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# 3D Sensitive Modeling of Proton Exchange Membrane Fuel Cell for Automotive Applications

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ABSTRACT - In recent years, the fault diagnosis in Proton Exchange Membrane Fuel cell (PEMFC) becomes challenging issues in order to increase performance of the Fuel cell electric vehicle (FCEV). In fact, the occurrence of faults on different operation conditions into the FC unavoidable thus, lead-up to malfunctions in the FCEV and consequently, reduces its detect faults based on operating condition in different points is one of the most tackle in this area. Therefore, the main purpose of this paper is to evaluate the fault's effect on stack PEM fuel cell on a based on diving cycle tests by using a proposed faults sensitive model.

## INDEX TERMS — fault diagnosis, driving cycle, PEM fuel cell, FCEV

#### 1. INTRODUCTION

Over the last years, the excessive increase of the number of automobiles in use around the world has caused serious problems for environmental and human life. In fact, the use of internal-combustion engine vehicles leads to increase of the greenhouse effect, responsible to global warming [1]. In Table I, an assessment of the exploitation duration of fossil resources is given based on BP statistical review of world energy [2]. In order to cope with air pollution problems and the depletion of the Earth's petroleum resources [2], FCEV will seem to be the most promising vehicles in the future by providing clean and enabling zero emission transportation (see in table 1).

Table1. Earth's petroleum resources

Fossil resources	Oil	Natural gas	Coal
Exploitation duration	53 years old	56 years old	109 years old

FCEV consists of many components (PEMFC, DC/DC converter, motor, DC/AC inverter, etc.). Indeed, PEMFC as a main power source in FCEV has an essential role in generating energy. Nevertheless, PEMFC is electrochemical power source consisting of many components, including catalysts, catalyst supports, membranes, and gas diffusion layers (GDL), bipolar plates, sealing, and gaskets. According to fuel cell operation conditions, each of these components can be degraded. In

previous works, we have published a thorough study on diagnosing and localizing faults in the sensitive model of the PEMFC. We have characterized several faults by the means of variations of the different resistances and capacitors according to the variations of temperature, pressure and humidity [3]. Following this study, the present paper focuses on fault diagnosis based on driving cycle with various operation conditions into the PEMFC automotive application. Depending on driving cycle, the performance of fuel cell will change based on variation operating condition. The durability and lifetime of fuel cell are affected by many parameters, including the material properties, fuel cell operating conditions, impurity inlet gases, environmental conditions and function modes. However, the most important degradation occurred in fuel cell due to driving cycles of the real vehicles [4, 5]. Due to irregular distributions of temperature, humidity and pressure the fuel cell could be affected by voltage losses such as ohmics, activation, concentration and Nernst voltage. This paper focuses on the sensitive modeling in 3D of PEMFC stack that can be able to simulate variations of operating condition regard to driving cycle. The proposed model is validated on really measured driving cycles. In section 2, the faults in PEMFC due to variation temperature are represented. Then a review of structure of the electrical circuit that effect by operating condition is introduced in section 3. Afterward, 3D sensitive model and validation study of this model is represented in section 4.

#### 2. FAULTS IN PEMFC ACCORDING TO OPERATION CONDITION

PEMFC is an electro chemical system based on electrocatalytic reaction, hydrogen oxidation in anode side and oxygen reduction in the cathode side. Fuel cell operations depend on many phenomena that occurred inlet of the fuel cell. Some of these phenomena are common source fault in the fuel cell, namely, improper water management (flooding, Drying) [6], catalyst degradation, fuel starving [7] and membrane electrode assembly (MEA) contamination [5]. The voltage drop and the reduction of the lifetime of the fuel cell can be affected by these faults. Indeed, different operating conditions cause to these faults. Fig.1. It shows a simplified scheme for processing fault classification with several levels of processing information. The lower level explains the processing data. Indeed, in these level different sensors collect data. In the medium level, faults are extracted from healthy mode and faulty mode. The higher level is belonged to fault classification and diagnosis [9].

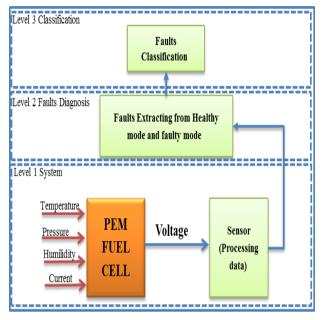


Figure 1. Fault's classification process in PEM FC.

