Towards a Study of the Operation of a Hydrogen-based Proton Exchange Membrane Fuel Cell for Power Generation

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ABSTRACT Energy challenges continue to grow due to the depletion of usual energy sources on the one hand, and climate change due to pollution on the other. The development of new energy production systems is therefore a priority for the scientific community. Hydrogen is a solution for the future that preserves the environment and makes it possible to obtain electricity through chemical reactions. Hydrogen technologies and in particular proton exchange membrane fuel cells (PEMFC) have many advantages to be the clean source of electrical energy of tomorrow. In addition, the fuel cell can operate with pure hydrogen, which can be produced not only from fossil fuels such as natural gas and oil, but also from renewable energies (wind, solar, hydraulic, biomass). Fuel cells (PEMFC) seem to be a promising alternative. One of the most important scientific and technical challenges for the design and production of a fuel cell is to know how a fuel cell behaves in its real environment of use. The purpose of this paper is precisely to analyze the performance of the PEMFC type fuel cell using a modeling and a numerical simulation carried out under the Matlab / Simulink software. In the light of this study, it would be possible to assess the behavior of the PEFMC and compare it to the actual data.

KEYWORDS Electrodialysis, Hydrogen, Matlab, Modeling, PEMFC

1. INTRODUCTION

Today, energy plays a very important role in our society. It is divided into renewable energy based on natural resources and other non-renewable sources. Currently, the main source of energy used to produce electricity is from fossil fuels (oil, natural gas and coal). However, it turns out that these resources are presented in limited and non-renewable quantities, and that their combustion generates greenhouse gases (GHG).

Green hydrogen has the potential to create a virtuous cycle for future renewable energy-based power grids, as it can provide much-needed flexibility to power systems, serving as a buffer to non-dispatchable renewable generation. This hydrogen is created by the electrolysis of water in an electrolyzer using energy generated by renewable sources including hydroelectricity, wind and solar. GHG emissions throughout the manufacturing process are zero if all electrical inputs come from renewable energy sources (and if desalinated water is required, it is powered entirely by solar and wind power).

Recently, the Hydrogen Fuel Cell (HFC) is identified as an alternative energy generator for transportation and portable applications because, it is such a simplified and compact system design, it does not have a unit fuel processing (reforming) and storage. The electrode/membrane assembly strongly influences the performance of fuel cells. Note that the phenomena that hinder the proper functioning of the cell relies on the membranes [1].

The obtained characteristics of a membrane should be used as inputs in a mathematical model to predict the performance of the corresponding HFC. Thus, instead of only having a prediction of HFC performance based on the results of research experiments, this type of model should allow a prediction. However, much of the research on HFC modeling is carried out in numerous settings in the literature [2].

In this paper, we will focus on Proton Exchanging Member Fuel Cells (PEMFCs). This type of battery is currently very studied because of its multiple applications in the stationary field as well as in the automotive and portable fields.

The first part of this paper presents general overview of fuel cells, the definition and the different types of a fuel cell, explaining how it works. The advantages and disadvantages of fuel cells will then be cited. In the second part we will present and study the characteristics of the PEMFC. The third part will be dedicated to the modeling and simulation of this type of fuel cell on Matlab/Simulink. By performing simulation, fuel cell performance can be analyzed before manufacturing, reducing the risk of failure and defects.

2. FUEL CELLS: CONTEXT AND ISSUES

2.1. International context

Despite its great advantages in terms of polluting emissions, the hydrogen fuel cell is sometimes the subject of criticism and has therefore only been partially developed commercially. The problem: transforming hydrogen into electricity requires an electrocatalyst which, in turn, is mainly composed of platinum – a rare and expensive metal.

Hong Kong researchers at the University of Science and Technology (HKUST) have now developed a fuel cell that not only uses around 80% less platinum, but also has a much longer lifespan [3].

