Water Distribution and the Impact of Relative Humidity in a PEMFC Energy System using Macroscopic Energy Representation by Inversion Control

Farid Saadaoui[1, 2*], Khaled Mammar[2], Abdaldjabar Hazzab[1, 2]
1- CAOSEE Research Laboratory Control, Analysis and Optimization of Systems Electro-Energetic systems, University of Tahri Mohamed Bechar, Bp417, Bechar, Algeria.
Email: f_saadaoui1969@yahoo.com (Corresponding author)
2- Department of Electrical Engineering, University of Tahri Mohamed Bechar, Bp 417, Bechar, Algeria.
Email: mammar.univ.dz@gmail.com

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ABSTRACT:
One of the most significant handicaps and disadvantages for the proper operation of the polymer membrane in a PEMFC fuel cell energy system is the distribution of water. In this paper, we propose a mathematical model for defining the static and dynamic characteristics of energy behaviour (voltage, electricity, and relative humidity) for various input operating parameters (hydrogen, oxygen, water flow rates, temperature and current). This energy phenomenon is used in a wide range of operating conditions to ensure the exploitation of the energy produced, which will be modeled by a recent practicable and achievable graphical formalism, the Macroscopic Energy Representation (MER), which is used because of its simplicity which feasibility, and is based on the action/reaction principle and controlled by a simple inversion method. This behavior is designed to deduce and recommend an energy management plan for the PEMFC system that takes into account the various states of flooding and drought and contributes to an optimal humidity level for the system's implementation. The simulation results show that to operate correctly for this model, the Relative Humidity must be in the neighborhood of 100% for the device to be effective.

KEYWORDS: PEMFC, FC, Water Distribution, Modeling and Control, RH, MER, MCS.

1. INTRODUCTION

The main goal of this paper is to view, investigate, and exploit the energy management of a PEMFC fuel cell that runs on hydrogen and oxygen, which is dependent on water delivery inside the cell to keep the electrolyte membrane moist and prevent flooding and drying, which can cause the FC to deteriorate in the first place, and to ensure the FC's long-term viability.

PEMFCs are excellent hydrogen and oxygen to electrical energy converters, where they are made up of [1-2 -25]:

-Anode: an emitter of electrons in the reaction is: $2H_2 \rightarrow 4H^+ + 4e^-$

-Cathode: an electron receptor in the reaction is:

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

-In the reaction, the support membrane (electrolyte) separates the anode from the cathode as follows:

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

Sets of cells can be connected in series to raise the voltage of an FC that can output from 0.8V to 1V [4-5]. A PEMFC consists of "Fig 1".

1-Fluidic domain:

-Oxygen enters the cathode from pure air.

-Hydrogen entry into the anode.

2-Water processing is the second area of water management.

3-Thermodynamic domain: energy generation (the nucleus of the cell).

4-Electrical domain: at a load, produce a constant aim voltage Vcell.

5-Heat generation is the fifth thermal domain.

For the realization and implementation of the PEMFC scheme, each of these areas is needed [1]-[25].

In order to keep the complexity of a mathematical model of a mechanism as low as possible while preserving the system's characteristics, different simplifying assumptions must be made: Let us make the following simplification assumptions to carry out

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our research:

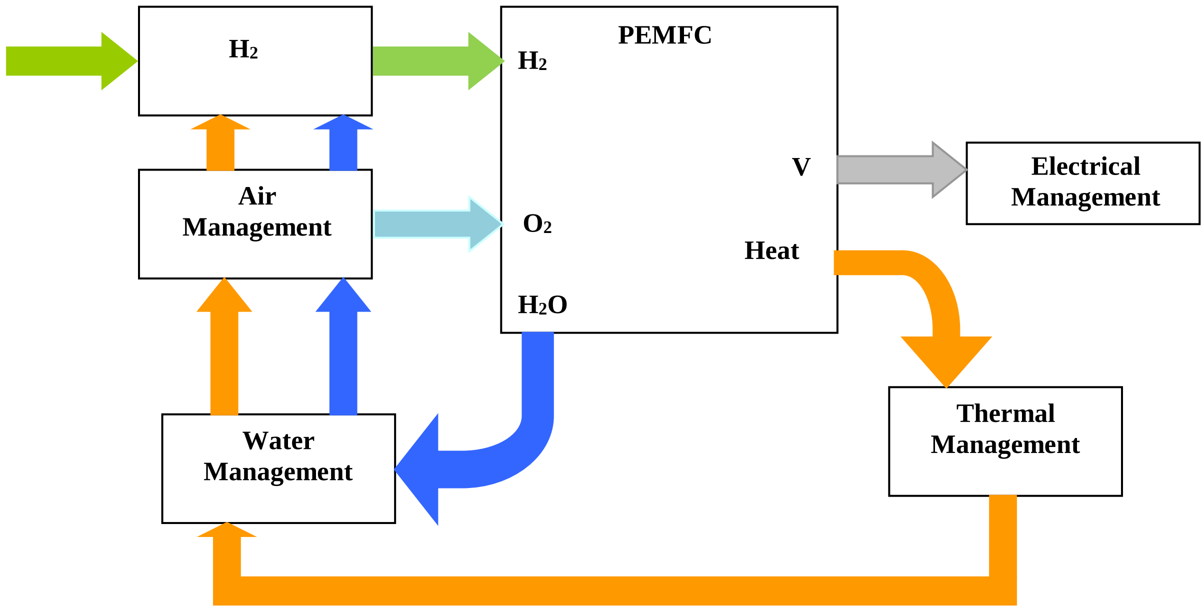


Fig. 1. Synoptic diagram for an operating fuel cell model [3]-[23].

