

Modeling and validation of fuel cell PEMFC

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Résumé – Dans cet article, un modèle mathématique de 1.2 W PEMFC est développé. Ce modèle décrit le comportement des PEMFC dans des conditions statiques et dynamiques. La nouveauté de ce modèle est l'intégration de toutes les équations dynamiques possibles comme la dynamique des équations de charge, telle que la dynamique débit molaire de l'hydrogène et de l'oxygène, pression, température, la tension de la pile, etc. La caractéristique V-I de PEMFC est obtenue pour différentes valeurs de paramètres d'entrée. La réponse transitoire du modèle PEMFC sur de courtes périodes et de longue date est analysée. Enfin, le comportement du modèle de pile à combustible PEM sous une charge résistive est évalué. Les résultats de simulation ont été validés en comparant les résultats prédits avec les résultats expérimentaux une pile composée de 4 cellules testées au CDER d'Alger, et ont été jugés en bon accord. Le résultat obtenu serait de conduire à des améliorations dans la conception des piles à combustible et son intégration dans des systèmes électriques.

Abstract - In this paper, a mathematical model of 1.2 W PEMFC is developed. This model describes the behaviour of PEMFC under static and transient conditions. Novel feature of this model is integration of all possible dynamic equations like dynamics of the charge equations like dynamics of the molar flow of hydrogen and oxygen, pressure, temperature, stack voltage, etc. The V-I characteristic of PEMFC is obtained for different values of input parameters. The transient response of the PEMFC model over short and long-time periods is analyzed. Finally, the behaviour of the PEM fuel cell model under a resistive load is evaluated. Simulation results were validated by comparing the predicted results with experimental results a stack consisting of 4 cells tested at CDER, Algiers, and were found to be in good agreement. The result obtained would lead to improvements in the design of fuel cells and its integration in electrical systems.

Keywords: PEM fuel cell – Modeling – Simulation – Static – Dynamic - Matlab-simulink™.

1. INTRODUCTION

The PEM fuel cell is considered to be a promising power source, especially for transportation and stationary cogeneration applications due to its high efficiency, low-temperature operation, high power density, fast startup, and system robustness [1]. PEM fuel cells are suitable for portable, mobile and residential applications [2].

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In most stationary and mobile applications, fuel cells are used in conjunction with other power conditioning converters and a circuit model would be beneficial, especially for power electronics engineers who in many cases have the task of designing converters associated with the fuel cell for various load applications [3]. In the last decade a great number of researches have been conducted to improve the performance of the PEM fuel cell, so that it can reach a significant market penetration [1].

A fuel cell consists of two electrodes, anode and cathode, and an electrolyte membrane which is inserted between them. Single fuel cell produces around 0.7 volts. For obtain higher voltage, multiple cells are stacked in series and called fuel cell stack (FCS) system [2]. The PEM fuel cells use pressurized hydrogen and oxygen as a fuel to produce electricity. Hydrogen in anode side will be dissociated into protons and electrons.

Protons flow through polymer electrolyte membrane to the cathode and the electrons flow from anode to cathode through external circuit to produce current. In the cathode side, oxygen will react with protons and electrons to produce water and heat [2, 3].

In order to utilize these systems in an effective way, mathematical models of the fuel cell stack are necessary so that the system behavior can be analyzed at the design stage by means of computer simulations in different conditions of load current, pressure of reactant gases, temperature, stack voltage, etc. [4].

The capability of predicting transient dynamics will also prove useful when attempting to develop a control strategy. In this study; firstly, general information about the fuel cells, their importance and applications are presented. Then mathematical models of the PEM fuel cell are investigated.

Finally, Dynamic modeling of the PEM fuel cell is performed. Various system dynamics such as fuel cell electrochemistry and reactant-flow are modeled, simulated and presented. On the other hand, the characteristic of 1.2 W PEM fuel cell is obtained by experiments.