Despite the low quantity of platinum, the hybrid catalyst retained approximately 97% of the performance of a platinum catalyst, after 100,000 current cycles under continuous load. For comparison, traditional catalysts drop to 50% of their life after the same number of cycles. During another test. No loss of performance was observed even after 200 hours of operation [3].

Hydrogen demand in 2020 was approximately 90 million tonnes, of which more than 70 million was used as pure hydrogen and less than 20 million mixed with carbon-containing gases in methanol production and steel manufacturing. Almost all of this demand was for refining and industrial uses. Currently, hydrogen is produced primarily from fossil fuels, resulting in nearly 900 Mt of CO2 emissions per year [4].

Figures 1 and 2 show global hydrogen demand by sector and by production technology.

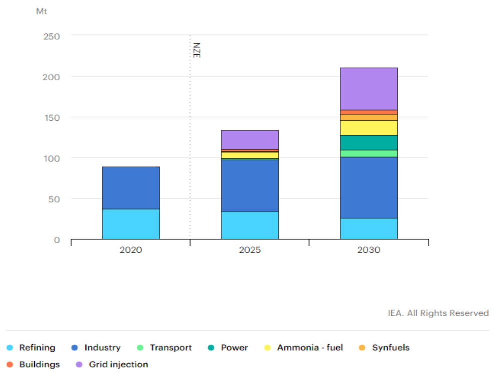

Figure 1. Global hydrogen demand by sector [4]

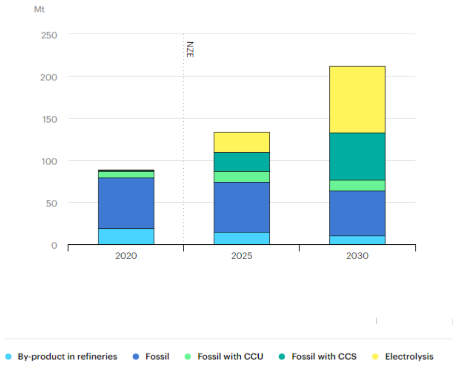

Figure 2.Global hydrogen demand by production technology [4]

2.2. Moroccan context

A conference on “solar hydrogen: potential for continued development of renewable energies in Morocco” was organized in mid-October 2019 jointly between the Amadeus Institute and the French Hydrogen and Fuel Cell Association (AFHYPAC) , in partnership with the Moroccan Association for Hydrogen and Sustainable Development (AMHYD). This seminar brought together different Moroccan and French actors who underlined the importance of creating a hydrogen sector at solar stations in Morocco, given the advantage that the country has in terms of infrastructure, which encourages a transition to hydrogen. Imminent action to introduce flexibility in the cost of hydrogen to create demand (Figure 3) [5,6].

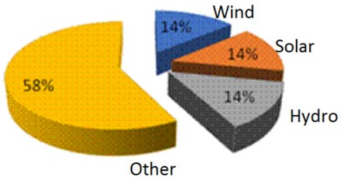

Figure 3. Moroccan energy mix in 2020

3. STUDY OF EXCHANGED PROTON MEMBRANE FUEL CELL: PEMFC

3.1. Presentation and principle of PEMFC

PEFMC is a low operating temperature battery that starts at around 25°C up to 80°C. It is also called: SPEFC (Solid Polymer Electrolyte Fuell Cell) or IEMFC (Ion Exchange Membrane Fuell Cell). This type of battery is the most famous thanks to its multiple advantages. It is made up of an electrolyte which is the membrane, electrodes, diffusion plates (backing) and bipolar plates. To better understand this type of battery in detail, let us observe the following diagrams (Figure 4).