-The simulation is about a cell.
-The temperature is assumed to be evenly distributed across the cell's components.
-The hydrogen and oxygen in the cell are pure and fine.

This presumption eliminates the difficulties created by impurities accumulating (nitrogen). Since the oxygen pressure accounts for 23% of the air pressure, the model still holds true when using air. In this situation, the nitrogen effect may be underestimated.
-Pressure losses in gas delivery systems are not taken into account (gas pressures are considered uniform in the supply pipes). According to a thorough study, these losses amount to around 3.5 percent of the supply strain.

Since this modeling is based on the MER approach, it is critical that we specify the various input variables on which we will operate, as well as the output variables characterizing the evolution of the mechanism, from the functional diagram mentioned in "Fig 1": measurable or observable quantities on the action of tension and relative humidity [3-23].

The input variables are (Ifc, P_{H2}, P_{O_2}, P_{H_2O}, RH et ΔSq) avec ΔSq : is the heat flow.

The output variables are ($q^r_{H_2}$, $q^r_{O_2}$, $q^r_{H_2O}$, $Vcell$, $Pcell$ et Tfc).

2. MODEL OF PEMFC WITH MER

The basic model is changed to create the control mechanism for a fuel cell design, which must have certain characteristics (energy, modularity, suitability for multi-complex physical domains of various domains, etc.). The MER modeling alternative is explained by the fact that it was created for the synthesis of complex systems (electromechanical, electrochemical, fluid mechanics, physical and electrical ...)[6].

The MER is a modern readable macroscopic representation that is more usable and simple to use, combining two graphical formalisms: the Informal Causal Graph (ICG) and the Band Graph (BG). The MER is made up of three pictograms [5]-[6] (source components, transfer elements, and aggregation elements) and is founded on the Action/Reaction theory of energetic processes according to integral physical causality (Table 1).

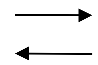
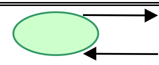
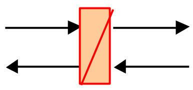
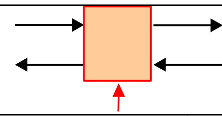
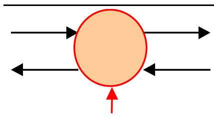
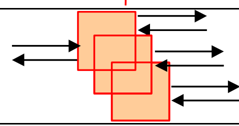
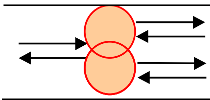
The L2EP Laboratory at the University of Lille in France first introduced the MER in 2000. It's a good method for making energy control systems like fuel cells, electromechanical systems, electric cars, tramways, metros, and wind turbines, among other things.

T. Zhoul suggested a model fuel cell that is a simpler version of Hissel's [7]. As seen in "Fig. 2" or the proposed model of the PEMFC stack with various couplings, our proposal consists of introducing the restriction of humidification of the membrane by the flow of water added into the air, as well as the effect of relative humidity on the proper functioning of the structure.

-The thermodynamic domain was linked to the physical domain by introducing flow speeds of hydrogen, oxygen, and water at the anode, cathode, and membrane.

- A thermal-thermodynamic coupling: Since temperature changes have a direct effect on the system, a constant temperature has been chosen in our case.
- A relation between the thermodynamic and humidification domains: This means a change in RH, which is something we are concerned with.
- A thermodynamic-electrical coupling is achieved by applying a Vcell voltage to the load, as seen in "Fig. 2."

Table 1. The basic elements of MER [6]-[8] Energetic Macroscopic Representation (EMR).

	Author affiliation		
	Action and reaction variables		Energy source (system terminals)
	Energy source (system terminals)		Mono-physical converter (energy conversion)
	Multi-physical converter (energy conversion)		Mono-physical coupling (energy distribution)
	Multi-physical coupling (energy distribution)		