2. MODELING OF PEMFC SYSTEM

2.1 Static model of PEMFC

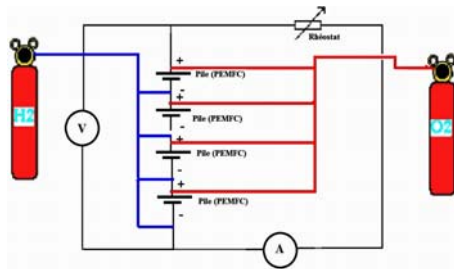


Fig. 1: Stack PEMFC system

2.1.1 Nernst voltage (E_{Nernst})

E_{Nernst} is the electrochemical thermodynamic potential of the cell and it represents its reversible voltage, which is an ideal output voltage. E_{Nernst} can be calculated by a modified version of the equation of Nernst, with an extra term to take into account changes in the temperature with respect to the standard reference temperature 25°C.

Using the standard pressure and temperature (SPT) values, the Nernst equation for the hydrogen/oxygen fuel cell for the above reaction is [5-7]:

$$E_{\text{cell}} = 1.229 - 0.85 \times 10^{-3} (T - 298.15) + 4.3085 \times 10^{-5} \times T \times (\ln P_{\text{H}_2} + 0.5 \times \ln P_{\text{O}_2}) \quad (1)$$

When we get the water production in the form of steam, 1.229 should be replaced by 1.18V. T is the cell operation temperature in [K], P_{H_2} and P_{O_2} are respectively the hydrogen and oxygen partial pressures in [atm].

2.1.2 PEMFC losses model

The losses considered here are activation losses, resistive losses and diffusion losses. These losses are described in the following sections.

$$V_{\text{cell}} = E_{\text{cell}} - \text{losses} \quad (2)$$

2.1.2.1 Activation polarization loss

The activation overvoltage is the voltage drop due to the activation of the anode and the cathode. Tafel equation, given below, is used to calculate activation overvoltage in a fuel cell [8]:

$$\eta_{\text{act}} = \xi_1 + \xi_2 \times T + \xi_3 \times T \ln(\text{CO}_2) + \xi_4 T \ln(I) \quad (3)$$

Where, I is the cell load current in [A], and $\xi_{(1-4)}$ are the parametric coefficients, defined on the basis of kinetic, thermodynamic and electrochemical phenomena (their values in the semi-empirical equations are given in the **Table 1**. CO_2 is the concentration of oxygen dissolved in a water film interface in the catalytic surface of the cathode in (mol/cm^3), estimated on the basis of the oxygen partial pressure and cell temperature by the law of Henry [8]:

$$\text{CO}_2 = \frac{P_{\text{O}_2}}{5.08 \times 10^6 \times \exp^{(-498/T)}} \quad (4)$$

2.1.2.2 Ohmic polarization loss

Ohmic polarization loss results from the inside resistance of the collecting plates and carbon electrodes, and also the resistance of transferring protons through the membrane. At a later stage, as current density rises, ohmic losses (η_{ohm}) prevail.

They are derived from membrane resistance to transfer protons and from electrical resistance of the electrodes to transfer electrons. The ohmic losses can be formulated as following [8]:

$$\eta_{\text{ohm}} = I \times (R_m + R_c) \quad (5)$$

where R_m is the equivalent resistance of the electron flow and R_c is the proton resistance considered as constant [1, 4]:

$$R_m = \frac{\rho_M \times l}{A} \quad (6)$$

In which ρ_M is the specific resistance of the membrane ($\Omega \cdot \text{cm}$). A is the membrane active area (cm^2), and l is the thickness of the membrane (cm). We can assume the membrane thickness to be 178×10^{-4} cm, which pattern is Nafion117:7 mil.

The following expression for the specific resistance is used [17, 5, 8]:

$$\rho_M = \frac{181.6 \left[1 + 0.03(T/A) + 0.062(T/303)^2 \times (I/A)^{2.5} \right]}{[\Psi - 0.634 - 3(I/A)] \times \exp^{[4.18((T-303)/T)]}} \quad (7)$$

where the term is $\frac{181.6}{[\Psi - 0.634]}$, the specific resistance ($\Omega \cdot \text{cm}$) at no current and at 30°C ; the exponential term in the denominator is the temperature factor correction if the cell is not at 30°C . The parameter Ψ is an adjustable parameter with a possible maximum value of 23.