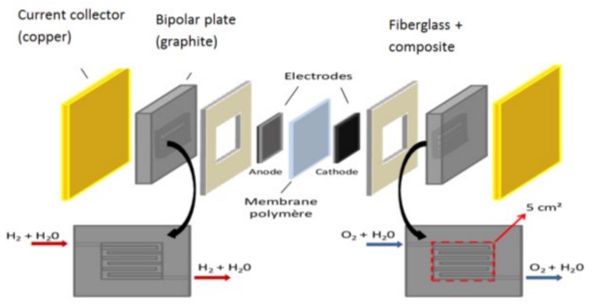

Figure 4. Diagram of the constituent elements of the PEMFC [7]

a. *Electrolyte*

The electrolyte here is an acid-type ionic polymer membrane. In general, it is a perfluorinated membrane onto which sulfonate acid groups are grafted. The most widespread model of these membranes is the “nation”, manufactured by the firm Du Pont de Nemours. This type of membrane retains negative ions and allows H ions (protons) to pass through, which are then mobile and free to transport as a positive charge through the membrane, from the anode to the cathode. This movement of charge thus described is internal to the battery.

If the anode and the cathode are connected by an electric wire via an ammeter, the latter will measure an electric current which would be the equivalent of a movement of electrons in this circuit outside the battery.

However, the ionic conductivity of the membrane depends on the temperature. The membrane must always remain saturated with water for better movement of protons

The membrane must prevent the passage of oxygen and nitrogen but also that of electrons.

Studies by Club PAC (fuel cell club) show that these membranes have a lifespan of 3500 to 4500 hours for operation between 25 and 90°C.

b. *Electrodes*

Electrodes makev it possible to dissociate hydrogen and transfer protons to the electrolyte. The electrodes are generally based on fine particles of platinum on black activated carbon so that the platinum content is 0.1 to 1mg/cm². Thus platinum catalyzes anodic and cathodic reactions.

$$H_2=2H^+2e^- \quad (1)$$

The cathode: The reduction of oxygen is carried out, according to reaction 2.

$$\frac{1}{2}O_2 + 2H^+ + 2e^- = H_2o \quad (2)$$

c. *The Catalyst*

For both half-reactions to be possible, a catalyst is needed. To enable the catalyst working effectively, the creation of active zones must be ensured. These zones involve the reactive gas, the electrons, the protons and the catalyst; this takes place at the level of the electrode-electrolyte interface [8].

d. *Backings (broadcast plates)*

They are conductive and porous. By surrounding the electrodes, allow the diffusion of gases to them on the one hand, then the transfer of electrons from the anode to the cathode on the other hand.

e. *Bipolar plates*

They are often made of graphite and are used to manage the distribution of gases, hydrogen and oxygen, and the evacuation of water resulting from the operation of the fuel cell. These plates are placed on the outermost parts of the pile.

3.2. Constraints on fuel cells

a. Temperature and pressure

Typically, polymer electrolyte membrane fuel cells (PEMFCs) operate at pressures between ambient pressure and a pressure of approximately 3 bar, and at temperatures between 50 and 90°C. High power density is achieved at higher operating pressures, but system efficiency may be lower due to the power required to compress the air. Higher air temperatures also increase power density, but can pose a significant challenge for water and heat management, particularly at lower operating pressures.

Therefore, the choice of operating temperatures and pressures for automotive PEMFC systems should be based on:

- The net yield of the system
- The small size of the components
- A neutral or positive water balance, so that the vehicle does not require an on-board tank.

The increase in operating power of a PEMFC system at elevated pressure results primarily from a reduction in cathode activation overvoltage, because the increased pressure increases the exchange current density, resulting in to record the open circuit voltage (OCV), as described in the Nernst equation [9].

b. Hydratation of the membrane

For PEMFCs, it is necessary to maintain satisfactory hydratation within the membrane, in order to ensure its ionic conductivity and to improve the transfer of protons (H+) from the anode to the cathode. The conductivity of the membrane located within the polymer electrolyte is quite complex because excess water can flood the active zone of the electrode and hinder the diffusion of gases. At the cathode, where water production is located, the flooding phenomenon is more recurrent [7].

Humidification is sensitive and can lead to drying or flooding of the membrane. A reduction in electrical energy production and lifespan may result. According to heat pump manufacturers, it is also necessary to humidify the hydrogen at the anode.