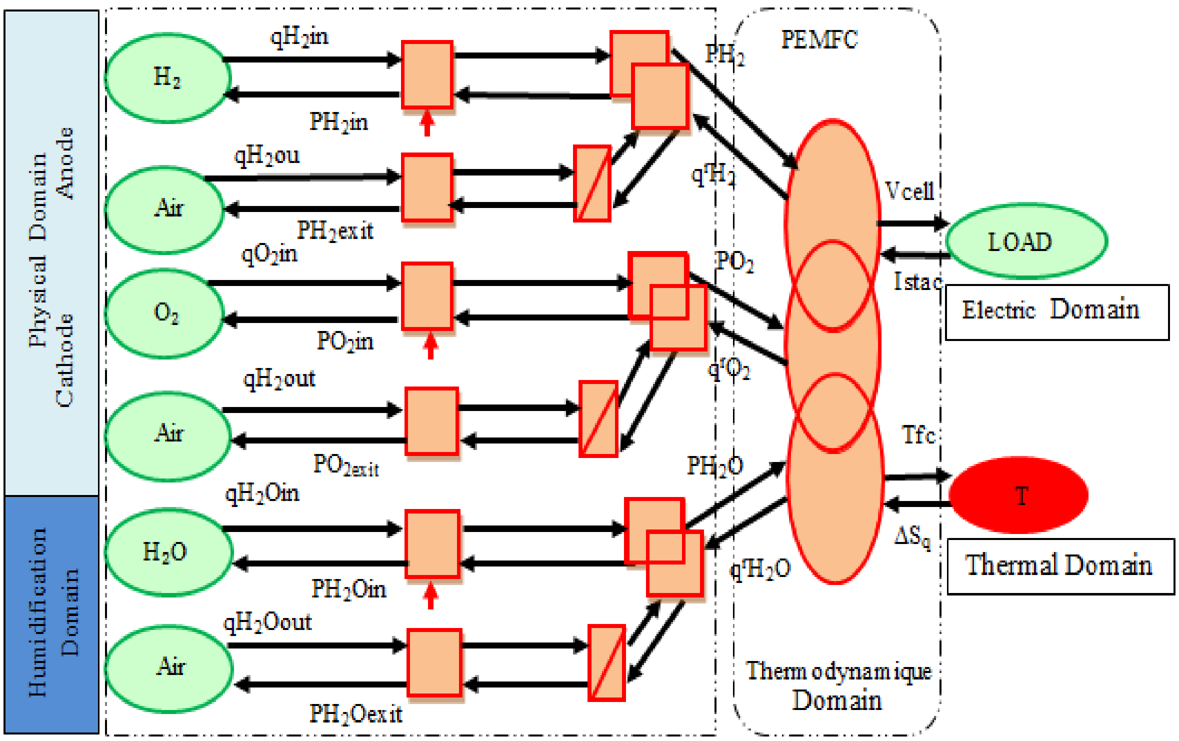


Fig. 2. The proposed PEMFC Representation by MER.

The equations for the various domains in this structure are as follows:

2.1. Domain of Thermodynamics

The voltage of a cell as determined by the ohm's rule [1-3]

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

Where, 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 below is the overall tension:

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

P_{H_2} : is the partial pressures of hydrogen (atm), P_{O_2} : is the partial pressures of oxygen (atm) and T is 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, ts is the operation state, and J represents the actual current density of the cell (A/cm).

$J_{max} = 1.5\mathrm{A/cm^2}$ 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 oxygen Co_2 :

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

σ_m :Nafion conductivity is the basic conductivity of the membrane proton (which is dependent on membrane water activity) and can be calculated experimentally using the equation [15]:

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

Alternatively, the following relation [8] gives the water content of the membrane.

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

2.2. Humidification and Physical Domain

The following electrochemical relationships formed by M. Y. El-Sharkh characterize the partial pressures of the three input gases and water at the PEMFC cell, as well as the output rates. The state equations become [1-3]:

$$\frac{d}{dt}(P_{H2}) = \frac{RT}{V_{an}}(q_{H_2in} - q_{H_2out} - q^r_{H_2}) \quad (5)$$

$$\frac{d}{dt}(P_{O2}) = \frac{RT}{V_{an}}(q_{O_{2in}} - q_{O_2out} - q^r_{O_2}) \quad (6)$$

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

q_{H_2} and q_{O_2} are the flow rate inlet of each gas and q_{H_2O} is the water inlet flow rate by air.

q_{H_2out} and q_{O_2out} are the outlet flow rates of each gas, and $q_{H_2O_{out}}$ represents water vapor.

In "Fig. 2," the MER's previously depicted fuel cell concept is clearly seen.

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

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

Or 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.

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

2.3. PEMFC Formula Water Activity

L. Boulon and all [3] created this method to quantify the relative humidity of a fuel cell at the gas outlet while researching the impact of air and water treatment on humidification issues.

In our simulation, the temperature is kept constant at T=363°K.

As a result, RH does not mechanically reach 100%, resulting in FC exhaust air saturation. This suggests that PEMFC can help to save water in the atmosphere. Furthermore, hot air contains more water than cold air, as is well known.

This research looks at the impact of the wet domain on the PEMFC model, using Rankine's experimental method, which is dependent on the temperature of the incoming air and has a saturation pressure that ranges from 0% (dry air) to 100% (humid air), which is the case we want [3].

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

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

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

P_{sat} : The saturated vapor pressure.

To calculate relative humidity, the water content of the outgoing air is measured.

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

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 is determined as a function of the incoming air molar flow and the moist air molar flow using the following equation:

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

$$q_{O_2in} = \frac{\lambda_a . I_{stack}}{4.F} \quad (14)$$

And

$$q_{rest} = 3.76.q_{O_2in} \quad (15)$$

q_{rest} is the remaining molar oxygen flux.

Finally, relative humidity is given by the following equation [3]:

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

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
Surface, A	50.6 cm^2
t_m membrane thickness	178 μm
Jn	1.2 A/cm^2
Istackn	60 A
R	8314.47 /Kmol.K

3. MODEL VALIDATION AND TESTING

The objective of this report is to better understand the effect of operating variables on the action of the FC voltage and to suggest a regulation to improve the efficiency of the PEMFC cell model. With this goal in mind, we used MATLAB/SIMULINK tools to model our method using semi-empirical equations and the parameters mentioned in Table 2, as well as to simulate and evaluate our 3D figures. The following are the simulation results:

3.1. A PEMFC's Static Characteristics

a) As seen in "Fig. 3," the FC voltage is directly affected by the current density and oxygen pressure. Voltage reduces at low oxygen concentrations and quickly rises at elevated pressures, resulting in a saturated voltage pressure characteristic.

