WATER ACTIVITY CONTROL OF PEM FUEL CELL USING ENERGETIC MACROSCOPIC AND INVERSION METHODOLOGY

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Abstract: *This paper describes how to control water activity in a PEM fuel cell using a new graphic formalism of energy systems called Macroscopic Energy Representation (MER). This methodology allowed us to model the behavior of a PEMFC (fuel cell voltage, power and relative humidity) as a function of operating variables such as (current, pressure, temperature, flows of hydrogen, oxygen and water). The validation of the simulation results shows the importance of the influence of relative humidity RH on the PEMFC cell behavior. In addition, these variables adjusted to take account of the RH in order to obtain better performance of the operation of the FC.*
For this reason, a control method based on inversion the Maximum Control Structure (MCS) used in order to ensure a relevant and adequate use of this energy system and to avoid the disadvantages of flooding and drying case, to achieve the desired relative humidity for relaxed operation of this PEMFC.

Key words:*.FC, PEMFC, Modeling and Control, Water Activity, Relative Humidity RH, Water Management, MER, MCS.*

1. Introduction.

The objective of this work is to study the energy management of a PEMFC fuel cell, based on water management and its influence inside the core of the Fuel cell as a function of the flow rates hydrogen and oxygen, taking into accounts the humidification of the membrane and its influence on the proper functioning of this system in electrical energy. In order to avoid the drying and flooding, which can cause the deterioration of the fuel cell.

Due to the high reliability and efficiency of a PEMFC in low temperature, drastic research have been carried out with the purpose of using its physical and electrochemical systems as renewable energy in different applications (mobile, stationary and residential ... etc.).

The PEMFC (Proton Exchange Membrane Fuel Cell) also called hydrogen cells, can be used at temperatures below 100 °C having a wide power range, the choice made is due to its flexibility operating, viscosity, performance, solid electrolyte and quick start. These are good converters of hydrogen and oxygen in electricity.

The heart of the PEMFC consists of [1]-[2]-[25]:

a- Anode: electron emitter whose reaction is:

$$2H_2 \rightarrow 4H + 4e^-$$

b- Cathode: electron receptor, the reaction of which is:

$$O_2 + 4H^- + 4e^- \rightarrow 2H_2O$$

c- Carrier Membrane (electrolyte) separates the anode and the cathode, thus the balance of the reaction is:

$$H_2 + \frac{1}{2}O \rightarrow H_2O \text{ + heat +electrical energy}$$

It is interesting and indispensable to acquire a long life of a FC and to optimize its performance to keep the rate of the relative humidity of the membrane constant.

A fuel cell (FC) produced from 0.7 to 0.8 V, in order to have higher voltages of the multiple cells that are stacked in series [4]-[5].

The various components of a PEM fuel cell system represented in Fig.1. as indicated below. This model consists of five fields of productions:

1-Thermodynamic domain: it is the main domain of electricity production (core of the cell: anode, cathode and membrane).

2-Electrical domain: it is the presence of the stack current, production of a desired constant voltage Vcell to a load.

3-Thermal domain: it is the heat production in the course of the electrochemical reaction.

4-Water management domain: it is the production of water flow required for moistening of the membrane.

5-Physical domain:

-At the cathode level: inlet of pure air (oxygen).

-At the level of the anode: hydrogen inlet.

The design of each area is an important part of the design of the complete system; it is a fundamental element in achieving high-performance fuel cell systems [1]-[25].

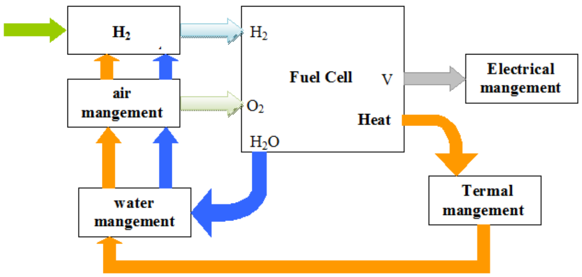


Fig.1. Synoptic diagram for operating fuel cell system

From the operational synoptic described in Fig.1. A model based on MER methodology of a fuel cell energetic system is developed to see the influence of input variables such as (current, flows rate of (hydrogen, oxygen and water)) on the behavior of tension and relative humidity [3]-[23].

The electrochemical and mathematical model of PEMFC, were developed by semi empirical equations, in order to obtain simulation results to develop and visualize the concern for the influence of water management on the system.

Therefore, we try to define the specific characteristics of the PEMFC and a control strategy by the MCS obtained through modeling and simulation by considering the different control structures for the exploitation of energy taking into account the inputs and outputs of the system.

The simulation results discuss and analyze the behavior of the system whose goal is to achieve a good design of such a model and lead to a direct chain of conversion of chemical energy from fuels to electrical energy

2. PEMFC Model Using MER

The specific model adapted to develop the control structure of a fuel cell system that must have the characteristics (energy, modular, suitable for multi-complex physical domains of different domains and the synthesis of the MCS). This is the reason why our choice of modeling was made on the MER. The MER is a graphical modeling process developed for the synthesis of complex systems (electromechanical, electrochemical, fluid mechanics, physical and electrical ...) [6].