There are different possibilities for hydrating the membrane. The simplest is to let the Fuel Cell self-hydrated with the water produced at the cathode during the electrochemical reaction. In low-power embedded applications, it is increasingly common to carry out micro short circuits which allow homogeneous hydration of the membrane. However, for higher power applications, it is preferable to rely on external hydratation. Indeed, too high air flow rates at the cathode could dry out the membrane and reduce the performance of the heat pump.

In order to better manage the water content of the membrane and above all to avoid condensation phenomena, the thermal management of this circuit is essential. It is often linked to the battery core cooling circuit [7] (Figure 5).

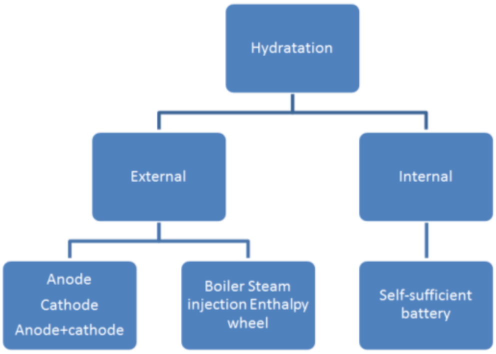

Figure 5. Different modes of PEMFC hydratation [10].

4. MODELING AND SIMULATION OF PEFMC

4.1. Electrochemical model of a PEFMC

When the PEMFC operates, the phenomena of polarization leads to irreversible losses that decreases the cell voltage. It mainly includes ohmic, activation and concentration losses as shown in equation (3).

$$V_{cell} = E_{nernst} - V_{act} - V_{ohm} - V_{conc} \tag{3}$$

The characteristic of the voltage in a fuel cell of figure 9 is composed of three zones which correspond to the preponderant phenomena versus the current density [6].

Figure 9 shows the characteristic of a single PEMFC. The OCV corresponds to a null value of the current density, which means no current is circulating in the cell. Then, the voltage is decreasing according to the losses mentioned above.

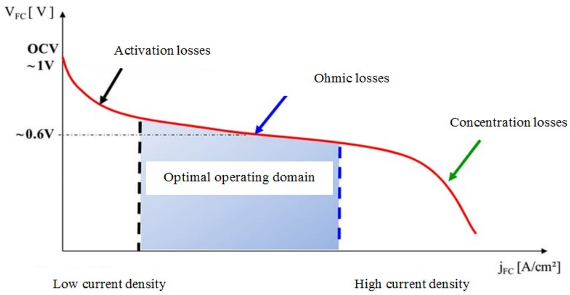

Figure 9. PEMFC polarization curve

The ideal voltage of a fuel cell can be represented by the Nernst equation :

$$E = E^0 - \frac{RT}{2F} \ln(PH_2 * PO_2{}^{0.5}) \tag{4}$$

Where :
E_0: EMF at standard pressure (ideal voltage).
E : thermodynamic equilibrium potential.
R : Universal gas constant
F : Faraday's constant
T: The temperature of the PEMFC.
PH_2 : Partial pressure of hydrogen (fuel) at the anode
Po_2 : Partial pressure of Oxygen (air) at the cathode.
The ideal voltage equation is then simplified as [11]:

$$E_{th} = 1.229 - 0.85 * 10^{-2} * (T - 298.15) + 4.3085.\,[ln(P_{H2}) + \frac{1}{2}(P_{o2})] \tag{5}$$

Figure 10 shows the ideal voltage simulation model in MATLAB/Simulink.

