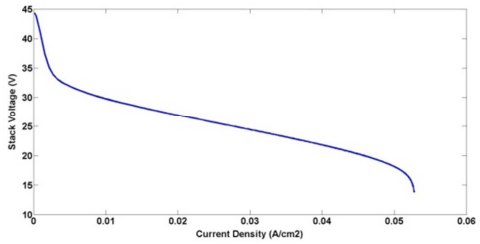

Figure 18: Dynamic Voltage.

3.3. Parameters Affects Performance

Ambient temperature and pressure were found that have a significant effect to the PEMFC performance. Input hydrogen pressure, Pa varies to get the partial pressure of hydrogen, Ph2 value in the range of 0.44 – 0.54 atm as stated in the practical H-500 fuel cell stack [28]. The ambient temperature is assumed constant at 303.15K, and the input oxygen pressure, Pc assume as 1 atm. Based on the Eq.6 the Ph2 is increase with the increasing Pa. Table 2 and figure 19 proof that the power deliver from the PEMFC is increased linearly with the increase input hydrogen pressure.

Table 2: Power performance in various input hydrogen pressure.

Input Hydrogen Pressure, P_a (atm)	Partial Pressure of Hydrogen, P_{H_2} (atm)	Power Deliver (W)
0.95	0.4519	395.9
1.00	0.4769	396.5
1.05	0.5019	397.0
1.10	0.5269	397.5
1.15	0.5519	398.0

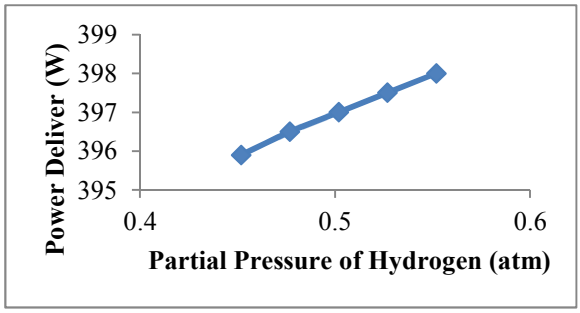

Figure 19: Relationship between partial pressure of hydrogen vs power deliver.

The operating temperature of fuel cell will affect by the different ambient temperature due to the behaviour of the reaction at warm or cold place. Hydrogen and oxygen pressure are set as constant 1.1 atm and 1 atm respectively. Table 3 and figure

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20 shows the fuel cell operation temperature performance is increase with the increasing ambient temperature. The ambient temperature is set to 278.15K – 303.15K as stated in data sheet of the Horizon H-500 fuel cell stack [28]. Besides, in increasing the ambient temperature, the power deliver of the fuel cell also increase linearly with the temperature as shown in table 4 and figure 21.

Table 3: Fuel cell temperature with increasing ambient temperature.

Ambient Temperature (K)	Temperature (K)
278.15	279.8
283.15	284.8
288.15	289.7
293.15	294.7
298.15	299.7
303.15	304.7

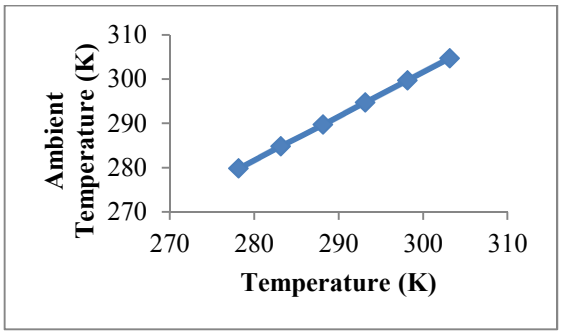

Figure 20: Relationship between ambient temperature and fuel cell temperature.

Table 4: Performance of power deliver with increasing ambient temperature.

Ambient Temperature (K)	Power Deliver (W)
278.15	373.30
283.15	378.30
288.15	383.20
293.15	388.00
298.15	392.90
303.15	397.50

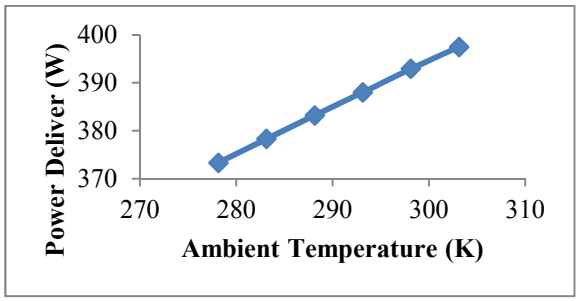

Figure 21: Relationship between ambient temperature vs power deliver.

3.4. Steady-State vs Dynamic Performance

Figure 22 shows the difference of the power performance between the steady-state and the dynamic modelling. 1.45 atm of input hydrogen pressure, Pa and 1.0 atm of input oxygen pressure, Pc are choosen to get the approximate performance of Horizon H-500 Fuel Cell. The temperature used for the steady-state model is 333.15K while for the thermodynamic model the temperature is feedback from the system using thermodynamic equation (20).

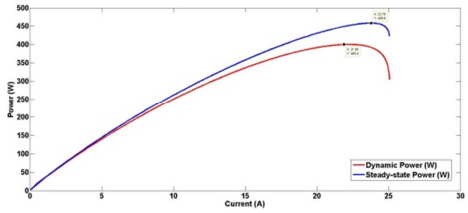

Figure 22: Comparison between steady-state and dynamic performance.

The power deliver from the steady-state model is 458.6W while for the dynamic model is 400.4W. There are 12.69% difference of the power deliver from the two models that due to the difference of the cell temperature performance and the dynamic losses of the system.

4. CONCLUSION

The simple steady-state and dynamic model of the PEMFC has been implemented in the MATLAB/Simulink environment based on Horizon H-500 fuel cell stack parameters. The performance of power, voltage and the three losses (activation, concentration and ohmic) have been visualized. It was found that the ambient temperature and input gas pressure are effecting the performance of the PEMFC power deliver.

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