Modeling and Analysis of a PEM Fuel cell for Electrical Applications

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Abstract - This paper presents a proposed three-Dimensional (3D) computational electrochemical simulation model for simulation and evaluation performance of Polymer Electrolyte Membrane (PEM) fuel cell. The proposed model is used to predict the output voltage, efficiency, hydrogen supply and study the transient response of PEM power plant when subjected to variable load connected to it. Additionally, the effects of temperature and current density have been studied. The effectiveness of the proposed model has been verified via extensive simulation using Matlab program to evaluate how the major operating variables affect the output performances. The results have indicated that the model provides an accurate representation of the dynamic and static behaviors of the fuel cell power module and guarantee a better analytical performance. On the other hand, the results show that the computer model can represent characteristics of the power system and it can be used in the study and design of fuel cell for electrical applications under different load conditions and temperatures.

Index Terms – Fuel cell, Modeling, Applications

I. INTRODUCTION

In 1838 Christian Friedrich Schoenbein discovered the fuel cell effect that marked the beginning of fuel cell research. Later on William Robert Grove invented the first fuel cell which started the development of the clean energy converter. The fuel cell, as a renewable energy source, is one of the most promising sources of electric power. They can be considered as green power sources because they are environmentally clean, have extremely low emission of oxides of nitrogen and sulfur, have very low noise, and high energy density. In addition, they can provide energy in a controlled way with higher efficiency than conventional power plants. The fuel cell is an electrochemical conversion device. It produces electricity from fuel (on the anode side) and an oxidant (on the cathode side), which react in the presence of an electrolyte. The reactants flow into the cell, and the reaction products flow out of it, while the electrolyte remains within it. Fuel cells have recently attracted a great deal of attention with some promising results in applications ranging from powering small cellular phones to large power generation in utilities [1-5]. There are several different types of fuel cells depending on the type of electrolyte materials used [6]. The commonly available fuel cells can be classified according to temperature, into low-temperature, medium-temperature, and high temperature fuel cells. The low-temperature fuel cells include the alkaline fuel cell, and solid polymer fuel cell or proton exchange membrane fuel cell (PEMFC). The medium-temperature class has the phosphoric acid fuel cell. The high-temperature class has the molten carbonate fuel cell and solid oxide fuel cell [1]. PEM fuel cells generally operate at lower pressure and lower temperature with higher power density compared to other types of fuel cells. Therefore, they are more suitable for applications in small to medium power levels, such as fuel cell powered automobiles or micro-grid power applications. The modeling and analysis of fuel cells is an important part to simulate and model of the fuel cell since they facilitate a better understanding of parameters affecting the performance of fuel cells and fuel cell systems. Several fuel cell models can be found in the literature. Amphlett et al. [2] used a semi-empirical approach to estimate the activation loss and to predict the voltage output of a Ballard Mark V 35-cell stack. El-Sharkh et al. [3] introduced a dynamic model for a stand-alone PEM fuel cell power plant. Then, Uzunoglu and Alam [4] modified the PEM fuel cell model described in [3] in Matlab and Simulink for stand-alone residential applications. Zhang et al. [5] presented the effects of the temperature and the equivalent internal resistance on the output characteristics of the PEM fuel cells. Baschuk and Li(489,950),(903,972) describe detailed model the PEMFC voltage in terms of the three aspects: 1) reversible voltage; 2) activation and mass transport loss of the cathode, and 3) ohmic losses of the electrode, membrane and flow channel plate. Many fuel cell models have been developed and reported in literatures but they didn’t focus on a 3D computational electrochemical simulation model for fuel cell performance and impact of individual operating parameters on fuel cell output characteristics. The paper implements a simple model to present a 3D computational electrochemical simulation model for fuel cell and it also presents impact of different operating temperatures on the performance of PEMFC characteristics against situations, like efficiency, power characteristics and load variations. Using the present dynamical model, it is also possible the development of several control techniques for the operation of the PEMFC.

