Simulation Analysis of Polymer Electrolyte Membrane Fuel Cell Using Aspen Plus

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Abstract. We present a simulation of proton exchange membrane fuel cell (PEMFC) system to convert the chemical energy stored in hydrogen into electrical power. The PEMFC model was developed using Aspen Plus and then analyzed to find the electricity generated. In the PEMFC system simulated in this study, hydrogen gas enters the heat exchanger prior to entering the anode to increase its temperature up to 80 °C. Around 80% of hydrogen used during electrochemical reactions with the oxygen, which entered from the cathode side. The proton and electron of the hydrogen combine, react with the oxygen provided, and produce water and heat. Based on the analysis, the power generated by the PEMFC system is 0.23 kW with current density of $1 \times 10^{-3}$ A/m² and MEA area of $3 \times 10^{-2}$ m², and the number of cells in stack is 135 cells.

1. Introduction

Indonesia is the country with the largest energy consumption in Southeast Asia and fifth in the Asia Pacific in primary energy consumption, placed after China, India, Japan, and South Korea [1]. An increase in energy consumption that results from human-related activities causes the depletion of fossil fuels and the global warming problem [2]. Currently, fuel cell has received much due to their high efficiencies and low emission [3]. The fuel cell is electrochemical devices that directly convert chemical energy stored in fuels such as hydrogen to electrical power. The efficiency for fuel cell can reach as high as 60% in electrical energy conversion, with an overall 80% in co-generation of electrical and thermal energies, and high in reduction emissions [4]. Five categories of fuel cell have received major efforts of research, namely, polymer electrolyte membrane (PEM) fuel cells or PEMFCs, solid oxide fuel cells (SOFCs), Alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), and molten carbonate fuel cells (MCFCs). PEM fuel cells are constructed using polymer electrolyte membrane as proton conductor and Platinum (Pt)-based material as the catalyst. The PEMFCs are considered as a possible answer to environment and energy problems and are expected to be a promising energy conversion device for automotive, stationary, and portable applications, because of their high-energy density at low temperatures, quick start-up and zero emissions [5-12], and high durability [13,14].

The primary application of PEMC is on transportation due to their potential impact on the environment, e.g. the control of emission of greenhouse gases. Other forms included distributed/stationary and portable power generation. Another promising area is portable power supply, considering that limited energy capacity of batteries unlikely meets the fast-growing energy
demand of modern mobile electric devices such as laptops, cell phones, and military radio/communication devices. PEM fuel cells provide continuous power as long as hydrogen fuel is available, and they can be fabricated in a small size without efficiency loss. Major electronics companies, such as Toshiba, Sony, Motorolla, LG, and Samsung, have in-house R&D units for portable fuel cells.

Hydrogen is an ideal fuel for PEMFC[20]. Hydrogen has the highest energy content per unit weight of any known fuel (142 kJ.g⁻¹) [21] more energy density than other existing biofuels such as methane, methanol, and ethanol [22]. In a traditional PEMFC system, hydrogen flows through the anode, and the un-reacted hydrogen is directly exhausted into the atmosphere, which reduces the efficiency of hydrogen utilization significantly[15]. The typical efficiency of hydrogen utilization for flow-through anode PEMFC is in the range of 65% - 95%, depending on the design of the stack and control strategy according to the PEMFC system [16]. To address this question, the additional fuel circulation system is often introduced to the PEMFC system, with which the un-reacted hydrogen is pump back from the outlet to the upstream region of the stack and is again supplied to the inlet with fresh hydrogen [17-19].

2. Description systems

2.1. The Basic of Fuel cell

The fuel cell works based on the concept of electrochemical reaction, and thus, it is considered to be more efficient then because of the maximum amount of chemical reaction is directly transformed into electrical energy instead of conversion to mechanical work through combustion (i.e., internal combustion engines) causing further loss of efficiency. The fuel used in operating in the fuel cell is hydrogen utilized to achieve the best possible electrochemical reaction [6]. The power and heat produced can be utilized for any cogeneration. Hydrogen flows in from the anode side plate and comes in contact with membrane coated with a catalyst. Upon contact with the membrane, hydrogen splits into electrons and protons. Electron is taken out from the plate with the help of circuit. These electrons go through a circuit, give out power and return to the cathode side flow plate to have a closed-loop. The protons that are left behind are allowed to pass through the membrane onto the cathode side of the cell. At the cathode side, oxygen is supplied through the cathode side flow plate. The proton and electron of the hydrogen combine, react with the oxygen provided, and produce water and heat.

