Modelling and validation of Proton exchange membrane fuel cell (PEMFC)

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Abstract. This paper is the outcome of a small scale fuel cell project. Fuel cell is an electrochemical device that converts energy from chemical reaction to electrical work. Proton Exchange Membrane Fuel Cell (PEMFC) is one of the different types of fuel cell, which is more efficient, having low operational temperature and fast start up capability results in high energy density. In this study, a mathematical model of 1.2 W PEMFC is developed and simulated using MATLAB software. This model describes the PEMFC behaviour under steady-state condition. This mathematical modeling of PEMFC determines the polarization curve, power generated, and the efficiency of the fuel cell. Simulation results were validated by comparing with experimental results obtained from the test of a single PEMFC with a 3 V motor. The performance of experimental PEMFC is little lower compared to simulated PEMFC, however both results were found in good agreement. Experiments on hydrogen flow rate also been conducted to obtain the amount of hydrogen consumed to produce electrical work on PEMFC.

1. Introduction

Fuel cell is an electrochemical device, which consists of negative charge electrode (anode), a positive charged electrode (cathode), and an electrolyte membrane. A fuel cell converts the chemical energy into electrical energy generally using oxygen and compressed hydrogen gas and produces only heat and water as byproduct [1]. Therefore, the fuel cell vehicles (FCV) are considered as zero-emission vehicle. Hydrogen fuel cell is identified as the most promising technologies as a power source, especially for transportation and stationary power application [2].

In a fuel cell, there are two electrodes, anode and cathode, and in the middle of it is an electrolyte membrane. A single fuel cell will generate about 0.7 volts [3]. In order to achieve higher amount of volts, multiple cells are stacked in series and it is called fuel cell stack system.

Hydrogen gas entering the fuel cell from the anode side and will split into proton and electron. Protons flow through the electrolyte to the cathode side forcing electrons to flow through external circuit producing electric current (figure 1). Oxygen gas fed into the cathode where oxygen, protons and electrons combine to from water which later given off from the exhaust as steam or vapors [4].
2. Fuel cell

Presently, there are various types of fuel cells that are under research and development. Each type has its particular properties, advantages, and disadvantage which makes them different in possible application. Table 1 below shows the characteristics of six main types of fuel cells that are already being developed and commercially used [5] [6].

Table 1. Types of fuel cell

| Fuel Cell Type | Polymer Electrolyte Membrane (PEMFC) | Direct Methanol (DMFC) | Alkaline (AFC) | Phosphoric Acid (PAFC) | Solid Oxide (SOFC) |
|---------------|--------------------------------------|------------------------|----------------|------------------------|---------------------|
| Fuel          | H₂                                   | CH₃OH + H₂O            | H₂             | H₂/CO/reformat         | H₂                  |
| Oxidizer      | O₂, air                              | O₂, air                | O₂, air        | O₂, air                | O₂, air             |
| Electrolyte   | Solid organic polymer                | Solid organic polymer  | Aqueous solution of potassium hydroxide soaked in a matrix | Liquid phosphoric acid soaked in a matrix | Solid zirconium oxide to which a small the amount of yttria is added |
| Operating Temperature | 40-100 ºC             | 60-130 ºC            | 65-220 ºC      | 205 ºC                | 600-1000 ºC          |
| Efficiency    | 50-60%                               | 40%                    | 50-70%         | 40 %                  | 50-60 %             |
| Applications  | -Electric equipment                  | -Electric equipment    | -Space         | -Stationary power generator | -All sizes of stationary power generation. |
|               | -Portable devices                    | -Portable devices      | -Military      | -Large vehicles        | -Electric utility   |
|               | -Transportation                      | -Specialty devices     |                |                        | -Transportation     |
|               | -lower power                         |                        |                |                        |                     |
|               | CHP system                           |                        |                |                        |                     |
|               | -Specialty                           |                        |                |                        |                     |
| Advantages    | -Solid                               | -Inexpensive           | -Cathode       | -Low cost              | - Non-precious      |
electrolyte reduces corrosion and management problem - Very strong bond, therefore, can be made into very thin film - Low operation temperature - Quick start-up - High power density - Compactness and lightness - Can absorb a lot of water - High power density - Easily transport and stored - Solid electrolyte advantages (see PEMFC) - Reaction faster in alkaline - High performance - Low cost material - Long time performance - Commercial electrolytes - Tolerant to impure H₂ - Low cost material - High performance - Compactness and lightness - Can absorb a lot of water - High power density - Easily transport and stored - Solid electrolyte advantages (see PEMFC) - Reaction faster in alkaline - High performance - Low cost material - Long time performance - Commercial - Can absorb a lot of water - High power density - Easily transport and stored - Solid electrolyte advantages (see PEMFC) - Reaction faster in alkaline - High performance - Low cost material - Long time performance - Commercial - Can absorb a lot of water - High power density - Easily transport and stored - Solid electrolyte advantages (see PEMFC) - Reaction faster in alkaline - High performance - Low cost material - Long time performance - Commercial - Can absorb a lot of water - High power density - Easily transport and stored - Solid electrolyte advantages (see PEMFC) - Reaction faster in alkaline - High performance - Low cost material - Long time performance - Commercial