2.1.2.3 Concentration polarization loss

The formation of concentration voltage loss is generated because the oxygen and nitrogen inside the cell cannot be delivered by constant pressure due to flow resistance. Therefore, it can be represented by the loss of the chemical reaction [7].

$$\eta_{\text{con}} = -B \times \ln(1 - (I/I_{\text{lim}})) \quad (8)$$

with, I_{lim} , Current density where fuel is used in a same rate as the maximum input rate (A/cm^2).

By replacing equations (3), (5) and (2), V_{cell} can be expressed by:

$$V_{\text{cell}} = E_{\text{cell}} - \eta_{\text{act}} - \eta_{\text{ohm}} - \eta_{\text{dif}} \quad (9)$$

Applying assumption that parameters for individual cells can be lumped together to represent a fuel-cell stack, the output voltage of the fuel-cell stack can be written as [10]:

$$V_{\text{stack}} = N_{\text{cell}} \times V_{\text{cell}} = N_{\text{cell}} \times (E_{\text{cell}} - \eta_{\text{act}} - \eta_{\text{ohm}} - \eta_{\text{dif}}) \quad (10)$$

Where, N_{cell} , number of fuel cell in stack, V_{cell} , fuel cell voltage; E_{cell} , thermodynamic potential of the fuel cell; η_{act} , η_{con} et η_{ohmic} are losses, introduced into the fuel cell.

2.1.3 Power of PEMFC

The electrical output of the cell can be linked to any load, with no restriction related to the load type, since the power supplied by the stack is enough to feed it.

The instantaneous electrical power supplied by the cell to the load can be determined by the equation:

$$P_{\text{fc}} = I \times V_{\text{fc}} \quad (11)$$

where V_{fc} is the cell output voltage for each operating condition, and P_{fc} is the output power.

2.1.4 Efficiency of PEMFC

The FC efficiency can be calculated from the equation [9]:

$$\eta_{\text{fc}} = 0.675 \times V_{\text{fc}} \quad (12)$$

where η is the fuel utilization coefficient, generally in the range of 95 %. V_m is the maximum voltage that can be obtained using the Higher Heating Value (HHV) for the

hydrogen enthalpy. The electrochemical potential (standard potential) corresponding to the HHV is 1.482 V per cell.

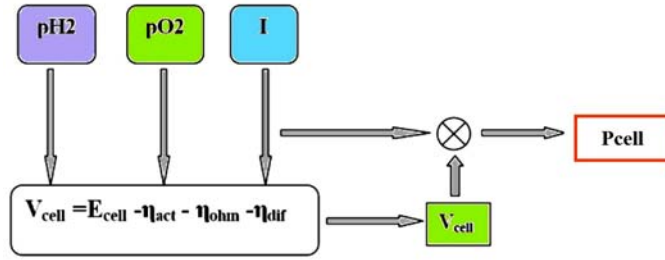


Fig. 2: Static Model of PEMFC

2.2 Dynamic model of PEMFC

In a PEM fuel cell, the two electrodes are separated by a solid membrane which only allows the H⁺ ions to pass, but prevents the motion of electrons [11, 12]. The electrons at the anode will flow through the external load and comes to the surface of the cathode, to which the protons of hydrogen will be attracted at the same time. Thus, two charged layers of opposite polarity are formed across the boundary between the porous cathode and the membrane [12].

These two layer separated by the membrane act as double charged layer, which can store electrical energy, due to this property this can be treated as a capacitor.

Circuitual model of fuel cell by considering all the effect discussed above is shown in Fig. 3, where the resistances are the equivalent resistance for different types of fuel cell losses.

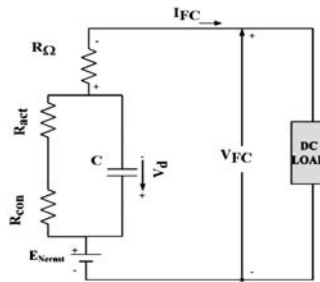


Fig. 3: Equivalent electrical circuit of PEM fuel cell [5]

This model of fuel cell is described by [6]:

$$\frac{d v_d}{d t} = \frac{1}{C} \times I - \frac{1}{\tau} \times v_d \tag{13}$$

Where V_d represents the dynamical voltage across the equivalent capacitor (associated with η_{act} and η_{com}), C is the equivalent electrical capacitance; and, τ is the fuel cell electrical time constant dependant of the cell temperature given by the equation:

$$\tau = C \times (R_{act} + R_{con}) = C \times \left(\frac{\eta_{act} + \eta_{con}}{I} \right) \tag{14}$$