Moreover, degradation of FC can occur under different operating condition, for instance, variable temperature, humidity and pressure. Fuel cell function generally improves with raise temperature. However, the increase of temperature has a negative effect in Nernst voltage [10]. Furthermore, augmentation of temperature leads to reduce of activation and concentration losses. It is obviously that the voltage enhances with the increase the temperatures [11], [12]. It should be noted that raising of the internal temperature makes to reduce the FC performances and causes irreversible damage of the fuel cell.

Increase in humidity leads to improve the membrane conductivity. Therefore, fuel cell performance will be improved [3].

Fuel cell is operated at the ambient pressure (1 bar), or it may be pressurized. The aim of the raising the pressure inlet gases are to increase cell voltage.

Besides, the driving cycle causes changing of the operating conditions and performance of each cell.

#### 3. STRUCTURE OF THE ELECTRICAL CIRCUIT PEMFC MODEL

In recent years, many researchers have widely investigated in the dynamic modeling of the fuel cell with an emphasis on electrical terminal characteristics [13], [14]. A detail explanation of electrochemical property of the fuel cell and simple equivalent circuit, including the dynamic effect are reported in [15]. The fuel cell can be modeled in the different way. One of the simplest models is electric as it is illustrated in Fig.2. One of the important aims of this kind of models is to design electric circuit connection to other electric components in the power train such as the power electronic powered converter. A dynamic model has been developed by MATLAB software. This model is based on, electrochemical and thermodynamic characteristic of the PEMFC. The FC output voltage in individual cells, which is the function of operating conditions and fuel cell current as the show in fig.2. In this model, with the inputs are included the influence of temperature, gas pressure (hydrogen and oxygen) and room temperature in voltage Nernst and other losses (Activation, Concentration and ohmics).

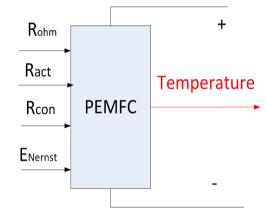


Figure 2. Electrical circuit model of the PEMFC

As shown in this figure, the activation, concentration and ohmics losses are represented by Ract, Rcon and Rohm respectively. The parameter C corresponds to the double-layer effect in order to explain of dynamic response of the PEMFC while E is the reversible voltage of the FC. Nevertheless, all parameters based on operating conditions will be changed.

Each cell is composed by Nernst voltage, activation, concentration and ohmics losses electrochemical are computed as follows [16]:

$$V_{act} = Aln\left(\frac{i_{fc}}{b}\right), A = \frac{R.T}{\alpha.n.F},$$

$$b = .001838e^{\frac{79422}{T}(1-\frac{T}{298.15})}$$
(1)

Where A, b depends on the electrode and cell condition while Vact is only valid for i>b (b=0.04 mAcm-2) [16].

Finally, the ohmics over voltage due to the membrane resistance Rm in PEMFC is given by the following expression [16]:

$$V_{ohm} = i_{fc} R_m, R_m = \frac{t_m}{\sigma_m}$$
(2)

A relationship for voltage loss due to concentration polarization is obtained as following:

$$V_{con} = \frac{RT}{nF} \ln \frac{I_{lim}}{I_{lim} - i_{cell}}$$
(3)

By adding capacitor, dynamic system is involved in this model. Therefore, the voltage of each cell is computed by equation as defined below:

$$V_c = V_{act} + V_{con}, \ C \frac{d_{VC}}{dt} + \frac{V_C - E}{R_{act} + R_{con}} = i_{cell}$$
(4)

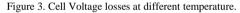
$$V_{fc} = E - V_c - i_{cell} R_{ohmic}$$
<sup>(5)</sup>

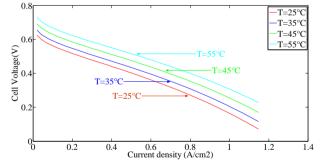
## 3.1 Effect of temperature in the PEMFC

3.1.1. Operational Effect

As explained above fuel cell voltage depends on many parameters, for instance, temperature, current... However, this model is not sufficient for modeling of the actual PEMFC. Because of the real model, PEMFC should be considered in 3D. Therefore, in this paper new model 3D stacks, fuel is proposed. The aim is present in an electric 3D model of PEMFC stacks that provide the three-dimensional steady-state distributions potential and temperature.

Mainly, in stack fuel cell, two parameters essentially influence to increase of temperature. Firstly, it is variationoperating condition of the fuel cell. Secondly is the driving cycling time. Indeed, increasing the temperature of the PEMFC leads to reduce the activation, concentration and ohmics losses. Fig.3 shows the effects of augmentation of temperature from 25°C-55°C on the polarization curves. It is obviously that the voltage rises with increasing temperature [15]. It should be noted that raising of the internal temperature of the PEMFC it makes to reduce in performances of the FC [5].