2.2. Design of PEMFC model system

Hydrogen enters the blower with discharge pressure 1.2 Bars then enters the heat exchanger to increase the temperature needed of 80 °C. Hydrogen enters the anode and is utilized, and 80% of hydrogen used enters the cathode, and the rest one comes to the burner. On the other side, air enters the blower with discharge pressure 1.2 Bars and enters the heat exchanger to increase temperature needed, 80 °C, and then air enters the separator to separate between oxygen and nitrogen. 32.5% of Oxygen comes the cathode, and the rest one plus nitrogen enters the burner. The heat produced in the burner distributes to the heat exchanger to increase temperature hydrogen and oxygen. In the cathode, electrochemical reaction takes place to provide water, heat, electrical energy.

In the preceding study [23], the PEMFC was modeled using Aspen Plus and analyzed in the working temperature of 120 °C. In this analysis, the system developed in Aspen plus simulation is shown Figure 1, with the working temperature of 80 °. The electrochemical model used to describe the electrical characteristic of the PEMFC is derived [7] under the following assumptions: steady-state and isothermal condition, ideal gas behavior, and no membrane swelling. Anode losses in the fuel cell are not considered due to the fast kinetics of the hydrogen oxidation reaction [8]. PEMFC using pure oxygen as oxidant is particular interest for specific application including aerospace and submarine application [9] for which the efficiency of fuel usage is required as high as possible. The overall voltage is obtained by determining the reversible cell potential and then subtracting the voltage losses, such as the kinetic voltage losses at the cathode and the ohmic resistance of membrane and electrodes [20].
2.3. Analysis of PEMFC stack module

The present PEMFC stack module is simplified from the previous three-dimensional HT-PEMFC CFD models developed by other researchers [17, 22, 24-25]. The output voltage of a single cell ($V_{cell}$) can be obtained by considering all the irreversible voltage losses from the thermodynamic equilibrium potential[26] as follows.

$$V_{cell} = U_O - \eta_{act} - \eta_{ohm} - \eta_{con}$$  \hspace{1cm} (1)

Where $\eta_{act}$, $\eta_{ohm}$, and $\eta_{con}$ represent the activation, ohmic, and concentration polarizations, respectively. The expression of $E_{Nernst}$ is given by Chippar and Ju[27]:

$$U_O = 1,1669 - 0,24 \times 10^{-3} (T_{cell} - 373,15)$$  \hspace{1cm} (2)

The activation overvoltage in Equation above, $\eta_{act}$, is calculated using the Bulter-Volmer equation for the hydrogen oxidation reaction (HOR) in the anode and oxygen reduction reaction (ORR) in the cathode [27] as determining as follows:

$$\eta_{act, a} = \frac{i_{ref}}{i_{0, a}^ref} \left( \frac{C_{H_2}^ref}{C_{H_2}} \right)^{1/2}$$ \hspace{1cm} (3)

$$\eta_{act, c} = \frac{i_{ref}}{i_{0, c}^ref} \ln \left( \frac{C_{O_2}^ref}{C_{O_2}} \right)^{3/4}$$ \hspace{1cm} (4)

where, $C_j$ and $\alpha$ represent the molar concentration and transfer coefficient, respectively. Also $i_{0, a}^ref$ and $i_{0, c}^ref$ denote the exchange current density of HOR and ORR, respectively. Their expression was driven by Chippar and Ju [26] as a function of temperature as follows:

$$i_{0, a}^{ref} (T) = i_{0, a}^{ref} (353,15K). \exp \left[-1400 \left( \frac{1}{T} - \frac{1}{353,15} \right) \right]$$ \hspace{1cm} (5)

$$i_{0, c}^{ref} (T) = i_{0, a}^{ref} (353,15K). \exp \left[-7900 \left( \frac{1}{T} - \frac{1}{353,15} \right) \right]$$ \hspace{1cm} (6)
The ohmic loss, $\eta_{ohm}$ is due to both proton and electron charge transport through various PEMFC stack components [27].

