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Modelling, simulation and testing of a proton exchange membrane fuel cell

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Abstract: Fuel cells are electrochemical devices that can convert chemical energy into direct electrical energy. Proton exchange membrane fuel cell is one of the several kinds of fuel cells .For understanding the electrical performance of the proton exchange membrane fuel cell, a voltage-current curve is used to explain the physical and chemical relationships and the fundamental operating principles. In this paper, a mathematical model of a proton exchange membrane fuel cellis developed and presented. The effect of various operating parameters (maximum current density, operative current density, cell temperature and the pressure of the reactant gases) on the performance of the proton exchange membrane fuel cellis investigated. The results are validated a previously done work. The results indicate that the model is quite good agreement with the experimental data. The mathematical model is very useful to reduce the investigating cost and avoid time waste for proton exchange membrane fuel cell controlling.
Keywords: Modelling; Computer Simulation; Proton exchange membrane fuel cell

1. Introduction

Proton exchange membrane fuel cell (PEMFC)is an electrochemical device that can convert chemical energy into direct electrical energy by a chain of reactions[1]. A typical PEMFC consists of two electrodes as an anode and a cathode which are separated by a proton exchange membrane (PEM) that acts as an electrolyte. The electrodes are coated with a catalyst layer loaded of platinum. Hydrogen (H_2) gas that is used as the fuel flows to the anodethrough a network of channels. H_2 breaks down into electrons and protons in the presence of the catalyst. While protons flow through the PEM, electrons flow over an external load (R_L) to the cathode [2]. Electrons that flow over R_L produce an electric current from the PEMFC. Oxygen (O_2) gas that is used as oxidant flows to the cathodethrough a network of channels, where it combines with electrons and protons to form water (H_2O). The reaction for H_2O formation is exothermic. Therefore heat is produced besides H_2O. The reactions on the electrodes are

$$H_2 \rightarrow 2H^+ + 2e^- \tag{1.1}$$

and

$$2H^+ + 2e^- + (1/2)\,O_2 \rightarrow H_2O \tag{1.2}$$

respectively. The total reaction is given as

$$H_2 + (1/2)\,O_2 \rightarrow H_2O + electricity + heat \tag{1.3}$$

To understand the electrical performance of the PEMFC, a voltage-current (V-I) curve, known as a polarization curve, is commonly used to explain the physical and chemical relationships and the fundamental operating principles. The V-I values depend on both the electrochemical reactions on the electrodes of the PEMFC and R_L[3, 4].

Many models [5-12] have been developed to understand the performance of the PEMFCs. But some of the models [13, 14] present the modelling without validation of any experimental data.

Models have been developed based on various operating parameters such as load current, flow rate, gaspressure, humidification temperature, etc. These models are a simple way to explain the dynamics of the PEMFC. They can be used for testingand simulatingthe PEMFC as close as possible to the effective working conditions. Modelling is useful for faster processingandmathematical model implementation [15, 16]. It can also be used for reducing the cost and time waste for PEMFC controlling.

In this work, a fuel cell model is developed for simulation a PEMFC. It can be modified for testing various operating conditions of the PEMFC. The developed model was based on maximum current density, operative current density, cell temperatureand the pressure of the reactant gases. The developed model has been

implemented and simulated by computer. Experimental data of a prepared cell on a previous work was used to validate the developed model[17].

2. Modeling of PEMFC

The cell voltage (V_{cell}) of PEMFC can be expressed as in Eq.1 [2, 18] as,

$$V_{cell} = E_{Nernst} - V_{act} - V_{ohm} - V_{conc} \quad (1)$$

where E_{Nernst} is the thermodynamic voltage, V_{act} is the activation loss which is interrelated with the reaction rates of the reactant gases on the electrodes, V_{ohm} is the ohmic loss which is interrelated with the electronic internal resistances and the proton conductivity of the PEM, and V_{conc} is the concentration loss which is interrelated with the change of the reactant gas and product (H_2O) concentrations.V_{act}, V_{ohm} and V_{conc} have a negative effect on Eq.1 to obtain the V_{cell} from E_{Nernst}.