Including this electrical dynamic behavior term, the resulting FC voltage is then defined by we can write (9) as given below:

$$V_{\text{cell}} = E_{\text{Nernst}} - V_d - I \times R_{\text{ohm}} \quad (15)$$

where R_{ohm} , R_{act} , R_{con} are respectively the representation for the ohmic, the activation and the concentration resistance; with C_{dc} corresponding to the membrane capacitance due to the double layer effect. This effect is incorporated in the output voltage of the PEM fuel cell.

Using (13), (14) and Laplace transformations, transfer function (15) was obtained, in which s represents Laplace operator:

$$V_{\text{cell}} = E_{\text{Nernst}} - \left(\frac{R_{\text{act}} + R_{\text{con}}}{sC \times (R_{\text{act}} + R_{\text{con}}) + 1} + R_{\text{ohm}} \right) \times I \quad (16)$$

An other hand, in some papers such as [19, 20], hydrogen pressure, P_{H_2} , and oxygen pressure, P_{O_2} , have been supposed constant value but these pressures are variable in different conditions.

Choosing constant value for these pressures can reduction of model accuracy. Since in our paper, cells have been divided to some category according to their characteristics so the pressure of input gases for each module may be differ from the other. The time constant, fuel cell current and number of cells in each module affect on oxygen and hydrogen pressure. The relationship between the molar flow of any gas (hydrogen) through the valve and its partial pressure inside the channel can be expressed as [15]:

$$\frac{q_{\text{H}_2}}{p_{\text{H}_2}} = \frac{k_{\text{an}}}{\sqrt{M_{\text{H}_2}}} = k_{\text{H}_2} \quad (17)$$

with, p_{H_2} , hydrogen partial pressure (atm), k_{an} , anode valve constant ($\text{kmol.kg}(\text{atm.s})^{-1}$), M_{H_2} , molar mass of hydrogen (kg/kmol), k_{H_2} , hydrogen valve molar constant, (kmol/atm.s).

$$\frac{d}{dt}(p_{\text{H}_2}) = \frac{R \times T}{V_{\text{an}}} \times (q_{\text{H}_2}^{\text{in}} - q_{\text{H}_2}^{\text{out}} - q_{\text{H}_2}^{\text{r}}) \quad (18)$$

with, R , universal gas constant [$(\text{atm})/(\text{kmol.K})$], T , absolute temperature, (K), V_{an} , volume of the anode (l), $q_{\text{H}_2}^{\text{out}}$, hydrogen output flow, (kmol/s), $q_{\text{H}_2}^{\text{in}}$, hydrogen input flow, (kmol/s), $q_{\text{H}_2}^{\text{r}}$, hydrogen flow that reacts (kmol/s).

According to the basic electrochemical relationship between the hydrogen flow and the FC system current, the flow rate of reacted hydrogen is given by [13, 14]:

$$q_{\text{H}_2}^{\text{r}} = NI / 2F = 2I \times K_r \quad (19)$$

where K_r , is a modeling parameter constant ($\text{kmol}/(\text{sA})$), which has a value of $N/4F$.

The model equations so far accept as inputs the partial pressures of the gases. Derivating the perfect gas equation, a specific relation is derived between the partial

pressure and the input flow rate of the fuel, the partial pressure of hydrogen and oxygen are given in Equations (20), (21). [13, 15]:

$$p_{H_2} = \frac{1/K_{H_2}}{(1 + \tau_{H_2}^S)} \times (q_{H_2}^{in} - 2I \times K_r) \quad (20)$$

$$p_{O_2} = \frac{1/K_{O_2}}{(1 + \tau_{O_2}^S)} \times (q_{O_2}^{in} - 2I \times K_r) \quad (21)$$

$$\tau_{H_2} = \frac{V_{an}}{R \times T \times K_{H_2}} \quad (22)$$

$$\tau_{O_2} = \frac{V_{an}}{R \times T \times K_{O_2}} \quad (23)$$

$$q_{H_2}^{in} = \frac{2K_r}{U_{opt}} \left(\frac{1}{1 + \tau_f^S} \right) \quad (24)$$

$$q_{O_2}^{in} = \frac{q_{H_2}}{r_{HO}} \quad (25)$$

with, K_{H_2} , valve molar constant for hydrogen (kmol/s.atm), K_{O_2} , valve molar constant for oxygen (kmol/s.atm), τ_{H_2} , response time for hydrogen (s), τ_{O_2} , response time for oxygen (s). By using equations (1), (3), (5), (8) and (20), (21), model for fuel cell unit can be modeled like Figure 4.