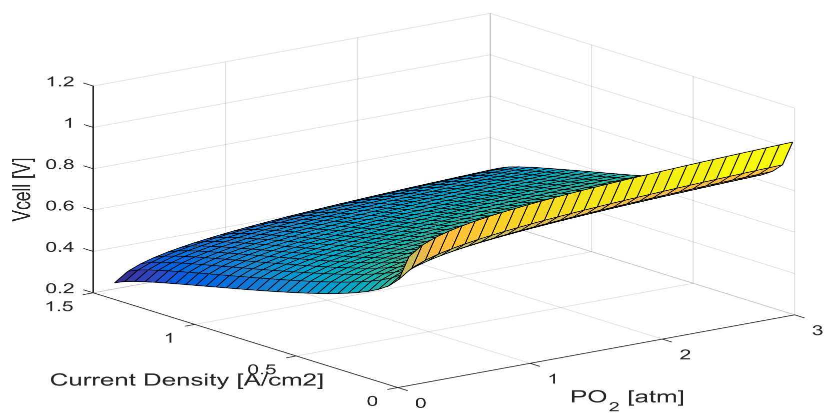


Fig. 3. Variation of PEMFC cell voltage as a function of current density and oxygen pressure with *(P_{H2}=P_{H2O}=1(atm),RH=100% and T=90°C).*

b) The range of the power relative to the same variables as in "Fig. 3" can also be seen in "Fig. 4."

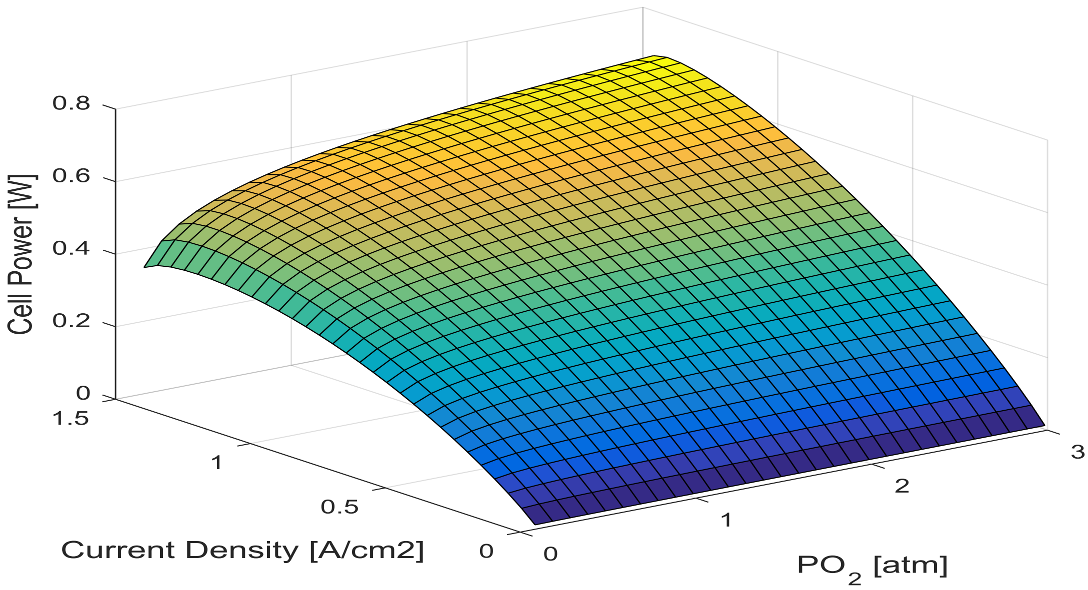


Fig. 4. Variation of PEMFC cell Power as a Function of Current Density and Oxygen Pressure with *(P_{H2}=P_{H2O}=1(atm),RH=100% and T=90°C).*

c) In terms of the effect of relative humidity RH on the action of the power displayed in "Fig. 5," it should be observed that when relative humidity exceeds 100%, cell power is at its peak, relative humidity increases by this value, and power drops rapidly for high current densities. As a result, a relative humidity of 100 percent is needed for proper fuel cell service.