E_{Nernst}, which is called as the reversible voltage, known as the Nernst voltage is the open circuit cell voltage at standard condition (1atm, 298.15K) of reactant gases without any R_L[3], and can be calculated as Eq.2[18] as,

$$E_{Nernst} = -\Delta G/nF \quad (2)$$

where ΔG (237,34 J) is the Gibbs free energy, n (2 electrons/mol) is the number of electrons per molecule of H_2, and F (96485 C/electron mol) is the Faraday constant.E_{Nernst} is a function of cell temperature (T) and pressure (P) of the reactant gases, and can be written as Eq.3[18, 19] as,

$$E_{Nernst} = 1{,}482 - 8{,}45x10^{-4}T + 4{,}308x10^{-5}T\ln\left(P_{H_2}{P_{O_2}}^{0,5}\right) \quad (3)$$

where T(T<373,15K, H_2O in liquid form[18]) is the cell temperature in (K), P_{H_2} and P_{O_2} are the partial pressures of the reactant gases in (atm), respectively. When T is higher than 373,15K, whereas H_2O is in gaseous form, contributes to the partial pressure effect, so E_{Nernst} is than written as Eq.4 as,

$$E_{Nernst} = 1{,}482 - 8{,}45x10^{-4}T + 4{,}308x10^{-5}T\ln\left(P_{H_2}{P_{O_2}}^{0,5}/P_{H_2O}\right) \quad (4)$$

where P_{H_2O} is the partial pressure of gaseous H_2O, otherwise P_{H_2O} is equal to 1.

To activate the PEMFC, it is necessary to transcensions the limit of the activation energy. For this transcensions, there is a need for voltage difference to continue the electrochemical reaction [18]. The main reason for the V_{act} is the slowness of the electrochemical reactions on the electrodes [2]. In open circuit or in a very low current density of a PEMFC, the V_{act} has a dramatic effect on the V_{cell} [18]. The V_{act} can be given as Eq.5 [7] as,

$$V_{act} = 9.514x10^{-1} - 3.12x10^{-3}T + 1.87x10^{-4}T\ln(i) - 7.4x10^{-5}T\ln(C_{O_2}) \quad (5)$$

where T is the cell temperature in (K), i is the current cell density in (A·cm^{-2}), and C_{O_2} is the O_2 concentration in (mol·cm^{-3}). The coefficients of Eq.(5) was indicated by the average confidence intervals of the related parameters [20]. The C_{O_2} is a function of the partial pressure of O_2 and cell temperature, and is expressed as Eq.(6) as,

$$C_{O_2} = P_{O_2}/5.08x10^6xe^{(-498/T)} \quad (6)$$

At intermediate current densities,V_{ohm} is nearly linear, and can be determined and expressedwith the Ohm's law as Eq.(7) as

$$V_{ohm} = iR_{cell} \quad (7)$$

where i is the cell current in (A) and R_{cell} is the total resistance in (Ω) of the PEMFC.R_{cell} includes the ionic resistance (R_i) of the PEM, the contact resistance (R_c) between the PEM and the electrodes, and the electronic resistance (R_e) of the electrodes as Eq.(8) [18] as,

$$R_{cell} = R_i + R_c + R_e \quad (8)$$

R_{cell} is a function of cell temperature in (K) and operative current density in (A·cm^{-2}), and can be rewritten as Eq.(9) [21] as,

$$R_{cell} = 1.605 \times 10^{-2} - 3.5 \times 10^{-5}T + 8 \times 10^{-5}i \quad (9)$$

The coefficients of Eq.(9) was indicated by the average confidence intervals of the related parameters [20].By combining the Eq.(7) and Eq.(9), the V_{ohm} is obtained as Eq.(10) as,

$$V_{ohm} = 1.605 \times 10^{-2}i - 3.5 \times 10^{-5}Ti + 8 \times 10^{-5}i^2 \quad (10)$$

At high current densities, V_{conc} increases dramatically due to the change in concentration of the gases at the electrodes [3]. The V_{conc} can be given as Eq.(11)[18] as,

$$V_{conc} = -4.08 \times 10^{-5}T\ln(1 - i/i_{max}) \quad (11)$$

where i_{max} is the maximum current density of the PEMFC in A·cm^{-2}, and i is the operative current density in A·cm^{-2}.