II. MATHEMATICAL MODEL

A. Fuel cell system

The PEMFC considered in the present study is based on the parameters of a Mark V cell, manufactured by the Canadian Company Ballard, whose operation and data are well known in the literature. Under normal operation, a simple FC typically produces 0.5 V to 0.9 V. For use in energy generation systems, where a relatively high power is needed, several cells are connected in series, arranging a stack that can supply hundreds of kW. The PEMFC primarily consists of three components: a negatively charged electrode (cathode), a positively charged electrode (anode), and a PEM. The simple
The electro-chemical reactions in the PEMFC are shown below:

1. \( H_2(g) \rightarrow 2 H^+ + 2e^- + \text{waste heat} \)
2. \( 2H_2(g) + O_2(g) \rightarrow 2H_2O(l) \)

Here, the waste heat produced in the stack module is removed through the cooling system.

**B. PEMFC Mathematical Model**

Useful amount of electrical energy could be obtained from a fuel cell only when a reasonable current is drawn from it. The PEMFC performance model developed by [8,9] is used to simulate the fuel cell stack. Fig. 2 shows the simplified circuit diagram of the actual PEMFC. The model predicts the voltage of a single cell at any specified operating conditions. The voltage of the entire stack is then obtained by multiplying the single cell potential with the number of cells in the stack.

\[
V_{cell} = E_{Nernst} - V_{act} - V_{ohmic} - V_{con} \quad (3)
\]

Where:

\[
E_{Nernst} = 1.229 - 0.85 \times 10^{-3} \times (T_k - 298.15) + 4.3085 \times 10^{-5} \times T_k \times [\ln(p_{H_2}) + 0.5 \times \ln(p_{O_2})] \quad (4)
\]

\( E_{Nernst} \) : The Nernst voltage or reversible voltage that exists at no load condition for a given temperature and pressure.

\[
V_{act} = -\xi_1 + T_k \times \xi_2 + T_k \times \xi_3 \times \ln(C_{O_2}) + T_k \times \xi_4 \times \ln(I_{fc}) \quad (5)
\]

\( V_{act} \) : The activation voltage drop due to the slowness of the chemical reactions taking place at electrode surfaces. Depending on the temperature and operating pressure, type of electrode, and catalyst used, this region is more or less wide, and.

\[
V_{ohmic} = I_{fc} \times (R_c + R_M) \quad (6)
\]

\( V_{ohmic} \) : The ohmic voltage drop results from the resistance to the electrons transfer through the collecting plates and carbon electrodes, and the resistance to the protons transfer through the solid membrane, and

\[
V_{con} = -B \times \ln \left( 1 - \frac{J}{J_{max}} \right) \quad (7)
\]

\( V_{con} \) : The voltage drop resulting from the reduction in concentration of the reactants gases or, alternatively, from the transport of mass of oxygen and hydrogen (also known as concentration over potential).

In the above equations, the parameters are:

- \( T_k \) : Cell operating Temperature (K),
- \( B \) (V) : Parametric coefficient, that depends on the cell and its operation state
- \( p_{H_2} \) : Effective partial pressure of Hydrogen (atm),
- \( p_{O_2} \) : Effective partial pressure of Oxygen (atm),
- \( \zeta \)'s : Represent parametric coefficients for each cell model, whose values are defined based on theoretical equations with kinetic, thermodynamic and electrochemical foundations [2, 10-12].
- \( C_{O_2} \) : Concentration of oxygen in the catalytic interface of the cathode (mol/cm³), it can be determined by:

\[
C_{O_2} = \frac{p_{O_2}^\gamma}{5.08 \times 10^6 \times \exp (-498/T_k)} \quad (8)
\]

- \( n \) : Number of exchange protons per mole of reactant,
- \( F \) : Faraday’s constant, 96,485 Coulombs.
- \( I_{fc} \) : Cell operating current (A), it can be calculated as follow:-

\[
I_{fc} = J \times A_a \quad (9)
\]