The MER is a combination of the two graphical formalisms: the Informal Causal Graph (ICG) and the Band Graph (BG), so it is a new readable macroscopic representation that is easy and more accessible. The MER is composed of three pictograms [5]-[6] (source elements, element of conversion and element of accumulation), it is based on the principle Action / Reaction of the energetic systems according to integral physical causality (table 1). The MER was introduced in 2000 in French by the University of L' ILLE by laboratory L2EP. It is a suitable method for developing the control of energy systems such as: (fuel cells, electromechanical system, hybrid vehicles, tramways, metro and wind turbines… etc).

A model fuel cell was proposed by T. Zhoul which simplified that Hissel [7]. Our proposal consists of adding the constraint humidification of the membrane by the flow of water introduced into the air, and the influence of relative humidity on the proper of functioning of the system, according to our Fig.2. The proposed model of the PEMFC stack with different coupling:

- From the thermodynamic domain with the physical domain: hydrogen, oxygen and water flow rates were introduced at the anode, the cathode and the membrane.
- A coupling of the thermodynamic domain with thermal domain: the temperature variation directly affects the system, for this in our case the constant temperature has been taken.
- A coupling of the thermodynamic domain with humidification domain: variation of the RH, which is our concern.
- A coupling of the thermodynamic domain with electrical domain: by producing a voltage Vcell to the load, as shown in Fig.2.

Thermodynamic Domain

The voltage of a cell, given according to the law of ohm [1]-[3]

$V_{cell} = E_{nerst} - V_{act} - V_{ohm} - V_{con}$

With E_{Nerst} is the Nernst equation, V_{act} is the activation loss, V_{con} is the concentration loss and V_{ohm} is the Ohmic loss.

The overall tension is as follows:

$$V_{cell} = 1.29 - 0.85.10^{-3}.(T - 298{,}15) + 4{,}31.10^{-5}.T\left[ln(P_{H_2}) + \frac{1}{2}ln(P_{O_2})\right] -$$
$$\left[\xi_1 + \xi_2 T + \xi_3 T ln(C_{O_2}) + \xi_4 ln(I_{stack})\right] -$$
$$B ln\left(1 - \frac{J}{J\max}\right) - I_{stack}\left(\frac{t_m}{\sigma} + Rc\right)$$

(1)

P_{H_2} : is the partial pressures of hydrogen (atm), P_{O_2} : is the partial pressures of oxygen (atm) and T the fuel cell temperature (°K).

Where $\xi_1 = -0.948$,

$\xi_2 = 0.00286 + 0.0002.ln(\mathrm{A}) + \left(4.3.10^{-5}\right) ln(C_{H_2})$,

$\xi_3 = 7.6.10^{-5}$ and $\xi_4 = -1.93.10^{-4}$ are experimentally defined parametric coefficients.

$B = \frac{RT}{nF} = 0.016V$: is a parametric coefficient, which depends on the cell and its operation state and J represents, the actual current density of the cell (A/cm).

$J_{max} = 1.5\text{A/cm}^2$ is the current density limit.

$Rc = 0.00003\,\Omega$ is the stack internal resistance and

t_m is the membrane thickness.

[14]-[24] give the concentration of the oxygen Co_2 :

$$Co_2 = \frac{Po_2}{5,08.10^6.e^{(-498/T)}} \quad (2)$$

σ_m: Is the specific conductivity of the membrane proton (which depends on the water activity in the membrane) calls Nafion conductivity, obtained experimentally by the following equation [15]:

$$\sigma_m = (0.00519\lambda - 0.00324)\exp\left(1268\left(\frac{1}{303} - \frac{1}{T}\right)\right) \quad (3)$$

Alternatively, λ is the water content of the membrane given by the following relation [8].

$$\lambda = \begin{cases} 0.043 + 17.81RH - 39.85(RH)^2 + 36(RH)^3, & 0 \le RH \le 1 \\ 14 + 1.4(RH - 1) & 1 \le RH \le 3 \end{cases} \quad (4)$$

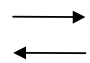
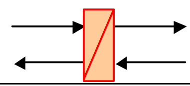
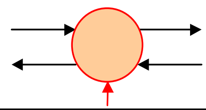
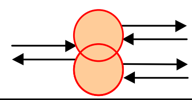
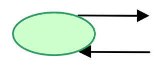
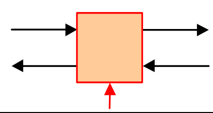
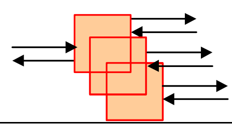
ENERGETIC MACROSCOPIC REPRESENTATION (EMR)	
	Action and reaction variables
	Energy source (system terminals)
	Multi-physical converter (energy conversion)
	Multi-physical coupling (energy distribution)
	Energy source (system terminals)
	Mono-physical converter (energy conversion)
	Mono-physical coupling (energy distribution)