3. Results

Eqs.(1)-(11) should be solved for V_{cell}, as a function of cell temperature, reactant gas pressures, maximum current density, and operative current density. A schematic diagram of the developed model is given in Fig.1.

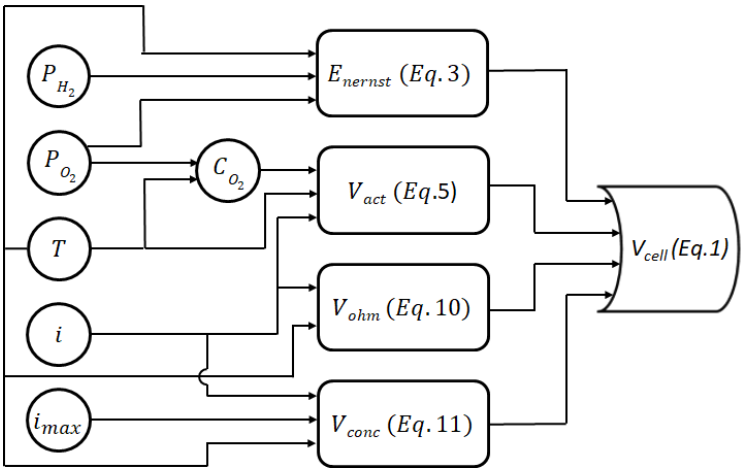

Fig.1. Schematic diagram of the developed model

The model validation involves comparing the model results with the PEMFC's experimental data. The experimental data are taken from previous work [17]. The parameters used for simulation are given in Table 1. Same parameters are previously used for operating the relevant PEMFC.

Table 1. Parameter values for simulating of the model and operating of the PEMFC.

Parameter	T	P_{H_2}	P_{O_2}	i_{max}	i
Value	293 K	1 atm	1 atm	1.451 A·cm^{-2}	0 – 1.7 A·cm^{-2}

Fig.2 shows the calculated polarization curves and power density curves of the model with the measured experimental data of the PEMFC. It can be seen that the curves are rather close to each other. Therefore, it can be concluded that the model is in quite good agreement with the experimental data.The non-homogeneous gas distribution can explain the small amount of the decrease of the PEMFC's experimental data curve.

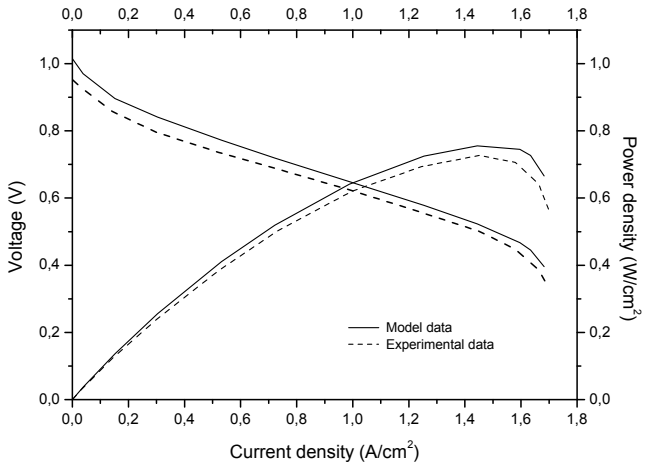

Fig.2. The computed polarization curves and power density curves of the model with the measured experimental data of the PEMFC.

4. Conclusions

In this paper, a mathematical model of a PEMFC with some operating parameters such as load current, flow rate, gas pressure, humidification temperature etc. has been developed and presented. The effect of the operating parameters acts on the PEMFC has been investigated. Besides, the results have been validated a previously done work. The results of this study indicate that the model is quite good agreement with the experimental data. It is also concluded that the mathematical model is very beneficial to reduce the investigating cost and avoid time waste for PEMFC controlling.

5. References

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