Disadvantages - Expensive catalyst - Sensitive to CO impurities - Crucial water management - All parts must be sufficiently hydrated - Intolerant CO₂ in impure H₂ and air - Corrosion - Expensive catalyst - Water management - Require more expensive catalyst - Corrosive and sulfur poisoning of electrolyte - Large and heavy - Slow start-up - Requires significant thermal shielding to retain heat - Corrosive electrolyte causes decreasing in cell life.

2.1 PEM Fuel cell for automotive application
PEM fuel cell is the most used technology in fuel cell vehicles. Many large automotive companies are focusing more on PEM fuel cell development. The main reason is the high power density of PEM fuel cell, which meets the requirement of space constraint in vehicles.

This is also because of PEM fuel cell’s lower operating temperature which allows a rapid start-up. The efficiency varies usually between 40-60% and output power can be changed to meet quickly demanded load [5]. Another characteristic of PEM fuel cell is the compactness and lightness. Thus, it is the best candidate for mobile application [7]. However, PEM fuel cell is sensitive to fuel CO impurities and requires precious metal as a catalyst which is expensive. Other than that, the electrolyte must be sufficiently hydrated. Thus, water management on stack becomes crucial [8]. In transportation, PEM fuel cell is used in hybrid configuration with electricity storage devices, such as batteries or super capacitor.

3. Modelling of PEMFC system

3.1 Nernst equation
In PEM fuel cell, the cell potential that obtained in open circuit thermodynamic balance is the reversible voltage of PEM fuel cell (E_Nernst). It can be defined mathematically by the following equation:

\[ E_{Nernst} = \eta_{anode} + \eta_{cathode} - \frac{RT}{2F} \ln \left( \frac{p_{H_2}}{p_{air}} \right) \]
\[ E_{Nernst} = E_r + \frac{RT}{2F} \ln \left( \frac{P_{H_2}P_{O_2}^{0.5}}{P_{H_2O}} \right) \]  

(1)

\[ E_{Nernst} \] can be calculated by modified version of the equation by taking the standard temperature as 25 °C [9]. Using the standard pressure and temperature values, the Nernst equation can be rewritten as:

\[ E_{Nernst} = 1.229 + 0.85 \times 10^{-3} (T - 298.15) + 4.3085 \times 10^{-5} \ln \left( \frac{P_{H_2}P_{O_2}^{0.5}}{P_{H_2O}} \right) \]  

(2)

When the byproduct is steam instead of water, 1.229 V should be replaced by 1.18 V. \( T \) is the cell operating temperature in Kelvin, \( P_{H_2} \) and \( P_{O_2} \) are hydrogen and oxygen partial pressure in atm.

3.2. Voltage losses

When the electrical energy is drawn from the fuel cell, the actual voltage decreases due to the several irreversible loss mechanisms. It can be defined as:

\[ V(i) = V_{rev} - V_{irrev} \]  

(3)

Three major classification of losses that cause the voltage drop from the circuit are as follows:

3.2.1. Activation polarization loss. Activation polarization loss is the voltage over potential required to overcome the activation energy of the electrochemical reaction on the catalytic surface. This type of losses dominates at low current density. Activation polarization loss can be used to measure the catalyst effectiveness at a given temperature [10]. The activation losses can be expressed simply by the Tafel equation:

\[ \nu_{act} = -\frac{RT}{anF} \ln \frac{i}{i_0} \]  

(4)

Where \( i \) is the current density, and \( i_0 \) is the reaction exchange current density. The reaction rate represents by the exchange current density. \( F \) is Farady’s constant, \( n \) is the number exchange protons per mole of reactant, and \( \alpha \) is the charge transfer coefficient used to describe the amount of electrical energy applied to change the rate of the electrochemical reaction.