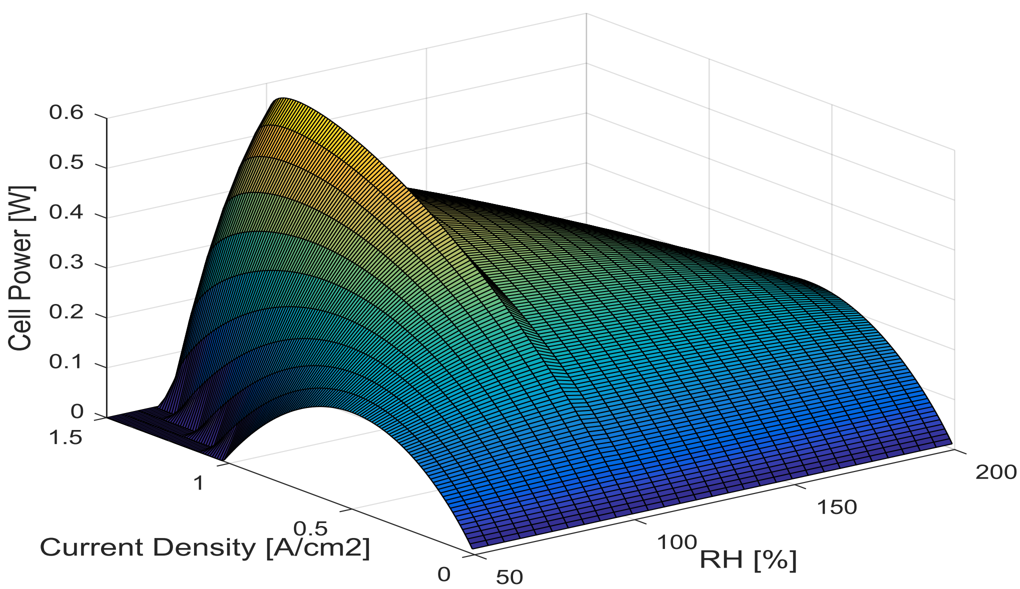


Fig. 5. Changes in cell power as a function of current density and relative humidity over time *(P_{H2}=P_{O2}=1(atm) and T=90°C).*

d) "Fig. 6" depicts the voltage difference as a function of both the current density and the relative humidity RH. The voltage reaches its limit when RH = 100 % and three distinct sections can be distinguished:
1- Drought period: when the relative humidity (RH) is less than 100. This is a non-essential component that can cause membrane damage due to the dryness created by the incoming air.
2- Flooding of the fuel cell occurs when the relative humidity (RH) is greater than 100 (excess water management); in this section, the incoming and generating water are not evenly dispersed, resulting in flooding of the fuel cell.
3- Saturation part: this is the aim of this work, where the flow of water from the inlet (from the incoming air and the electrochemical reaction) equals that from the outlet, resulting in a RH of 100 percent and, of course, a perfectly maximal voltage [25].

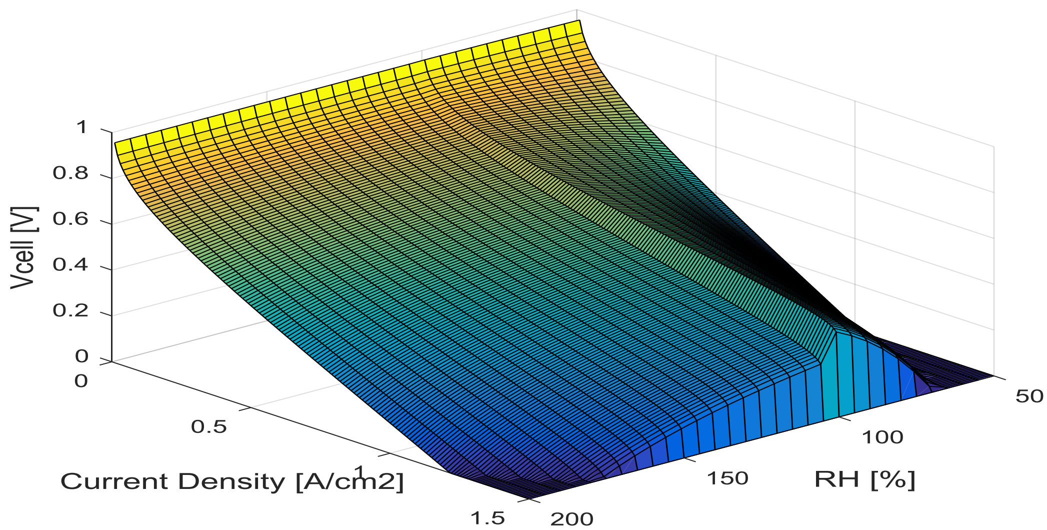


Fig. 6. Variation of cell voltage with respect to current density and relative humidity *(P_{H2}=P_{O2}=1(atm) and T=90°C).*

e) The variance of power as a function of current density and temperature is depicted in "Fig. 7." For high current densities, power rises as a function of temperature in this diagram.

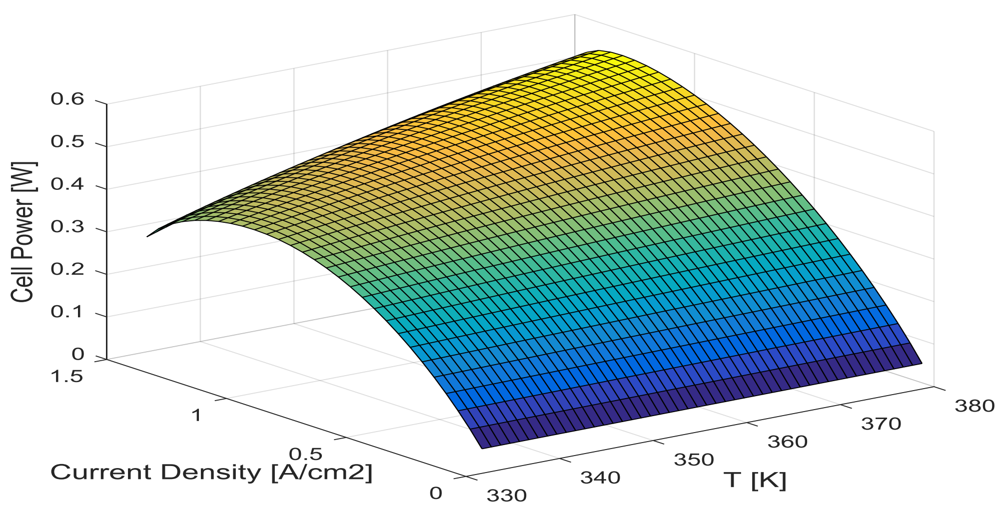


Fig. 7. Changes in cell power as a function of current density and temperature over time *(P_{H2}= P_{O2}= 1(atm)* and *RH=100%).*