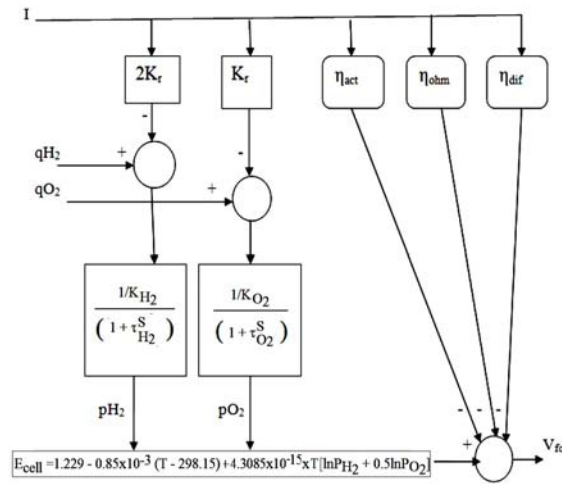


Fig. 4: PEMFC system model

The unique feature of the dynamic model discussed in this paper is the integration of all possible dynamic equations by including dynamics of the molar flow of hydrogen and oxygen, pressure in the anode and cathode channels and current density.

3. SIMULATION RESULTS

The performance of the PEM fuel cell HT-PEMFC is characterized through experimental tests. A comparison between simulation and experimental results was made for several variables for the validation of the developed model. The whole simulating process is divided into two parts which are:

1. Static simulating which is carried out in Matlab environment.
2. Dynamic simulating which is implemented using Simulink.

3.1 Static operations of PEMFC

Using (2) – (12) and the data in **Table 1**, the polarization curve presented in Fig. 5 was established for the 1.2 W HT-PEMFC stack, which also allows a comparison between the manufacturer's [17] and the simulated data. This stack is composed of 04 unit cells, with a membrane active area of 16 cm². Hydrogen and air are supplied at the atmospheric pressure (0.01 atm, 0.02 atm). For this test, the stack runs at a temperature of 25° C. The maximum current for this stack is 0.745 A.

3.1.1 Voltage and power output

Figure 5 shows the result of output voltage and output power against load current at steady state for operating temperature 298.15 K. The V–I characteristic curve experiment is conducted and the proposed model is simulated for comparison as shown in Fig. 5.

Figure 6 shows the power increases gradually to the maximum power point and then decreases. The maximum power produced by this model of fuel cell is 0.39 W, when the load current is 0.07895 A and the voltage output is 0.54 V. There is a small difference between the experiment data and the simulated data [17] at a low current, because of the nonlinear behaviors' of a fuel cell.

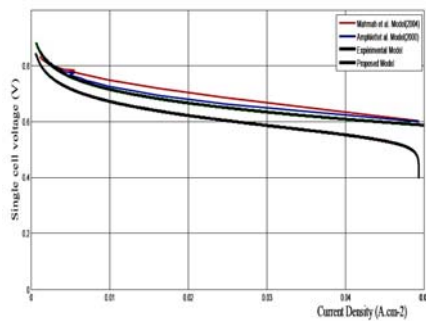


Fig. 5: The output voltage characteristic against current graph

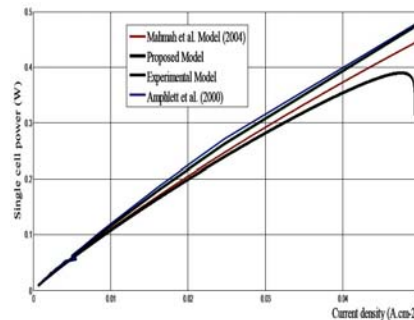


Fig. 6: The output power characteristic against current graph

3.1.2 Effect of operating temperature

Figure 7 plots the predicted performance of the cell based on the model and other simulated determined response in output voltage for various independent changes in the operating temperature.