$$\eta_{ohm} = i \left( R_{H^+} + R_{elec} \right) \quad (7)$$

In equation above, the area-specific resistance due to the proton transport, $R_{H^+}$ was obtained by considering the membrane and catalyst layer properties as follows [27]:

$$R_{H^+} = \frac{\delta_{mem}}{K} + \frac{0.5 \delta_{ACL}}{V_{ACL} K} + \frac{0.5 \delta_{CL}}{V_{CL} K} \quad (8)$$

In equation above, $V_{ACL}$ and $V_{CL}$ denote the volume fractions of the electrolyte in the anode and cathode catalyst layer, respectively. The number 0.5 appearing in the number of the second and third terms is due to the assumption that the average proton transport path through the catalyst layer is half of its thickness. Finally, the concentration polarization, $\eta_{con}$ is expressed as follows [27]:

$$\eta_{con} = \frac{RT}{4F} \ln \left( \frac{i_{lim}}{i_{lim}-i} \right) \quad (9)$$

In equation above, $i_{lim}$ represent the limiting current density that is determined by the interfacial oxygen concentration between the cathode gas channel and gas diffusion layer (GDL), and porosity and thickness of cathode GDL, which can be expressed as [27]:

$$i_{lim} = V_{GDL}^{1.5} D_{O_2} \frac{c_{O_2}}{\delta_{GDL}} \quad (10)$$

Once the single cell voltage, $V_{cell}$, is calculated from the equation above, the stack voltage, $V_{stack}$, and stack power, $P_{stack}$, can be estimated depending on stack configuration. If the cells are connected in series, $V_{stack}$ and $P_{stack}$ are as follows [27].

$$V_{stack} = n_{cell} V_{cell} \quad (11)$$

$$P_{stack} = n_{cell} V_{cell} \cdot i \cdot A_{MEA} \quad (12)$$

where $n_{cell}$ and $A_{MEA}$ are the number of cells in the PEMFC stack and the area of the membrane electrode assembly (MEA) for each cell, respectively.

The electrical efficiency of the PEMFC system, $\epsilon_e$, is defined as the ratio of the net output electrical power produced by the PEMFC system to the low heating value of the fuel supplied as follows [27].

$$\epsilon_e = \frac{P_{stack} - \sum_i bh_{pi}}{m_{fuel} x LHV_{fuel}} \quad (13)$$

**Table 1.** Input parameters and geometric/operating condition [26].

| Parameter                          | Value          | Ref. |
|-----------------------------------|----------------|------|
| MEA area, $A_{MEA}$               | 300 cm$^2$     | -    |
| Operating Temperature, $T_{cell}$ | 165 °C         | -    |
| Number of cell in a stack, $n_{cell}$ | 135          | -    |
| Anode/cathode stoichiometry, $\xi$ | 1.2/2.0       | -    |
| Thickness of anode/cathode GDLs, CLs, $\delta_{GDL}, \delta_{CL}$ | 0.35/0.015 mm | -    |
| Thickness of anode/cathode membrane, $\delta_{MEM}$ | 0.07 mm    | -    |
3. Results and Discussion
The influences of current density to cell voltage and cell power are shown in figure 2. The cell voltage decreased along with the incremental values of current density. The Nernst voltage value is around 1.172 Volt. The voltage drop during operation due to activation losses, ohmic losses, and concentration losses. From Figure 2, the cell power increase along with increasing the current density.

![Figure 2. Graphic of cell voltage, cell power, and current density.](image)

The influences of various temperature conditions towards the cell voltage and current density are shown in Figure 2. It showed that the graphs trend tend linear among cell voltage at the working temperature of 80°C, 90°C, 100°C, 110°C, and 120°C. Meanwhile, the incremental temperature influences the performance of cell voltage, which causesthe cell voltage drops. Thus, The PEMFC is proper to work at low-temperature conditions.
4. Conclusion
The operational characteristic of proton exchange membrane fuel cell has been investigated under various operating conditions. The incremental temperature influences the performance of cell voltage, which causes the cell voltage drops. By utilizing of 80% hydrogen, during electrochemical reactions in the processes, the PEMFC can produce 1.172 Volt. Several experimental under simulation conditions are under processing to investigate the effect of different fuel utilization and air utilization to the PEMFC performance.

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