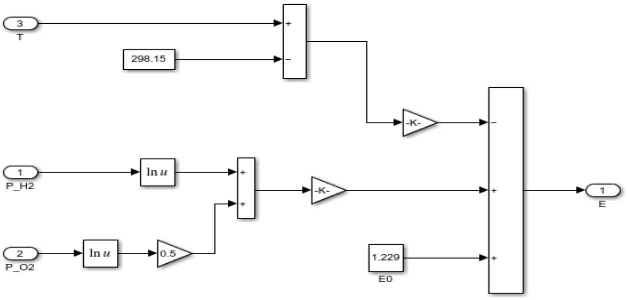

Figure 10. Ideal voltage simulation model (E Nernst)

- Activation voltage:

Activation polarization represents the amount of activation energy that comes form a certain pressure drop, which is due to the the transfer process of the protons (H^+) obtained by the electrolysis of H_2 at the anode, through the proton exchange membrane to reach the catalytic layer of the cathode. The activation voltage V_{act} is formulated according to equation 6.

Tafl's law describes the activation vvoltage of the PEFMC [12].

$$V_{act} = \xi_1 + \xi_2 * T + \xi_3 * T * ln(C_{o2)} + \xi_4 * T * ln(I) \quad (6)$$

Where
I : cell's current,
ξ : Coefficients of the cell model.
Co_2 : Concentration of Oxygen. It's calculated by Henry's law [12]:

$$Co_2 = \frac{PO_2}{5.08 * 10^6 * e^{(-\frac{498}{T})}} \quad (7)$$

Matlab Simulink model of the activation voltage is represented on figure 11.

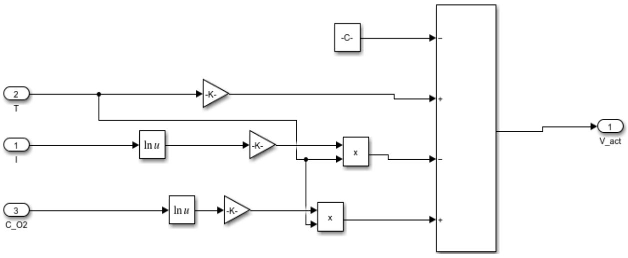

Figure 11. Activation voltage

- Ohmic voltage :

The voltage loss at the PEFMC is modeled by the equivalent resistance R_m of the proton exchange membrane, but also by the resistance R_c that prevents the proton of crossing the membrane [13]. The voltage losses are then written as [9]:

$$V_{ohm} = (R_m + R_c) * I \quad (8)$$

$$R_m = \frac{\mathrm{r_m . l}}{\mathrm{A}} \quad (9)$$

A :The effective activation area,
r_m The proton exchange membrane resistivity. This last is calculated as follows [13]:

$$r_m = \frac{181.6[1+0.03i+0.062(\frac{T}{303})^2 i^{2.5}]}{(\lambda - 0.634 - 3i)e^{4.18(\frac{T-303}{T})}} \quad (10)$$

$$i = \frac{I}{A} \quad (11)$$

I : current density,
λ: The proton membrane water. Matlab Simulink model of the activation voltage is represented on figure 12.

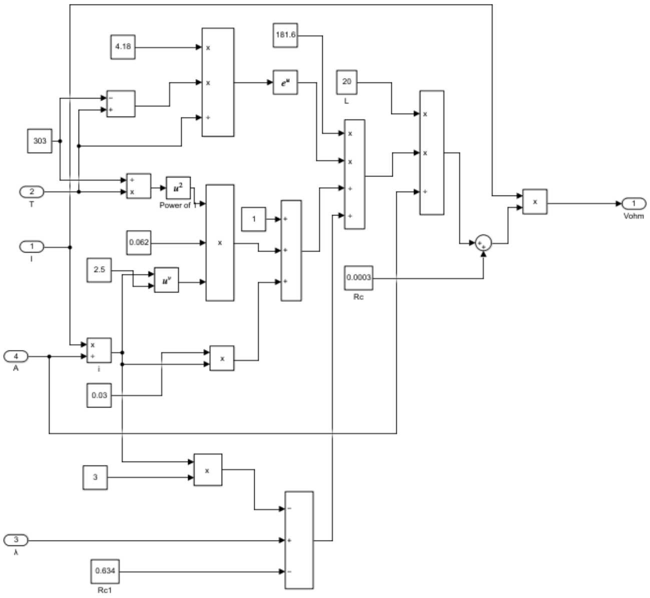

Figure 12. Ohmic bias voltage modeling

- Concentration voltage :