Fig.2. Proposed PEMFC MER Representation

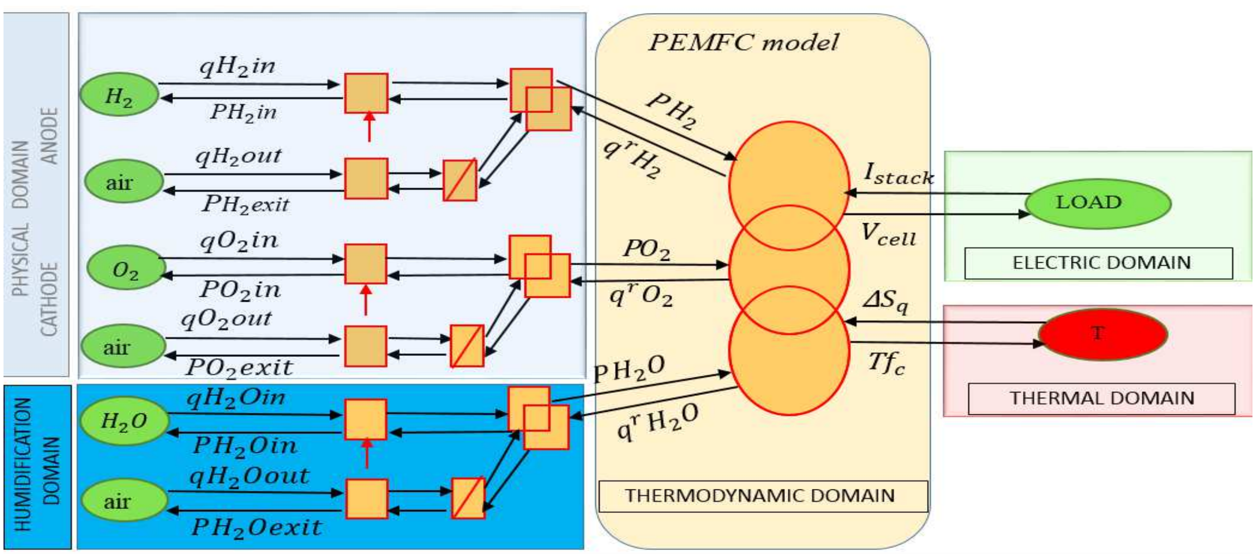


Table 1 The basic elements of MER [6]-[8]

For this configuration, the equations of the different domains are as follows:

Physical and Humidification Domain

Either the partial pressures of the three inputs gas and water at the PEMFC cell and the output rates defined by the following electrochemical relationships developed by M. Y. El-Sharkh. The equations of state become [1,3]:

$$\frac{d}{dt}(P_{H2}) = \frac{RT}{V_{an}}(q_{H_2 in} - q_{H_2 out} - q^r_{H_2}) \tag{5}$$

$$\frac{d}{dt}(P_{O2}) = \frac{RT}{V_{an}}(q_{O_{2in}} - q_{O_2 out} - q^r_{O_2}) \tag{6}$$

$$\frac{d}{dt}(P_{H_2O}) = \frac{RT}{V_{an}}(q_{H_2Oin} - q_{H_2Oout} - q^r_{H_2O}) \tag{7}$$

q_{H_2} and q_{O_2} : The inlet flow rate of each gas and

q_{H_2O} : The water inlet flow rate by air.

$q_{H_2 out}$ and $q_{O_2 out}$: The outlet flow rates of each gas and $q_{H_2O_{out}}$: The water vapor.

The fuel cell model previously depicted by the MER shows us visible in (Figure 2).

The input variables are (*Ifc*, P_{H2}, P_{O_2}, P_{H_2O}, I_{stack} *and RH).*

The output variables are *(Vcell and Pcell).*

Where in the reaction rates of hydrogen, oxygen and water flow rates in the cathode, anode and membrane (electrolyte) of the electrochemical relationships are:

$$q^r_{H_2} = 2q^r_{O_2} = q^r_{H_2O} = \frac{N_0 . I_{stack}}{2.F} = 2.K_r . I_{stack} \tag{8}$$

N_0: Is the number of stacks in the PEMFC.

$K_r = \frac{N_0}{2.F} = 0{,}996.10^{-6}$: is a constant in Kmol / S.A and F is the Faraday constant.

$$q_{H_2out} = K_{H_2}P_{H_2} ; q_{O_2out} = K_{O_2}P_{O_2} ; q_{H_2Oout} = K_{H_2O}P_{H_2O} \tag{9}$$

Water Activity in PEMFC Formula

This formula developed by L. Boulon and all [3] in order to calculate the relative humidity of a fuel cell at the outlet of the gases, studying the influence of air and water management on humidification problems. In our simulation case we consider the temperature as constant as T=363°K. Thus RH does not physically exceed 100%, hence the exhaust air saturation of the FC. This indicates that the PEMFC can conserve water in the air. Moreover, it always known that hot air can contain more water than cold air. We are studying the influence of the wet domain on the model PEMFC which is the purpose of our paper in reference to the experimental approach of Rankine that depends on the temperature of the incoming air has saturation pressure whom tends from 0% (dry air) to 100% (humid air) which is our desired case [3].

$$RH = \frac{P_{H_2O}}{P_{sat}(Tair)} \tag{10}$$

With P_{H_2O} : The partial pressure of water vapor and

$$P_{sat} = 10^5 \exp\left(13.7 - \left(\frac{5120}{T_{air} + 273.15}\right)\right) \tag{11}$$

P_{sat} : The saturated vapor pressure.