#### 3.1.2. Driving Cycle Effect

Simulation results of voltage and current have been compared to experimental ones as illustrated in Fig.4. In this test, the PEMFC supplied an electronic active load reproducing the power of the DC-bus of an electric vehicle during a real driving cycle. Indeed, temperature has a relationship with current regarding to electrochemical process. According to passing time, the output voltage refuses to obey to current profile, i.e. the current vanishes just after 8100s. Because of long operating driving cycle, conditions in PEMFC are changed.

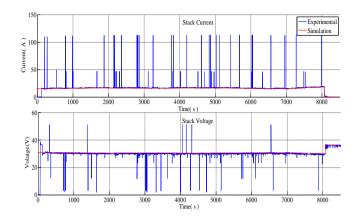


Figure 4. Stack voltage of FC

As the show in Fig.5 temperature is raised in each step of the current profile due to the high operating performance of the PEMFC (Time operating or driving cycle time). Thus, driving cycle time and operational aspect (chemical reaction and current density) are affected by the influence of temperature on the performance of the fuel cell.

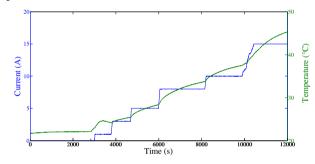


Figure 5. dynamic load profile and behaviour of the stack temperature

In addition, environment temperature could affect the performance of fuel cell. As illustrated in Fig.6 the stack voltage of fuel cell has been improved by increasing outside temperature. To illustrate of this effect fuel cell located in climatic room, (see Fig.7). In this test, the temperature of room has been regulated between 10 and 30  $^{\circ}$ C (Fig.7).

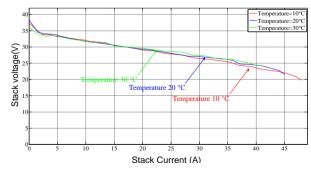


Figure 6. Comparison of polarization curves for different temperatures

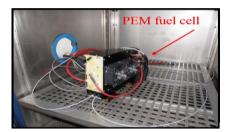


Figure 7. PEM fuel cell in chamber room

Therefore, one of the most important operating conditions in the PEMFC is temperature. It can be most effective at the performance of fuel cell. Even at short time without control of temperature, irreversible fault might be happened in fuel cell namely, drying in membrane.

Modeling of the PEM fuel cell in the past decade more has been developed generally in 1D and exceptionally in 2D. However, no attempt has been done in modeling of the PEM fuel cell in three-dimensional distributions of potential and temperature. For this reason in this paper proposed, the 3D fault sensitive model (X, Y and Z-axis) is based on 3D distributions of temperature and voltage. This model is developed in order to localize fault effects in each of the three space directions of the fuel cell stack.

#### 4. EXPLANATION OF THE 3D SENSITIVE MODEL

This paper proposes a 3D sensitive model. It considers distributions of temperature and voltage in X, Y and Z-axes. An illustration of the 3D model is shown in Fig.8. An equivalent circuit of this model is included the parallel and series impedances. These Impedances account the temperature effect. Without considering of temperature, effect then fuel cell electrical model is included of the activation loss, consideration loss, ohmics loss, double layer capacitor and Nernst voltage. By Adding impedances in parallel and series Z1, Z2... we can significantly marker the effect temperature in the electric model of PEMFC in different 3D directions. This is because of; there are physical relationships between temperatures and these impedances.

Furthermore, considering these impedances to simulate the PEMFC the accuracy of the PEMFC model is improved. Thus, for any reason variation temperature in different directions in the FC stacks makes to change the value of these impedances.

In brief, each cell in the FC stacks has been divided into many branches, which include of reversible voltage, activation, concentration, ohmics losses and impedances. Because of the variation operating condition in each direction, voltage has different values in each branch. Therefore, reversible voltages and other losses are connected by impedance in the X, Y and Z direction.

In this model because of significance effect of temperature in comparison to other operating conditions. The temperature distribution was considered in 3D space.

Hence, any fault that related to variation temperature such as flooding and drying, and degradations are able to consider in this model. The calibration of this 3D model, the Newton Raphson algorithm will help to determine the values of the related impedances in different directions.

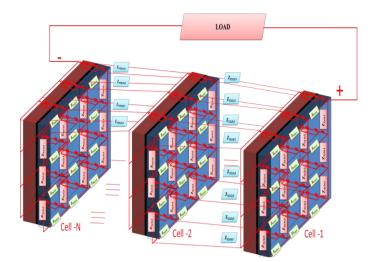


Figure 8. Stack PEMFC based on elementary cell in three dimensions (3D).