The polarization curves of the fuel cell at different operating temperatures showed that fuel cell performance was improved with increasing temperature from 298 to 373 K. As the result, if the operating temperature of fuel cell is high, the voltage produced by fuel cell is high.

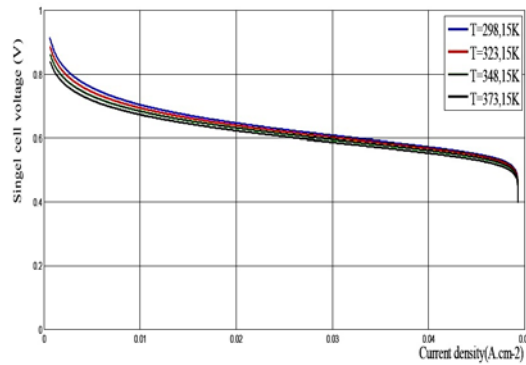


Fig. 7: The output voltage versus current density at different operating temperature graph

3.1.3 Effect of operating pressure

Fuel cell performance is also largely influenced by operating pressure. In this study, operating pressure was varied from 0.01 to 1 atm at a constant operating temperature of 25 °C. The polarisation curves for different operating pressure are shown in Figure 8.

When the oxygen and hydrogen partial pressure is equal to atmospheric pressure (0.01 atm). The voltage generated is the lowest compare to other gasses partial pressure. When the gasses partial pressure is increased to 0.02 atm, the characteristic of output voltage is also increased. At 1 atm, the voltage produced by fuel cell is the highest value.

The difference voltage characteristic between partial pressure 0.01 atm and 0.02 atm is smaller compare to the difference voltage value between partial pressure 1 atm and 2 atm. Therefore, the higher gasses partial pressure, the higher voltage generated by PEMFC.

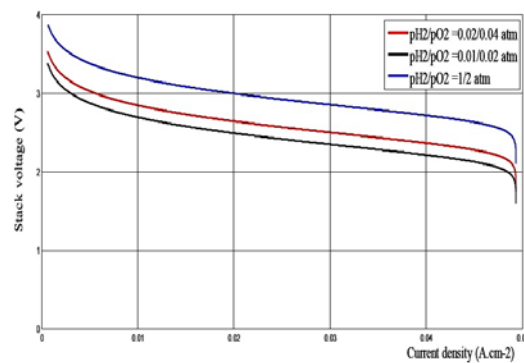


Fig. 8: The output voltage versus current density at different gasses partial pressure graph

Table 1: PEMFC Parameters [17], [This model]

Parameters	Value	Parameters	Value
T	298.15 K	U_{opt}	85
F	96487 C/mol	τ_{H_2}	3.37 s
R	8.314 J/kmol.K	τ_{O_2}	6.74 s
E^0	1.229 V	τ_f	0.8 s
N	4	R_m	0.126 Ω
K_{H_2}	4.22×10^{-5} kmol/s.atm	K_{O_2}	2.11×10^{-5} kmol/s.atm
K_r	1.0364×10^{-5} kmol/s.A	R_c	0.0003 Ω
B	0.016 V	C	V
Γ_{H_2O}	1.168	L	230 μm
$\xi_{1 \text{ theoretical}}$	-0.949 V	$\xi_{1 \text{ experimental}}$	-1.053 V
ξ_2	$0.02866 \ln(A) + 4.3 \times 10^{-5} \ln(CH_2)$		
ξ_3	7.6×10^{-5}	ξ_4	1.93×10^{-4}
J_{lim}	0.0496 A/cm ²		

3.2 Dynamic operation of PEMFC

Also, the simulation results with the H-P PEM fuel cell stack has been studied. The simulation results are compared with the simulation results and the experimental data of the Mahmah *et al.* [17].

Figure 9 and 10 shows changes in fuel cell voltage and current for varying loads. The equivalent capacitor will basically change the stack electrical constant, then, it will change the time response. As observed in Figure, the fuel cell voltage and current takes about 3 ms for the base parameter ($C = 3 \text{ F}$).