The water content of the outgoing air is analysed to estimate the relative humidity

$$P_{H_2O} = P_{exit}\left(\frac{0.420 + \lambda_a \psi}{\lambda(1+\psi) + 0.210}\right) \tag{12}$$

Where P_{exit} ; is the pressure at the output of the stack, for an atmospheric fuel cell = λ_a (atmospheric).

λ_a = 2. The air stoichiometry calculated as a function of the molar flow of incoming air and the molar flow of moist air given by the following relation:

$$\psi = \left(\frac{q_{H_2Oin}}{q_{O_2in} + q_{rest}}\right) \tag{13}$$

$$q_{O_2in} = \frac{\lambda_a . I_{stack}}{4.F} \tag{14}$$

$$q_{rest} = 3.76. q_{O_2in} \tag{15}$$

q_{rest} : Is the remaining molar oxygen flux.

Finally, the relativity humid given by the following equation [3] :

$$RH = \frac{P_{H_2O}}{P_{sat}(T)} = \frac{P_{exit}\left(\frac{0.420+\lambda_a\psi}{\lambda(1+\psi)+0.210}\right)}{10^5 \exp\left(13.7 - \left(\frac{5120}{T_{air} + 273.15}\right)\right)} \tag{16}$$

3. Model Test and Validation

The aim of this section is to understand the impact of the operating variables on the behavior of the FC voltage and to improve the performance of the PEMFC cell model by a proposed regulation. We are using the MATLAB and SIMULINK tool to model our system through semi-empirical equations with the parameters cited in Table.2 and simulating our 3D figures to analyze the results. These simulation results are as follows:

TABLE. 2. Model parameters [8]-[9]-[10]-[12]-[24]

Parameters	Values
parametric coefficient, B	0.016 V
Faradays Constant, F	9684600 C/Kmol
Universal gas Constant R	8314.47 j/Kmol.K
Number of cells, N_0	100
Hydrogen valve constant K_{H2}	$4.22*10^{-5}$ Kmol/S.A
Oxygen valve constant K_{O2}	$2.11*10^{-5}$ Kmol/ S.A
Stack internal resistance Rc	O.00003 Ω
K_r constant	$0.996*10^{-6}$ Kmol / S.A
air stoichiometry, λ_a	2
Surface, A	50.6 cm^2
t_m membrane thickness	178 μm
Jn	1.2 A/cm^2
Istackn	60 A
R	8314.47 j/Kmol.K

The Static Characteristics of a PEMFC

a) The current density and the oxygen pressure directly affect the FC voltage as shown in Fig.3. For low oxygen pressures the voltage decreases and for high pressures the voltage increases rapidly and the voltage pressure characteristic is saturated.

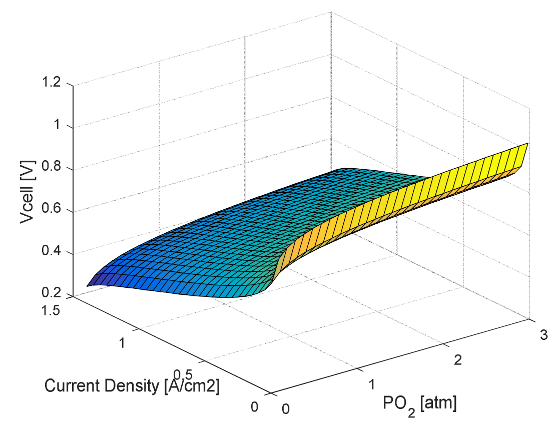


Fig.3. Variation of PEMFC cell voltage as a function of current density and oxygen pressure with *(P_{H2}=P_{H2O}=1(atm),RH=100% and T=90°C).*

b) It is also possible to see in Fig.4, the range of the power according to these same variables of Fig.3.

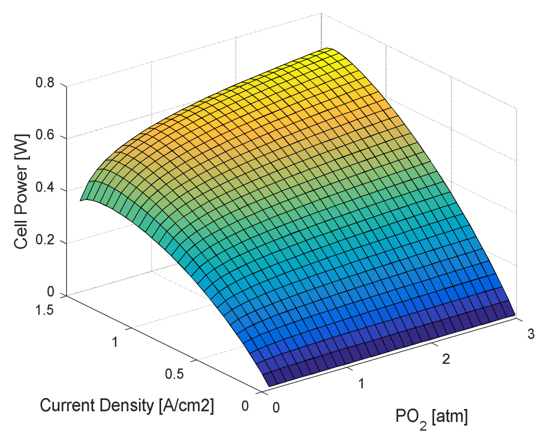


Fig.4. Variation of PEMFC cell Power as a Function of Current Density and Oxygen Pressure with *(P_{H2}=P_{H2O}=1(atm),RH=100% and T=90°C).*

c) Concerning the influence of the relative humidity RH on the behavior of the power shown in Fig.5, it is noted that when the relative humidity reached 100% the cell power is maximum, more relative humidity increases by this value the power decreases rapidly for high current densities. Therefore, the correct operation of the fuel cell requires a 100% relative humidity.