#### 4.1. Multi variable Newton-Raphson (NR) method

The voltage of each cell in the mesh group of stack must be the same values [17]. However, as discussed above the voltage will be changed with variations of the operating conditions. We have considered the parameters such as voltage revers, activation, concentration, ohmics losses and the impedances (parallel and series) to be non-liner relation functions of current, temperature, pressure and humidity.

In this paper, we focus on the temperature effect only. The partially advantage of the Newton Raphson method is to avoid applying some empirical parameters. This method is applied to find the impedance in 3D direction regarding to temperature variations in different points of PEMFC stack.

The Newton-Raphson is used to calculate voltage cell and current for each element. As shown in Fig.9 voltage cell one  $(n^{\circ}1)$  in x, y direction can be calculated as follows:

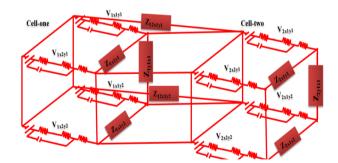


Figure 9. Uneven distributions temperature in 3D model.

$$V_{1x1y1} = V_{1x2y1} + I_{1x2y1} \cdot Z_{1x2y1}$$
(6)

$$V_{1x1y2} = V_{1x2y2} + I_{1x2y2}.Z_{1x2y2}$$
(7)

$$V_{1x1y2} = V_{1x2y2} + I_{1x2y2}Z_{1x2y2}$$
(8)

$$V_{1x1y1} = V_{1x1y2} + I_{1y1x1} \cdot Z_{1y1x1}$$
(9)

In the same way for cell two in x, y direction voltage can be calculated as below:

$$V_{1x1y2} = V_{2x1y2} + I_{12x1y2}.Z_{12x1y2}$$
(10)

In Z direction between cells, one and two impedances in Z direction will be added, and voltage can be calculated as following:

$$V_{cell\,12} = V_{1x1y1} + V_{2x1y1} \tag{11}$$

Finally, voltage in 3D direction can be calculated as bellow equation:

$$V_{cell12} = 2V_{1x2y2} + 2I_{1x2y2}.Z_{1x2y2} + 2I_{1y1x1}.Z_{1y1x1} - I_{12x1y1}.Z_{12x1y1}$$
(12)

$$V_{stack} = 2 \sum_{i=1}^{N} V_{ix2y2} + I_{ix2y2} \cdot Z_{ix2y2} + I_{iy1x1} \cdot Z_{iy1x1} - \sum_{i=1, j=2}^{N} I_{ijx1y1} \cdot Z_{ijx1y1}$$
(13)

This system as the show in Fig.5 with impedance in x, y and z direction can be replaced by the entire function F(x) which is a dimensional and X is a dimension vector:

$$F(x) = \begin{pmatrix} V_{cell} - f(i_1) \\ V_{cell} - f(i_2) \\ \vdots \\ \vdots \\ V_{cell} - f(i_n) \end{pmatrix}, \ x = \begin{pmatrix} V_{cell} \\ i_1 \\ i_2 \\ \vdots \\ \vdots \\ i_n \end{pmatrix}$$
(14)

$$f(i_1) = V_{1x2y2} = E_{rev} - V_{act} - V_{con} - V_{ohm}$$
(15)

The purpose is to minimize F(x) to F(x) = 0.

F(x) can be solved by using the Newton-Raphson method.

$$X^{(\nu+1)} = X^{(\nu)} + \Delta X^{(\nu)}$$
(16)

$$X^{(\nu+1)} = X^{(\nu)} - J(\Delta X^{(\nu)})^{-1} f(X^{(\nu)})$$
(17)

With J the Jacobian of F,

$$J = \begin{bmatrix} 1 & \gamma_1 & 0 & \dots & 0 \\ 1 & 0 & \gamma_2 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 1 & 0 & \dots & 0 & \gamma_n \end{bmatrix}$$
With  $\gamma_i = \frac{2T\xi_4}{I_i} + 2.Z_i +$ (18)  
2. $Z_i + Z_i + m.n. \exp(n.I_i) - R_m$ 

.

#### 5. CONCLUSIONS

In this paper, it has been proved that a difference of  $5^{\circ}$ C temperature exists between the middle and the two extremities of the studied PEMFC stack. This means that, the performances of the fuel cell are deeply changed. These phenomena can now be taken into account through the proposed 3D model.

Furthermore, it has been shown that this model can evaluate the fault's effect on PEMFC stack. This 3D model has been developed by using an electrical network approach. The latter provides the three-dimensional steady-state distributions, potential and temperature. To calibrate such a model the Newton Raphson algorithm has been used.

The future of the proposed model is the training of an ANN algorithm for the PEMFC diagnosis purpose.

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