f) "Fig. 8" depicts the variance in voltage as a function of current density and temperature; for high current densities, it reduces as the temperature decreases, and vice versa. This trait is extremely temperature sensitive, necessitating the use of temperature control [18].

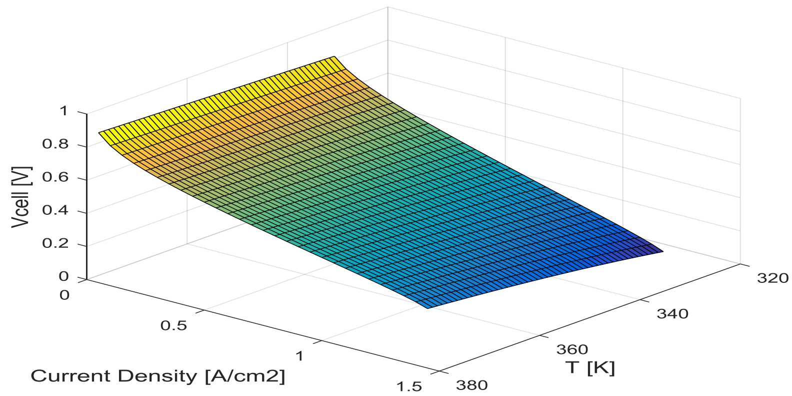


Fig. 8. Cell voltage variation as a function of current density and temperature with *($P_{H2=}$ $P_{O2=}$ 1(atm)* and *RH=100%).*

With these characteristics, changes in the electrical response (voltage, strength, and relativity) of the device with varying operating parameters (current and incoming hydrogen, oxygen, and water pressures) at a constant temperature can be observed in a time limit of 100 seconds.

For active and effective activity, the temperature of the PEMFC is controlled to a constant value.

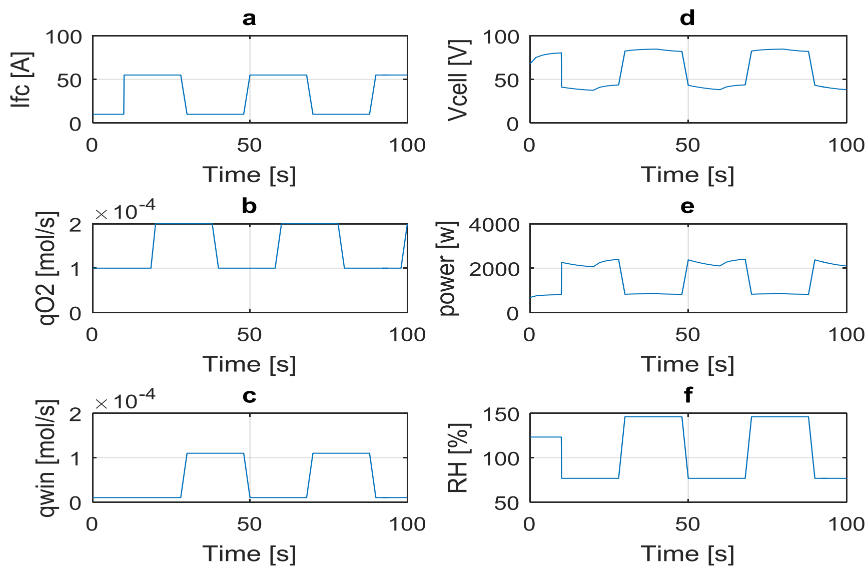


Fig. 9. The dynamic characteristics of a PEMFC *(Ifc, q_{O_2in} , q_{H_2Oin} , Vcell, Pcell and RH).*

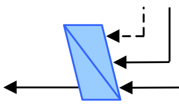
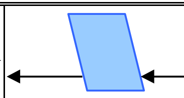
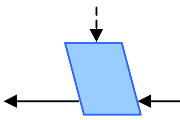
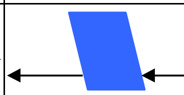
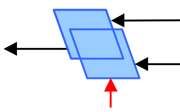
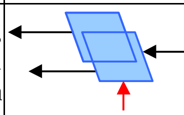
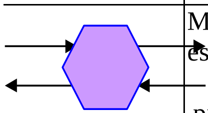
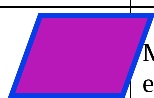
3.2. A PEMFC's Dynamic Characteristics

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

RH (Relative Humidity) varies directly in response to the same input variables. The fact that it is between 50 and 150%, i.e. very far from 100%, allows one to consider improving this relativity and therefore performance parameters (Vcell, Pcell), both of which are governed by a well-defined strategy for proper and adequate commissioning of this energy system.

Table. 3. MCS's fundamental components [6,8, 18].