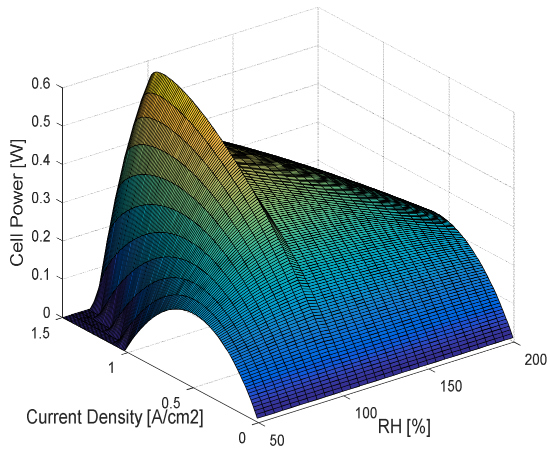


Fig.5. Variation of cell power as a function of current density and relative humidity with *($P_{H2=}P_{O2=}1$(atm) and T=90°C).*

d) The Fig.6 shows the variation of the voltage simultaneously as a function of the current density and of the relative humidity RH. It is noted that for RH = 100% the voltage is the maximum and three different parts can distinguish:

1. Drought part: when RH less than 100. This is the non-prerequisite part, which can cause the membrane defect through the dryness caused by the incoming air.

2. Critical part of flood: RH is greater than 100 (excess water management) in this part incoming and the producing water is not sufficiently and totally distributed which causes the flooding of the fuel cell.

3. Saturation part: it is our goal of this work, where the flow of water from the inlet (coming from the incoming air and the electrochemical reaction) is equal to that of output which gives us an RH of 100 % and the voltage produced is of course perfectly maximum [25].

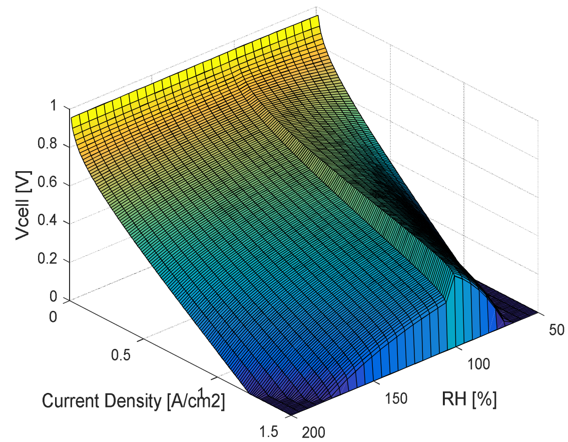


Fig.6. Variation of cell voltage as a function of current density and resistive humidity with *($P_{H2=}P_{O2=}1$(atm) and T=90°C).*

e) The Fig.7 shows the variation of the power as a function of the current density and the temperature. In this figure, the power increases as a function of the temperature for high current densities.

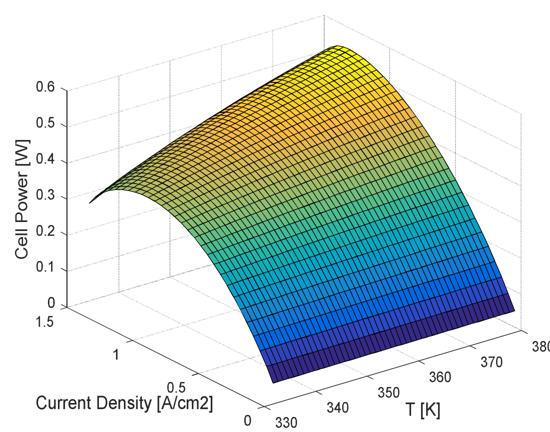


Fig.7. Variation of cell power as a function of current density and temperature with *($P_{H2=}$ $P_{O2=}$ 1(atm) and RH=100%).*

f) The Fig.8 shows the variation of the voltage as a function of the current density and the temperature, it decreases when the temperature decreases for high current densities and vice versa. This characteristic is very sensitive to temperature, which requires us to introduce a temperature control [18].