- \( A_a \) : Active intersection area of fuel cell stack, (cm²)
- \( J \) : Current density. Typical values for current density are in the range of 500 to 1500 mA/cm².
- \( R_c \) : Resistance to the transfer of protons through the membrane usually considered constant.
- \( R_M \) : Equivalent resistance of the membrane, It can be calculated by:-

\[
R_M = \frac{\rho_M}{A_a} \quad (10)
\]

Where,

- \( \rho_M \) : Specific resistivity of the membrane for the electron flow (Ω cm),
- \( l \) : Thickness of the membrane (cm).
The membranes of the type Nafion® considered in this work, is a registered trademark of Dupont and broadly used in PEMFC. Dupont uses the following product designations to denote the thickness of the membranes Nafion:
Nafion 117: 7 mil (l = 178 μm)
Nafion 115: 5 mil (l = 127 μm)
Nafion 112: 2 mil (l = 51 μm)
The following numeric expression for the resistivity of the membranes Nafion is used [10]:
\[
\rho_M = \frac{181.6}{\psi} \left[ 1 + 0.03 \left( \frac{T}{303} \right) ^2 + 0.062 \left( \frac{T}{303} \right) ^{2.5} \right] \left( \frac{303}{T} \right) ^{0.634 - 3 \left( \frac{T}{303} \right) ^2 + \exp \left[ \frac{4.187 - \left( \frac{T}{303} \right) ^2}{\left( \frac{T}{303} \right) ^2} \right] \right) \tag{11}
\]
\( \psi \) : The membrane water content.
The parameter \( \psi \) is an adjustable parameter with a possible maximum value of 23 and minimum value of 14 [10]. This parameter is influenced by the preparation procedure of the membrane and it is a function of relative humidity and stoichiometry relation of the anode gas. It may have a value of 14 under the ideal condition of 100% of relative humidity. The effective partial pressure for Hydrogen and Oxygen can be obtained through the following procedure.
First the saturation water vapor pressure for the system at the temperature of operation, \( p_{sat}^{H_2O} \), is calculated by [6,11]:
\[
\log_{10}(p_{sat}^{H_2O}) = -2.1794 + 0.02953 * Tc - 9.1837 * 10^{-5} * Tc^2 + 1.4454 * 10^{-7} * Tc^3 \tag{12}
\]
where, \( T_c \) : Temperature in Celsius and calculated by:
\( T_c = T_0 - 273.15 \)
The partial pressure \( p_H^2 \) and \( p_O^2 \) at cathode O2 H2 and anode are calculated by:
\[
p_H^2 = 0.5 \left( \frac{p_H^2}{\exp \left[ \frac{1653.1}{T_k} \right]} - p_{sat}^{H_2O} \right) \tag{14}
\]
\[
p_O^2 = \frac{p_O^2}{\exp \left[ \frac{1392.9}{T_k} \right]} - p_{sat}^{H_2O} \tag{15}
\]
Finally, the power output for the fuel cell system can then be calculated by the equation:
\[
P_{fcsystem} = n_{stack} * n_{cell} * V_{cell} * I_{fc} \tag{16}
\]
Where, \( n_{stack} \) and \( n_{cell} \) are number of stacks in the system and number of cells in a stack, respectively.
The power system model presented as shown in Fig. 3 consists of four major subsystems: the PEMFC stack module, the air compression subsystem, the hydrogen supply subsystem, and the cooling subsystem. The PEMFC stack module is the heart of the power system. The air compressor component of the system module provides pressurized oxygen in the form of air, to the stack. The pressurized air is cooled down in a heat exchanger and humidified in a humidifier before being fed to the stack. Similarly, compressed hydrogen stored on-board is humidified in a humidifier before feeding to the stack. Humidification of inlet streams is necessary to prevent dehydration of the membranes in the fuel cell stack. Non of all the hydrogen supplied to the fuel cell is consumed by the fuel cell stack, and therefore the unreacted hydrogen leaving the stack is recirculated. The purpose of the cooling loop is to remove the heat produced by the exothermic reaction of hydrogen and oxygen. The cooling loop consists of a radiator, cooling pump, radiator fan. The cooling pump directs coolant through the stack to remove the waste heat via radiator. In order to produce electricity, a fuel cell must be supplied continuously with fuel and oxidant. In addition, product water must be removed continually to insure proper fuel and oxidant at the catalyst layers to maintain high fuel cell efficiency. Voltage losses occur in the fuel cell due to activation losses, ohmic losses, and mass transport limitations. The hydrogen mass flow rate (g/s) is:
\[
m_{H2,in} = S_{H2} \cdot \frac{M_{H2}}{2F} \cdot n_{cell} \cdot I_{fc} \tag{17}
\]
The oxygen mass flow rate (g/s) is
\[
m_{O2,in} = S_{O2} \cdot \frac{M_{O2}}{4F} \cdot n_{cell} \cdot I_{fc} \tag{18}
\]
The air mass flow rate (g/s) is
\[
m_{air,in} = \frac{S_{O2} \times M_{air}}{r_{O2} \times 4F} \cdot n_{cell} \cdot I_{fc} \tag{19}
\]
In the above equations, the parameters are:
\( M_{H2} \) : Molar mass of hydrogen being 2.016 × 10⁻³ kg mole⁻¹,
\( S_{H2} \) : Hydrogen stoichiometric ratio.
\( M_{O2} \) : Molar mass of Oxygen being 31.9988 × 10⁻³ kg mole⁻¹,
\( S_{O2} \) : Oxygen stoichiometric ratio.
\( M_{air} \) : Molar mass of air which is equal to 28.85 × 10⁻³ kg mole⁻¹,
\( r_{O2} \) : Oxygen content in the air, which is equal to 0.2095.