Maximum Control Structure MCS

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

4. MCS CONTROL STRATEGY

Using inversion rules [3] (Table 3), the MCS structure is successively deducted from the MER in the following steps:

1- Defining the control chain (objective setting variables): in our case, we aim to change the voltage Vcell, electricity, and relative humidity RH "Fig. 9,"

2- For inversion, reverse the mechanism of block by block up adjustment of the adjustment chain.

3- Each block must be changed individually.

Table 3 shows the key components of the optimal control structure:

-Sources that have not been reversed (in green).

-Reversed coupling and conversions.

-The aggregation factors that keep their absolute causalities and are not reversed.

Controlling the variables (Ifc, q_{O_2in}, q_{H_2in}, q_{H_2Oin}) of the mechanism adjustment system with the aim of controlling the Vcell voltage and RH is the goal of this control technique.

4.1. PEMFC Process MCS Regulation.

By operating on input flows, the control component built in this study aims to regulate voltage, membrane humidification, and pressure distribution.

The control technique given by MCS, as seen in "Fig. 10," is used for this purpose. Incoming flow speeds (hydrogen, oxygen, and water) regulate the power cell and relative humidity.

The voltage Vdc (load voltage) is controlled by a chopper.

This converter's conversion feature is used in the system's energy conversion to monitor the change chain, allowing the PEMFC model to run at a constant reference or expected reference voltage (Vref = 60 V) corresponding to the maximum power point relative humidity reference RH_{ref} =100%, as required, by specifying an error ε_3 such that : $\varepsilon_3 = RH - RH_{ref} \approx 0$

4.2. Conversations and Interpretations

A DC/DC chopper is attached to the PEMFC model's output, the FC is assimilated as a regulated voltage source (the voltage of the load is checked), and this voltage is used as a reference using a PI (Proportional Integrator) controller. The controller of option has shown its adaptability to the process.

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 is made in the reaction flow rates: $q^r{}_{H_2}$, $q^r{}_{O_2}$ and $q^r{}_{H_2O}$ after electrochemical reaction, it is 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 $\varepsilon_2 = q_{O_2} - q_{O_2ref} \approx 0$.

The control system needs an estimator to estimate relative humidity based on the relationship (16). The relative humidity relation RH_{ref} =100% desired controls this relativity by specifying an error ε_3 such that: $\varepsilon_3 = RH - RH_{ref} \approx 0$

The control effects are seen in "Fig. 11," which shows how the various output parameters of the PEMFC model vary as a function of the input parameters over a time interval of 150 seconds.

The control technique entails setting the Vdc voltage at the model's output to a fixed value of 6OV as a reference. Power converters are typically used to increase this voltage with a variable current.

At the model's production, relative humidity ranges from 50% to 150 percent, as seen in "Fig. 9." As seen in "Fig. 11," the relative RH is monitored so that it is close to 100%. The inversion-based control rests on step-by-step inversion (input and output elements).

This method of regulation prevents flooding and dryness in the fuel cell. As a result, water control is efficient.