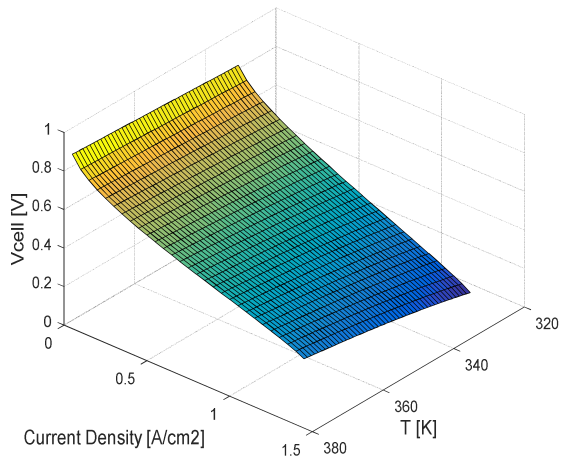


Fig.8. Cell voltage variation as a function of current density and temperature with *($P_{H2=}$ $P_{O2=}$ 1(atm) and RH=100%).*

The Dynamic Characteristics of a PEMFC

These characteristics make it possible to see the variations of the electrical response (voltage, power and relativity) of the system with variable operating parameters (current, incoming pressures (of hydrogen, oxygen and water)) at a constant temperature in a time of 100 seconds.

In practice, the temperature of the PEMFC is regulated to a constant value for active and efficient operation.

The Fig.9 shows the variations of the voltage cell, power cell and RH as a function of the variations of the various parameters *(Ifc, q_{O_2in} , q_{H_2Oin})* characterizing the uncontrolled PEMFC model. The voltage Vcell varies as a function of the current variation, of the oxygen, hydrogen and water flows [16].

The relative humidity RH undergoes direct variations according to these same input variables, notice it is between 50 and 150%, very far from 100%, which encourages us to take into consideration to improve this relativity and thus output parameters (*Vcell, Pcell)* and controlled by a well-defined strategy for the proper and adequate commissioning of this energy system.

3. Control Strategy by MCS

The MCS structure is deducted successively from the MER using inversion rules [3] Table.3 by the following steps:

1- Define the control chain (the objective variables of settings): in our case we want to adjust the voltage Vcell, power and relative humidity RH Fig.9.

2- Reverse the system of adjustment block by block up the chain of adjustment for the inversion.

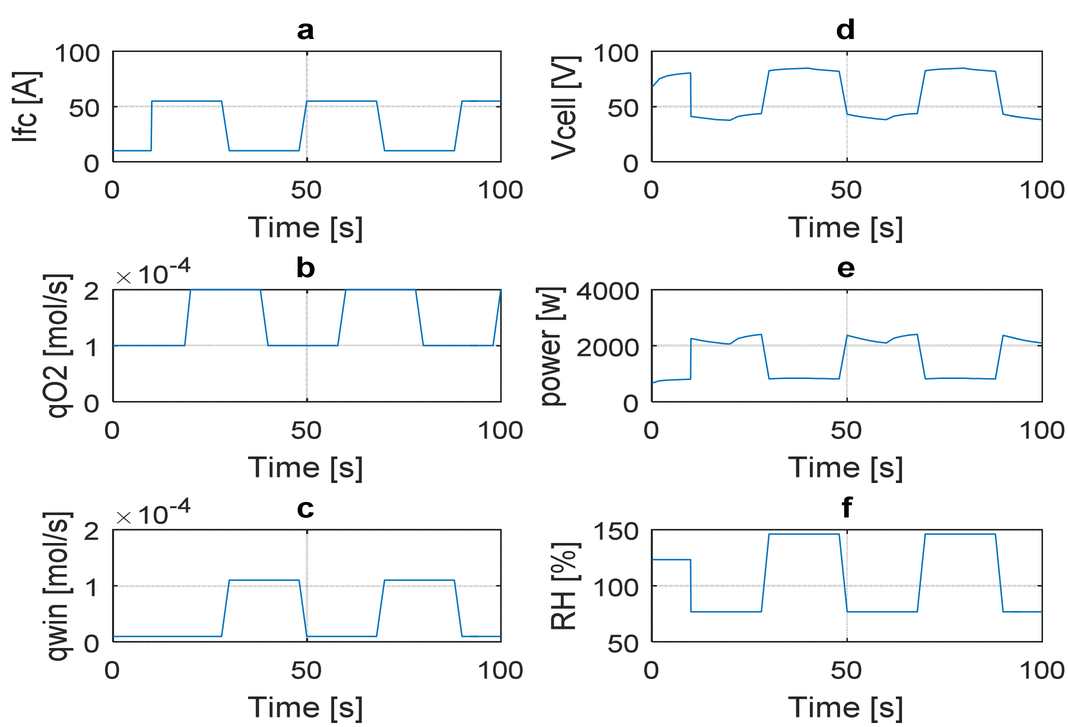


Fig.9**.** The dynamic characteristics of a PEMFC.

3- Each block must be individually adjuster.

The main elements used in the maximum control structure are (Table 3):

- Sources (in green color) are not reverse.
- Coupling and conversions are reverse.
- The elements of accumulation which, retain their total causalities and which, are not reverse.

This control methodology consists in controlling the variables (*Ifc*, q_{O_2in}, q_{H_2in}, q_{H_2Oin}) of adjustment of the system in the objective is to control the voltage Vcell and the RH.

MCS control of PEMFC system

The control part designed in this study is to manage voltage, humidification of the membrane and pressure distribution by acting on input flows. For this purpose, the control strategy given by MCS illustrated in Fig.10 is used. The power cell and the relative humidity are controlled by the incoming flow rates (Hydrogen, Oxygen and water). The voltage Vdc (load voltage), is controlled by a chopper.