3.2.2. Ohmic polarization loss. Ohmic polarization loss is due to natural resistance upon charge flow in conductors which occurs because of electrical resistance in the cell components [11].

\[ \nu_{ohmic} = iR_{ohmic} = i(R_{ionic} + R_{elec}) \]  

(5)

Where the current of the fuel cell is \( i \) (A), while \( R_{elec} \) is the total electric resistance of all other conductive components (Ω), and \( R_{ionic} \) is the ionic resistance of the electrolyte. Since the ohmic overpotential for the fuel cell is mainly due to ionic resistance in the electrolyte, this can be expressed as:

\[ \nu_{ohmic} = iR_{ohmic} = jA_{cell} \frac{\delta_{thick}}{\sigma A_{cell}} = \frac{j\delta_{thick}}{\sigma} \]  

(6)

3.2.3. Concentration polarization loss. The fuel cell concentration losses (or mass transport losses) can be express by the following equation:

\[ \nu_{conc} = \ln \left( \frac{i}{i_L} \right) \]  

(7)

Where the limiting current density is \( i_L \), while \( i \) is the current density of the fuel cell, and \( c \) is a constant. The value of \( c \) is approximately:
\[ c = \frac{RT}{2F} = \frac{(8.314)(373.5)}{2(96485)} = 0.016 \]  \hspace{1cm} (8)

The absolute temperature is assumed at 373.5 K (100 °C) which is the boiling point of water [9]. This is due to voltage drop occurs at the high-temperature condition as well as high current density. Therefore, the voltage loss by concentration equation can be expressed as:

\[ \nu_{conc} = 0.016 \ln \left( \frac{i_k}{i_k-I} \right) \]  \hspace{1cm} (9)

3.3.4. Reactant gasses diffusion in the electrode. To find Nernst voltage and voltage losses, the partial pressure of water must be calculated first and after that the partial pressure of hydrogen and oxygen. To calculate the partial pressure, the assumptions are as follows [5]:

i. Ideal and uniform gas distribution
ii. The fuel cell gas flow channel at constant pressure
iii. One-dimensional treatment
iv. \( H_2 \) is humidified and oxidant is humidified by air. The effective anode water vapor is at 50\% of the saturated vapor pressure while the effective cathode water pressure is 100\%.

Thus, the saturation pressure of water can be express as:

\[ \log_{10}(P_{H_2O}) = -2.1794 + (0.02953 \times T_c) - (9.1837 \times 10^{-5} \times T_c^2) + (1.4454 \times 10^{-7} \times T_c^3) \]  \hspace{1cm} (10)

Where the operating temperature at degree Celcius is \( T_c \), the partial pressure of hydrogen and oxygen are:

\[ P_{H_2} = 0.5 \times \left[ \frac{P_a}{\exp \left( \frac{1.653T_c}{4.192T} \right)} \right] - P_{H_2O} \]  \hspace{1cm} (11)

\[ P_{O_2} = \left[ \frac{P_c}{\exp \left( \frac{4.192T_c}{7T} \right)} \right] - P_{H_2O} \]  \hspace{1cm} (12)

Where the saturated vapor pressure in atm is \( P_{H_2O} \), while \( T \) is the absolute temperature (K), \( P_c \) is the partial pressure at the cathode, and \( P_a \) is the partial pressure at anode.

4. Results and discussions

4.1 Experiment on performance of PEM fuel cell

An experiment has been conducted using Horizon FCSU-12 PEM Mini fuel cell to determine its performance. To express the performance of a fuel cell, current voltage dependency is the most important property due to kinetics of electrochemical reaction of oxygen and hydrogen [12]. Figure 3 represents polarization curve of fuel cell used. The polarization curve shows the electrochemical efficiency of the fuel cell at operating current. At first, the output voltage was recorded directly from the fuel cell without connecting it to the motor which will determine its open circuit voltage. As can be seen on figure 4, both experimental and simulation data are in good agreement. The open circuit (no load) voltage of the experimental PEM fuel cell is almost similar with the simulation data. But after that, the activation losses that occurred on the experimental PEM fuel cell are greater compared to simulation. This shows that the efficiency of the experimental fuel cell seems to be much lesser compared with the simulation. This may be due to the circuit of the motor that contain more resistance since there are two LED light attached to
the motor circuit. The voltage reading only can be take maximum at 0.5 A due to the motor specification. Larger than 0.5 A of load will damage the motor.