The difference between the concentration of ions of the electrode and the electrolyte cell mass solution, leads to the appearance of a concentration voltage that can be folmulated using equation 12:

$$Vconc = \frac{4F}{3RT}\ln(1 - \frac{i}{i_m}) \quad (12)$$

R : The ideal gas constant,
F : Faraday constant,
I_m is the maximum current density, it depends on the conductivity of the electrode materials and the diffusion rate of the pores of the catalytic layer.

Matlab Simulink model of the concentration voltage is represented on figure 13.

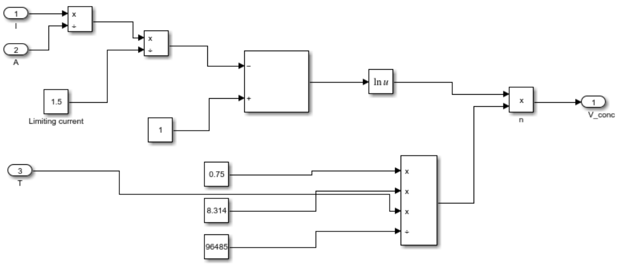

Figure 13. Concentration voltage

4.2. Modeling of PEFMC Stack

All the voltages calculated above correspond to a single cell. The PEFMC is an arrangement of a number *n* of cells. The total voltage of the stack is then obtained as follows [11].

$$V_{stack} = n.V_{cell} \tag{13}$$

- **Fuel cell efficiency**

The efficiency of fuel cells can be defined as the ratio between the output voltage of the cell and the theoretical voltage of the cell. It can also be defined as the ratio between the produced electricity and the produced hydrogen [14].

$$E_{eff} = \frac{W_{el}}{W_{H2}} \tag{14}$$

W_{el} is the electricity produced and W_{H2} is the energy value of the hydrogen consumed in watts.

$$W_{el} = i * V \tag{15}$$

Efficiency is therefore the ratio between the cell voltage and the current voltage can be calculated according to equation 16 [11]:

$$E_{eff} = \frac{V_{cell}}{V_{actual}} \tag{16}$$

Where V_{cell} : the fuel cell voltage

and E_{eff} : the efficiency. Figure 14 shows the total assembly of the model in steady state.

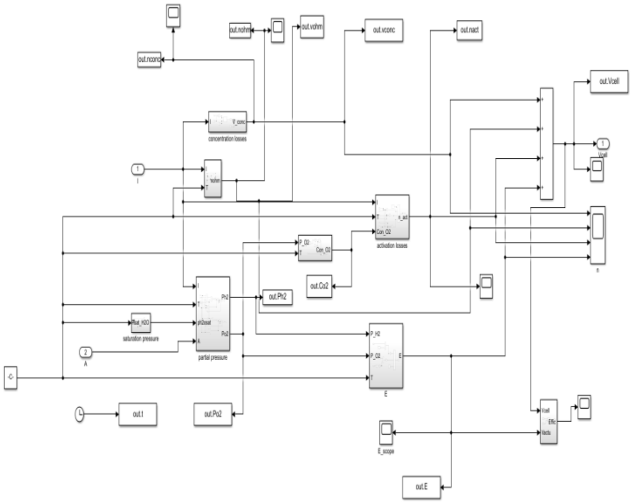

Figure 14. the total assembly in steady state

The Matlab simulink diagram of the Fuel cell is shown on Figure 15.

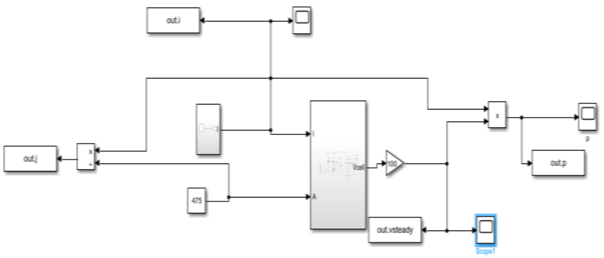

Figure 15. Fuel cell block diagram

4.3. Results and interpretations

Table 1 presents the parameters used in this model.