### C. Efficiency of PEMFC

Fuel Cell is characterised by a high efficiency and comparatively small emissions. The fuel cell efficiency is the ratio between the electrical power output and the fuel input as shown in Eq. (21).
\[
\eta_{fc} = \frac{(Electrical \ Power \ Output) \ P_{fc}}{(Fuel \ Input) \ P_{in}} \tag{21}
\]
Where,
\( P_{fc} \) : The electrical power output of the fuel cell as shown in Eq. (16).
\( P_{in} \) : The input fuel (in power units). It is a product of fuel (hydrogen) consumption rate (in g/s) and its energy content, usually given as enthalpy (AH) or higher heating value. Hydrogen’s higher heating value is 142,000 J/g.

Hydrogen consumption rate (in g/s) and its energy content, usually given as enthalpy (AH) or higher heating value. Hydrogen’s higher heating value is 142,000 J/g. Hydrogen consumption rate (in g/s) can be calculated from Equ. (17).
\[
F_{in} = m_{H2,in} \cdot \Delta H = S_{H2} \cdot \frac{M_{H2} \cdot \Delta H}{2F} \cdot n_{cell} \cdot I_{fc} \tag{22}
\]
The expression \( \frac{M_{H2} \cdot \Delta H}{2F} \) has a value of 1.482 V. This is called reversible potential which corresponds to the maximum possible energy (both electrical and thermal) resulting from the electrochemical reaction as shown in Equ. (1) and (2).
Therefore, by combining equations (21), (16), (17) and (22),

\[ \eta_{fc} = 0.675 \times V_{fc} = 0.675 \times \frac{P_{fc}}{I_{fc}} \]  

\[ \text{(23)} \]

III. RESULTS AND DISCUSSION

First, the paper discusses the influence of operating cell temperature on the behavior of a single fuel cell as well as a stack, which include the typical polarization curves and efficiency at different working temperatures and transient responses of the stack on a current.