![Figure 2. Experiment setup](image)

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For further validation, the experimental and simulation data are compared with the results from other studies as can be seen on figure 5. All results are in good agreement. The result from S. Haji [10] is conducted at 25°C which is similar to the condition of this experiment, while T. Selyari et al. [13] fuel cell is conducted at 50°C. Both are using a fuel cell with an active area of 25 cm². However, T. Selyari et al. fuel cell performance are much higher due to greater fuel cell operating temperature. This can validate that higher temperature does improve the performance of the fuel cell. Meanwhile, L. Patularu et al. [14] conducted the study at 23°C with 92 cm² active area. Although, the operating temperature is much lower, the greater active area improves the performance of the cell. More hydrogen and oxygen are utilized to produce higher electrical work.
Figure 3. Polarization curve of experimental PEM fuel cell

Figure 4. Comparisons between experimental and simulation value of PEM fuel cell polarization curve
4.2 Experiment on hydrogen flow rate

Figure 6 shows the configuration of the hydrogen fuel cell flow rate measurement system. The input of flowmeter is connected to the hydrogen supply system while the output flowmeter is connected to the fuel cell. The reading on the flowmeter is taken with one minute interval.

From both graph on figure 7 shows the variation of hydrogen flow rate based on the change of voltage and time. Both graphs show that there is no rapid change on the amount of hydrogen flow rate. From figure 7, the graph shows a little increasing trendline which proves that higher hydrogen flow rate produce higher voltage. This result also achieved by Khazaee et al. [16] where the experiment was done on different hydrogen and oxygen flow rate to determine the performance of the cell. It is
observed that the increasing of oxygen flow rate from 0.5 L/min to 0.9 L/min and hydrogen flow rate from 0.3 L/min to 0.7 L/min enhances the performance.

From the equation of the trendline on the graph in figure 7 which is,

\[ y = 0.0297x + 0.1519 \] (13)

It can be assumed that the slope of the trendline is \( m = 0.0297 \). This value also can represent that 0.0297 l/min of hydrogen is needed to produce 1 Volt.

![Figure 7. Hydrogen flow rate versus time and voltage](image)

### 4.3 Simulation of PEM fuel cell using MATLAB Simulink

#### Fuel cell nominal parameters:
- Stack Power: Nominal = 558.8 W, Maximum = 633 W
- Fuel Cell Efficiency = 0.7833
- Open circuit voltage of one cell (V) = 1.218 V
- Nominal Utilization:
  - Hydrogen: 7.2% - 8.4%
  - Oxygen: 95% - 99%
- Nominal Consumption:
  - Fuel: 0.3 l/min
  - Air: 14.27 l/min
- Exchange current density: 0.22059 A/cm²
- Exchange coefficient (global): 0.00545

#### Fuel cell signal variation parameters:
- Fuel composition (\% H₂): 92.05%
- Oxygen composition (\% O₂): 21%
- Fuel flow rate (Fuel Flow) of nominal Hydrogen utilization:
  - Nominal = 39.35 l/min
  - Maximum = 58.5 l/min
  - Minimum = 30.3 l/min
- Air flow rate (Air Flow) at nominal Oxygen utilization:
  - Nominal = 308.0 l/min
  - Maximum = 558.4 l/min
- System Temperature (T₁) = 290 K/36°C
- Fuel supply pressure (Fuel): 1.5 bar
- Air supply pressure (Air): 1 bar

![Figure 8. PEM fuel cell stack simulation parameters and setup](image)
In this simulation, we want to observe how the fuel flow rate may affect the fuel cell stack voltage which will affect the stack efficiency, fuel consumption and air consumption. For the first 10 secs, the utilization of hydrogen is set to constant ($u_f \text{H}_2 = 99.56\%$) by via a fuel flow rate regulator. After 10 secs, the flow rate regulator is bypassed and the fuel flow rate is increased from 50 lpm to maximum 85 lpm. The increase of fuel flow rate has resulted in the increase in stack voltage and decrease in stack current as shown in figure 10. From figure 9, stack efficiency is at its highest at 0.7 sec which nearly 76%, and after that it starts to decrease as the load increases. The stack efficiency
once again starts to drop after 10 secs from 55% to 33% at 13.5 second. This drop of stack efficiency after 10 second seems to be affected by the decreasing amount of hydrogen utilization, stack consumption and current.

5. Conclusion
Fuel cell are a new promising technology for generation of electrical energy, not just for automotive application but for other applications as well. This technology involves in using hydrogen and oxygen to produce electrical work through electrochemical process within the fuel cell. The experiment and simulation of fuel cell have been conducted using mini PEM fuel cell to measure the output voltage on certain amount of load which can prove the efficiency of the fuel cell. An experiment and simulation on hydrogen flow rate on PEM fuel cell also have been conducted to determine the effect of hydrogen flow rate on the fuel cell voltage and to measure the amount of hydrogen needed for the fuel cell to produce electricity. From the study it can be concluded that:

i. Both experimental and simulation results are in good agreement although the voltage losses on experimental result is little greater.

ii. It is observed that the increasing fuel flow rate will increase the voltage produced by the fuel cell.

iii. It is also observed that higher operating temperature and pressure of the cell improve the performance of the fuel cell.

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