Table 4
Used parameters

Parameters	Values
Number of cells	100
The surface of the cell	475 (A/cm^2)
Temperature	303.15K
Anode pressure	1.45atm
Cathode pressure	1atm
Concentration loss coefficient (B)	0.016

- **Performance of the PEMFC**

Figure 16 represents the the polarization characteristic of the PEMFC with the parameters mentioned above.

The voltage begins with a maximum value when there is no current density at the cell. The three potential losses make the volatge decreasing. Activation losses dominate at low current densities. The ohmic losses represent the linear part in the middle. The concentration voltage is then represented by a significant drop at the end.

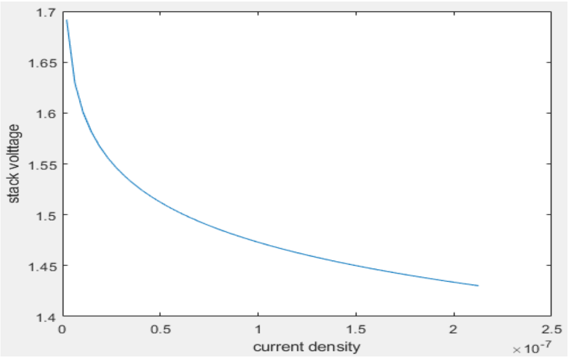

Figure 16. Polarization curve of a fuel cell

The ideal cell voltage is shown on Figure 17. Whatever the current changes, this voltage remains constant.

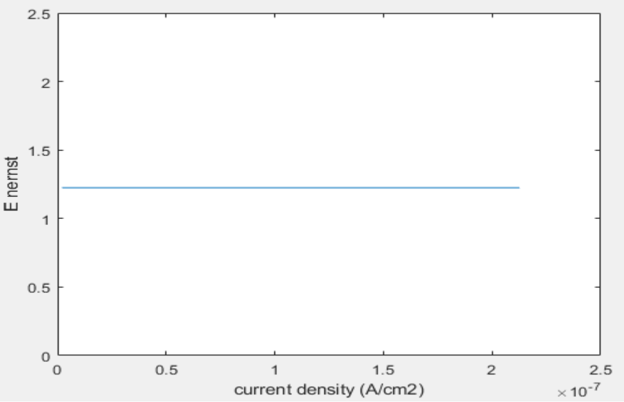

Figure 17. Ideal cell voltage

The ohmic losses are represented on Figure 18. This voltage increases in a linear law versus the current density. The resistance offered by the fuel cell components increases when the reaction proceeds and the current density reached high values. This is mainly due to the resistances of the wire, the bipolar plate and the proton exchange membrane.

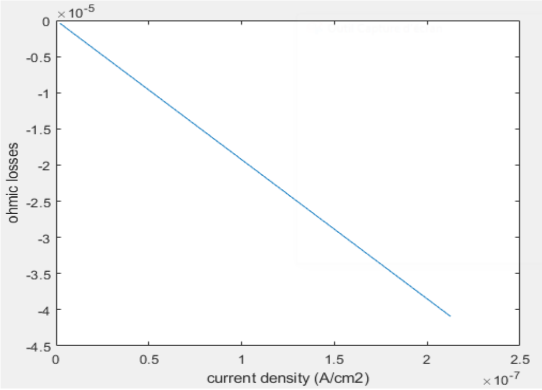

Figure 18. Ohmic loss

The steady-state activation voltage versus the current density is shown on Figure 19. We can observe that due to the slow start of the reaction, activation losses dominate at low current density, and a steep drop off can be noticed at first. The role of the initial voltage is to overcome the activation energy of the reaction. Also, the activation losses depend on the concentration of oxygen, that's why the reaction at the cathode, and the water formation is a slow process.