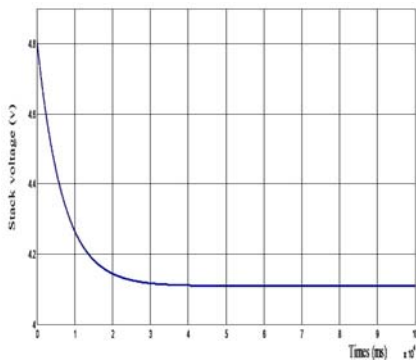


Fig. 9: Transient state of load current

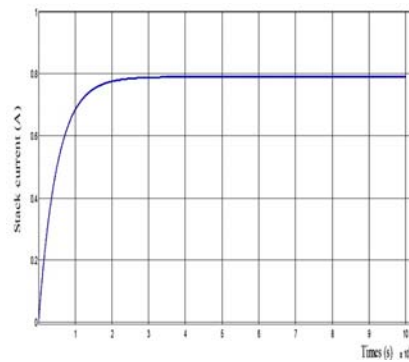


Fig. 10: Transient state of output voltage

Shows the input molar flow of fed hydrogen after gas processing response and this hydrogen flow will be fed to PEM stack unit. From Figure 11 and 12, we can see that the gas reaction process requires a short time of delay to response.

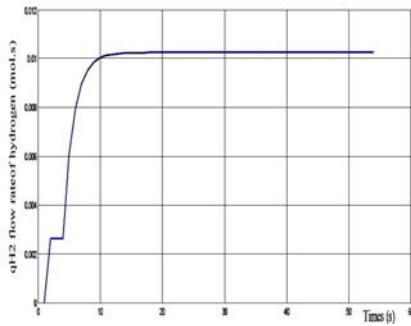


Fig. 11: Hydrogen gas input flow q_{H_2}

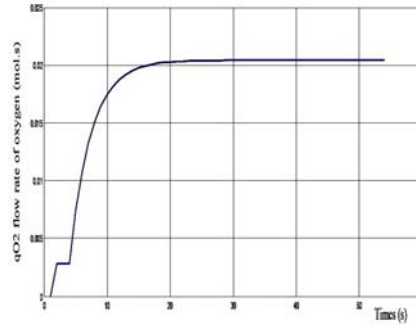


Fig. 12: Oxygen gas input flow q_{O_2}

Figures 13 and 14 shows a comparison of the experimental and simulation for the different loads (resistances of rheostat) from 0 to 45 Ω .

For example, if loads increases from 35 Ω to 45 Ω for the same current density at 0.00569 A/cm², the operating voltage increase from 3.175 to 3.373 V and Power output decrease from 0.2898 to 0.2519 W resulting in high efficiency of 67.46 %.

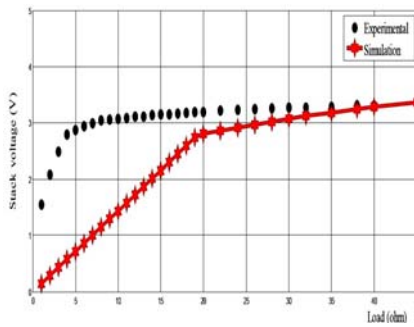


Fig. 13: Output stack voltage at transient state for different load

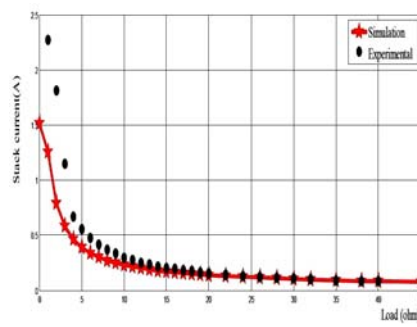


Fig. 14: Stack current at transient state for different load



Fig. 15: The PEMFC Test Bench station (CDER) [18]

4. CONCLUSION

In this paper, a mathematical model is proposed to simulate the steady –state and transient phenomena in a PEMFC system. The V-I characteristics of the fuel cell are obtained for different values of the input parameters and it is found that by operating the fuel cell at the higher values of input variables, voltage losses can be reduced.

The complete set of equations were developed to characterize the effects the dynamics of the molar flow of hydrogen and oxygen and pressure in the anode and cathode channels features in the fuel cell body. The simulation results obtained using the proposed model lays a foundation in designing controllers for fuel cell based power generation.

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