A. Parameters

In this work, the parameters of a Mark V cell, manufactured by the Canadian Company Ballard, are used, whose operation and data are well known in the literature as shown in Table I.

<table>
<thead>
<tr>
<th>Param.</th>
<th>Value</th>
<th>Param.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T )</td>
<td>20-100 °C</td>
<td>( z_{ij} )</td>
<td>-0.948</td>
</tr>
<tr>
<td>( A_a )</td>
<td>50.6 cm²</td>
<td>( z_{ij} )</td>
<td>0.0026+0.0002 Ln(A_a)²+4.3.10^{-5}.Ln(cH₂)</td>
</tr>
<tr>
<td>( L )</td>
<td>178μm</td>
<td>( \xi_{ij} )</td>
<td>7.6x10^{-5}</td>
</tr>
<tr>
<td>( PH_2 )</td>
<td>3 atm</td>
<td>( \xi_{ij} )</td>
<td>-1.93.10^{-4}</td>
</tr>
<tr>
<td>( PO_2 )</td>
<td>3 atm</td>
<td>( J_{act} )</td>
<td>1.5 A/cm²</td>
</tr>
<tr>
<td>( B )</td>
<td>0.016 V</td>
<td>( J_{act} )</td>
<td>1.2 mA/cm²</td>
</tr>
<tr>
<td>RC</td>
<td>0.0003 Ω</td>
<td>( J_{act} )</td>
<td></td>
</tr>
</tbody>
</table>

B. Effect of operating temperatures

Study the effect of fuel cell temperature on PEMFC performance was carried out in humidified and dry inlet gases conditions. Fig. 4 shows the temperature dependent \( f-V \) characteristics from 20 to 100°C with a step of 10°C with the externally humidified anode and cathode sides. Humidification temperatures were equal to the cell temperatures. Backpressures were constant in 3 atm. An increase in the cell voltage at the same current density is viewed in this figure, particularly under high current densities. In other words, the performance of the fuel cell is improved under elevated cell operating temperature in humidified inlet gases conditions. The increase of the fuel cell performance with the increase of the cell temperature can be explained by two reasons. First, with increasing temperature the diffusivity increases and mass transport resistance decreases, which reduces activation losses as shown in Fig. 5 and second, the increase in ohmic-ion conductivity of Nafion membrane which reduces voltage ohmic losses as shown in Fig. 6.

In Figure 7, the power curves are obtained with different values for current density and cell temperatures from 20 to 100°C with a step of 10 °C. Operation at higher temperature is essential to obtain high power density in the PEMFC system, since both will improve electrode kinetic performance and increase the ionic conductivity in the membrane and electrodes. However, a higher operating temperature will give more severe thermal management and membrane dryout problems.

Fig. 4. Temperature effect on the cell voltage of a PEM.
In this paper, the fuel cell efficiency is directly proportional to the cell potential, as shown from equation (23); So, the efficiency is a function of power and current density moreover temperature. Figs. 8-10 show the effect of cell voltage, power and current density with variable operating cell temperature on the performance surface of a PEMFC. From the presented data in Figs. 6-8, it can be seen that the potential and efficiency are higher values for low current densities and power densities. On the other hand, for higher values of power, the efficiency and the voltage are smaller values. Therefore, the control system for PEMFC needs to find the optimum operation point for the cell. The PEMFC cannot operate with a very high voltage (and, consequently, high efficiency and low current density) because the possible output power would be much reduced, meaning that the cell should be overestimated for this case. On the other hand, PEMFC cannot also operate with a very high output current, because, in this case, the potential and efficiency would be much reduced, besides decreasing the useful life of the PEMFC. Table II shows the exact values for maximum power and its corresponding values for efficiency, Voltage, current density and input hydrogen. A control system should be established among the demand of the load, the power supplied from the PEMFC and temperature. For example, if temperature increases from 60°C to 100°C for the same current density at 1.4629 A/cm², the operating voltage increase from 0.8190 to 0.8258 V and Power output decease from 61.2373 to 61.1304 W resulting in high efficiency of 60.44%.