The concentration voltage is represented on Figure 20. When the current limit occurs, this voltage drops dramatically and the PEMFC stops working. At this time, the concentration of reactants at the electrode is null. When the current drawn from the fuel cell exceeds the current limit, the reactants involved become greater than the reactants supplied.

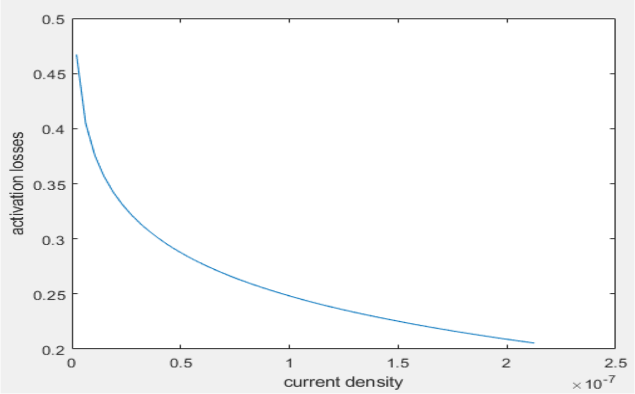

Figure 19. Activation Losses

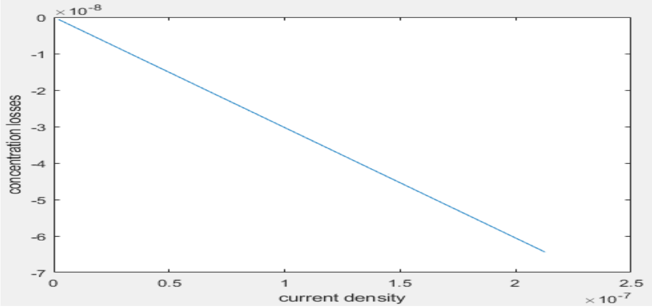

Figure 20. Concentration losses

The steady-state power output of the PEMFC is shown on Figure 21. The maximum output power is reached at the nominal current value. If we want to increase the current beyond this point, we need to lower the output power. This is due to the current limit that begins to occur.

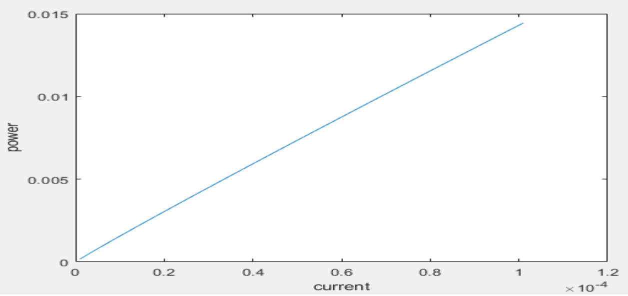

Figure 21. Steady state output power

5. CONCLUSION

In this paper, we have presented a model based on the study of the performance of the proton exchange membrane fuel cell. To obtain the polarization curves which describe the performance of the battery, we established a modeling on the electrochemical model.

In the first part we discussed the generalities on renewable energies and hydrogen, then in the second part, we have developed a presentation of fuel cells, particularly PEMFC type cells and their technological evolution. Later, we have cited the challenges, also an overview of the models that describe the PEMFC.

The third part represents the modeling of a proton exchange membrane fuel cell, performed on Matlab Simulink.

From the results above, under stable conditions, and taking into account fixed input parameters, the maximum output power of the fuel cell is 0.014 W which corresponds to a current of 1 A.

The modeling and the simulation presented in this paper is important in terms of it's ability to expect the fuel cell performance before manufacturing, reducing the risk of failure and defects. This simulation, can be applicable to static systems and can be used with a wide range of fuel cells.

We can extend the study in order to reach a higher efficiency of the PEMFC, by considering in the physical constitution of the latter. Also, and in order to obtain results the most close to the experimental data, it's imoprtant to explore the dynamical behavior of this stack.

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