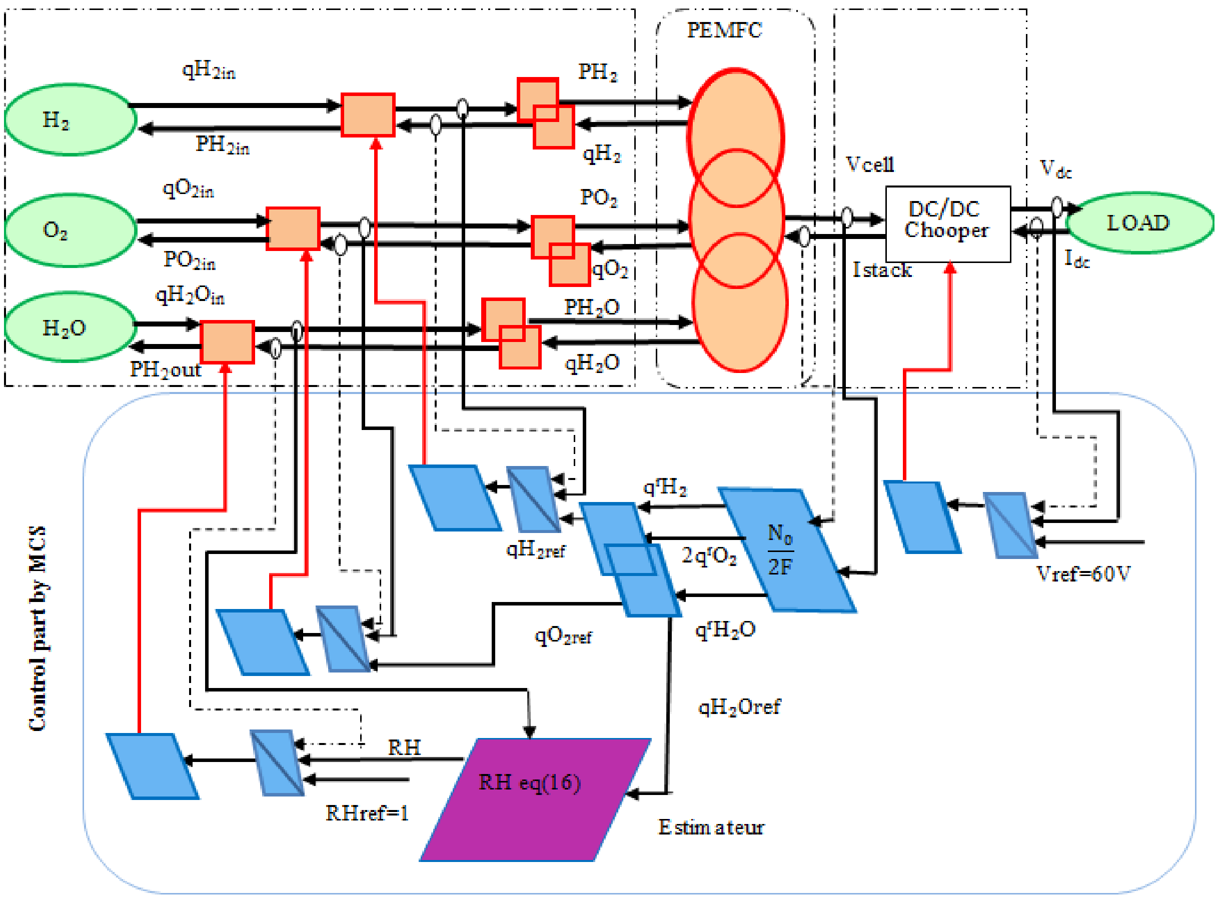


Fig. 10. PEMFC Synoptic Control Strategy with MCS Proposed.

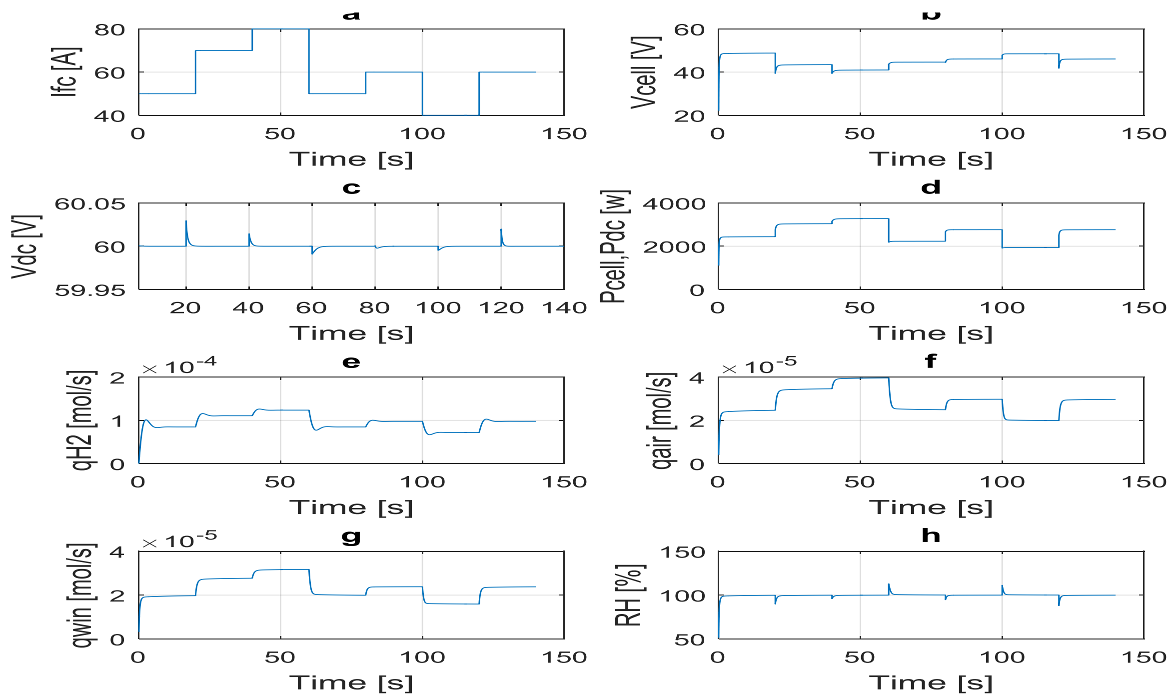


Fig. 11. PEMFC operational variables are under control.

5. CONCLUSION

This paper discusses the impact of water treatment and control in fuel cell systems.

The Macroscopic Energetic Representation (MER) graph technique is used to model the configuration of the PEMFC model as a power source. This formalism is straightforward; it examines the energy exchanges within this energy system and helps the designer to derive a clear, accurate, and applicable control technique directly.

The degradation and removal of water in the PEMFC stack results in a significant drop in voltage, which can lead to device deterioration and the end of its useful life.

The amount of incoming water within the fuel cell as well as the effect and range of humidification in the air, have an impact on the PEMFC's efficiency.

The relative humidity RH must be about 100% to reach optimum voltage and power.

The Maximum Control Structure was used as the control technique in this study (MCS). The model's inversion entails changing the voltage.

The simulation results demonstrate that this energy system can adapt to a variety of operating conditions with ease.

As a result, it is preferable for the supply of electrical energy to better design these parameters under appropriate conditions in order to reduce voltage losses and mitigate fuel cell drawbacks in order to achieve the goal of using PEMFCs with high cell efficiency and using them in energy production.

There has not been an automated estimation system that can assist in the construction of a RH controller before now. The authors' goal is to develop a system that will enable them to estimate and monitor relative humidity in PEMFCs.

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