<table>
<thead>
<tr>
<th>Tem. p., °C</th>
<th>Power, W</th>
<th>Efficiency</th>
<th>Voltage, V</th>
<th>Current density, A/cm²</th>
<th>mH₂, Kg/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>39.0543</td>
<td>42.24 %</td>
<td>0.5771</td>
<td>1.3373</td>
<td>2.4869e-005</td>
</tr>
<tr>
<td>40</td>
<td>46.2685</td>
<td>46.69 %</td>
<td>0.6379</td>
<td>1.4334</td>
<td>2.6655e-005</td>
</tr>
<tr>
<td>60</td>
<td>52.2351</td>
<td>51.64 %</td>
<td>0.7056</td>
<td>1.4629</td>
<td>2.7204e-005</td>
</tr>
<tr>
<td>80</td>
<td>57.1154</td>
<td>56.19 %</td>
<td>0.7677</td>
<td>1.4703</td>
<td>2.7342e-005</td>
</tr>
<tr>
<td>100</td>
<td>61.2373</td>
<td>59.94 %</td>
<td>0.8190</td>
<td>1.4777</td>
<td>2.7479e-005</td>
</tr>
</tbody>
</table>
C. Transient response

For electrical application use, the fuel cell stack is tested with the stack supplies 40 A to the load; after 3 seconds of simulation, the current is increased to 140 A, staying at this value until the simulation time reaches 7 seconds. Finally, the load current is decreased again to 40 A, until the end of the simulation (t = 10 seconds). The results correspond to the use of a PEMFC stack Ballard Mark V, consisting of an association of 35 cells, with an active area for each cell of 232 cm², with a power of 5 kW @ 960 mA/cm². The other parameters are the same ones as described in the Table I. The partial pressures of hydrogen and oxygen influence the resulting stack voltage. In the simulations that proceed, air was used as the oxidizer and, then, the partial pressure of oxygen becomes 0.319 atm.

Fig. 10 depicts variable load current. Fig. 11 shows the voltage during variation of load. It can be noticed that the values of the voltage are 35.21 V before the load increase, 31.13 V during the load pulse and, again, 35.21 V when the current is decreased. Fig. 12 shows the stack power output during a load variation. A peak can be observed at the load insertion instant, with a maximum value of 4.375 kW. When the load is decreased, the power presents a minimum value of 1.449 kW. On the other hand, hydrogen supply in kg/s during load variation presents in Fig. 13. In the real behavior of the fuel cell in the same operating conditions, there are snapshots during a transient from load variation.

The stack efficiency is shown in Fig. 14. The behavior is similar to the voltage, since these are directly related. The steady-state values for the efficiency are: 73.641% for a current of 40 A and 65.10% for a current of 140 A. It can be noticed that there is a significant reduction in the efficiency for variations of the demanded current, which should be taken into consideration when one evaluates a certain system.
IV. CONCLUSIONS

The paper presents a 3D computational electrochemical simulation model for PEMFC, on the other hand, it presents a computer modeling to analysis the performance of a PEMFC stack in similar circumstances as those commonly in small-scale power generation systems, such as load variations. From the results obtained above, the following salient conclusions can be drawn:

1. Computer model presents in this paper can represent characteristics of the power system and it can be used in the study and design of fuel cell for electrical applications under different load conditions and temperatures.
2. Voltage, power, hydrogen supply and efficiency affect by load demand and temperature.
3. The potential and efficiency are higher values for low current densities and power densities.
4. Higher values of the power, the efficiency and the voltage are smaller values. Therefore, the control system for PEMFC needs to find the optimum operation point for the cell.
5. If temperature increases from 60°C to 100 °C for the same current density at 1.4629 A/cm², the operating voltage increase from 0.8190 to 0.8258 V and Power output decrease from 61.2373 to 61.1304 W resulting in high efficiency of 60.44%.

References


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