This converter by means of its conversion function is used in the energy conversion of the system in order to control the adjustment chain, making it possible to operate the PEMFC model at a constant reference or predicted reference voltage (Vref = 60 V) corresponding to the maximum power point relative humidity reference RH_{ref} =100%, desired by defining an error ε_3 such as $\varepsilon_3 = RH - RH_{ref} \approx 0$

Results and discussions

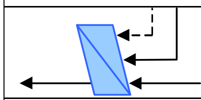
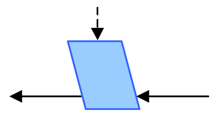
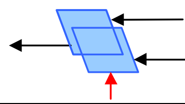
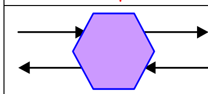
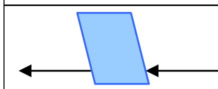
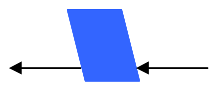
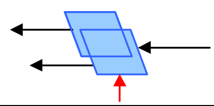
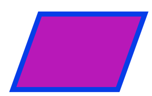
At the output of the PEMFC model a DC / DC chopper is connected, the FC is assimilated as a controlled voltage source (the voltage of the load is checked) using a PI controller this voltage is taken as a reference. The choice of controller has shown its adaptation to the system.

In the physical domain the flows q_{H_2}, q_{O_2} and q_{H_2O} are controlled for our operation.

The coupling control in the MCS part made in the reaction flow rates: $q^r{}_{H_2}$, $q^r{}_{O_2}$ and $q^r{}_{H_2O}$ after electrochemical reaction compared with reference flow rates $q^r{}_{H_2ref}$, $q^r{}_{O_2ref}$ and $q^r{}_{H_2Oref}$, in such a way as to have errors $\varepsilon_1, \varepsilon_2$ such as $\varepsilon_1 = q_{H_2} - q_{H_2ref} \approx 0$ and $\varepsilon_2 = q_{O_2} - q_{O_2ref} \approx 0$.

An estimator is appropriate to the control system to estimate the relative humidity according to the relationship (16). This relativity is controlled by the relative humidity reference RH_{ref} =100% desired by defining an error ε_3 such as $\varepsilon_3 = RH - RH_{ref} \approx 0$

TABLE.3. The basic elements of the MCS [6]-[8]-[18]

Maximum Control Structure (MCS)	
	Indirect inversion (closed-loop control)
	Direct inversion using a disturbance rejection
	Coupling inversion (weighting)
	Model or estimator (any pictogram)
	Direct inversion (open-loop control)
	Strategy (energy management)
	Coupling inversion (distribution)
	Model or estimator

The control results checked up as shown in the following (Figure 11), where we can see the variations of the different output parameters of the PEMFC model as a function of the input parameters in a time interval of 150 seconds

The control strategy consists in setting the voltage Vdc at the output of the model to a constant value of 6OV intended as reference. Generally, power converters, are used to raise this voltage with a variable current.

Relative humidity varies from 50% to 150% as shown in Fig.9 at the output of the model this relative RH controlled in such a way that it is close to 100% as shown in Fig.11.

The inversion-based control rests on step-by-step inversion (input and output elements).

This type of control keeps the fuel cell away from flooding and dryness. Therefore, the water management works properly.

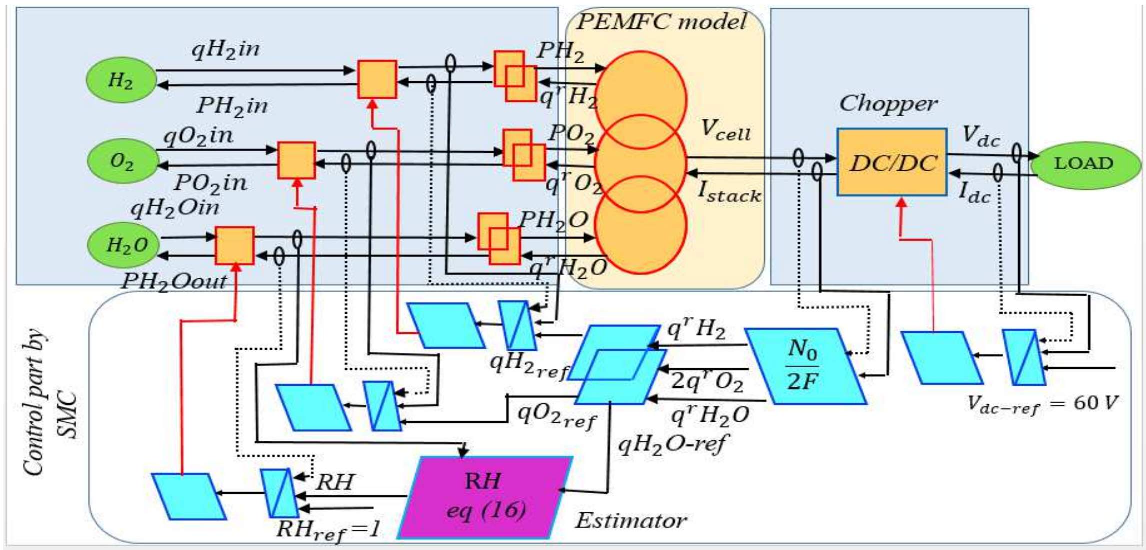


Fig.10. Proposed synoptic control strategy of PEMFC using MCS.

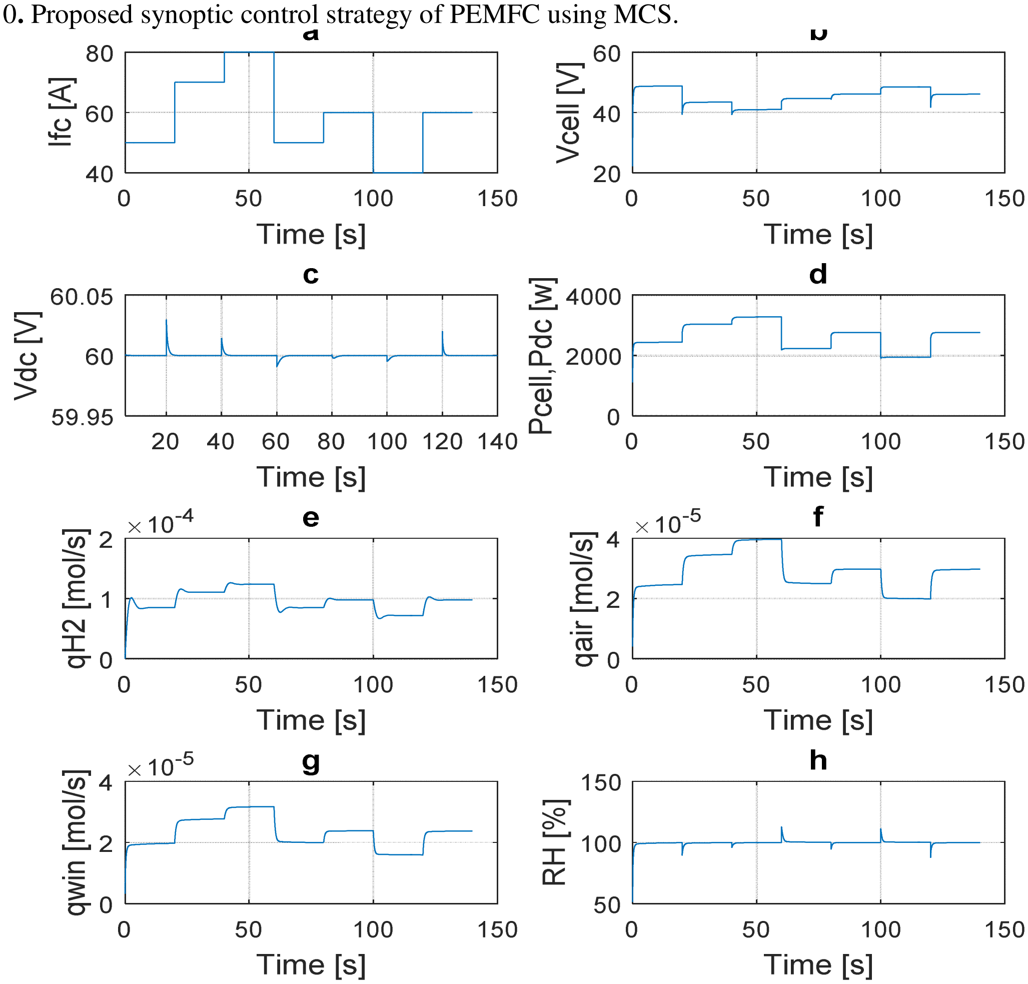


Fig.11. Control of PEMFC operating variables

4. Conclusion

The influence of water management and control in fuel cell system has presented in this work.

The structure of the PEMFC model treated as a power source modeled, using the Macroscopic Energetic Representation (MER) graph tool. This formalism is simple, it analyses the energy exchanges of this energy structure and it allows the designer to directly, deduce a simple reliable and relevant control methodology.

The degradation and depletion of water in the PEMFC stack, causes a large drop in voltage and can cause aging and the end of life of the system.

The effect and range of the humidification in the air and the amount of incoming water inside the fuel cell act on the performance of the PEMFC.

To achieve maximum voltage and power, the relative humidity RH must controlled around 100%.

The control strategy adopted in this work is the Maximum Control Structure (MCS). The inversion of the model consists of adjusting the voltage.

The simulation results show that this energy system can respond easily to the different changes in operating conditions.

Consequently, it is preferable for the supply of electrical energy to design these parameters properly under suitable conditions in order to reduce the voltage losses and to minimize the disadvantages of the fuel cell in order to achieve the objective of using the PEMFC with a High performance and for powers used in production of energy.

Until now there has been no electronic estimation device that can help us to realize an RH controller, the future work is to realize this device which allows us to estimate and control this relative humidity in the PEMFC.

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