

## Modeling and Optimization of the Transport Phenomena of Water in a Fuel Cell $H_2 / O_2$

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### Abstract

One way to store electrical energy takes place by electrolysis of alkaline water, hydrogen and oxygen obtained are stored and thereafter be re-used as fuels in internal combustion engines or in fuel cells which are cheaper, safer than the latter. Among these fuel cells, CFLs we find English Alkaline Fuel Cell. The electrolyte of the fuel cell is a potassium hydroxide solution, the chemical reaction that occurs within the fuel cell is the recombination of hydrogen with oxygen to give water, electric energy and heat energy.

One of the major challenges for the proper functioning of the fuel cell is discharging water and heat that can damage the electrolytic solution; therefore, it is essential to master the phenomena of mass transfer of water that operates within the fuel cell, and the optimum temperature of the inlet gas, knowing that fuel cells typically operate in isothermal conditions. This mastery must first go through the modeling of these phenomena then the real-time simulation of the main factors involved ensuring good cell efficacy. This model is articulated around Nernst-Planck equations, the equation of continuity and the two of Fick laws. The resolution of these equations requires a numerical approach of the partial differential equations.

**Keywords:** Water transport; AFC Alkaline Fuel Cell; Hydrogen; Oxygen; Mathematical Model

### Introduction

During the 20<sup>th</sup>, the world has experienced a surprising proliferation of unusual weather events (heat waves, persistent droughts, floods, rising sea level, hurricanes). At that environmental concerns must be added the one that posed by the decline of world reserves of fossil resources. For these reasons, we are witnessing the emergence of cleaner energy technology, and the coming years will be those of the diversification of renewable energy sources. The hydrogen carrier is a realistic solution in terms of alternative energy source, especially for embedded or mobile systems. The fuel cell uses chemical energy of hydrogen and oxygen to generate electricity without pollution. Other products are simply pure water and heat. The system is efficient and clean because it produces no emission of toxic gases [1, 2]. The AFC batteries are the oldest variants of fuel cells. They were developed in the early sixties, and they had a renewed interest with the European space program.

Also A. Khalidi et al., [3] based their study on the implementation of an alkaline with  $H_2$ - $O_2$  immobilized electrolyte which is intended in space applications. After optimizing the flow of hydrogen to the accuracy of the removal of water produced by the overall reaction of the cell, another problem has appeared to them after a long operating time of the cell which is the accumulation of  $OH^-$  ions on the cathode side of the electrolyte.

Jang-Ho Jo and Sung-Chul Yi. [4] presented a mathematical model for a single cell of an alkaline fuel cell AFC. Parameters and operating conditions of the model are based on fuel cells Obiter, which are used as an energy source for space shuttles from NASA. Simulated

result is obtained, which shows good agreement with some experimental data. The profiles of the variables (local density and the overvoltage current) are also obtained based on the cell voltage. A study of the influence of the electrolytes indicates that the initial concentration of the performance of the AFC is maximized at a concentration of 35%.

Ivan Verhaert et al. [5] have also worked on the AFC. They give a thermodynamics model. The alkaline fuel cells are the ones of static low-temperature applications, such as cogeneration in buildings, is a promising market. To ensure a long life for the fuel cell, water and thermal management must be done carefully.

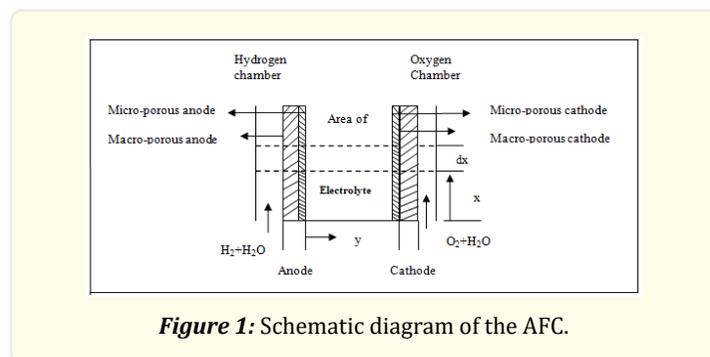
S.Rowshanzamir et al. [6] also conducted a study on the performance of hydrogen-air fuel cells in the fuel cell along with the immobility of the alkaline electrolyte. They developed a one-dimensional mathematical model of partial based on the principles of transport phenomena in the gas phase, for alkaline fuel cell that checks the operating conditions resulting in water balance, and that determines a set of optimum values for the current density, the gas flow rate, the rate of humidity, temperature and pressure to ensure that the cell operate without a water deficit or excess.

Betty Y.S. Lin and al. [7] worked on the alkaline fuel cell (AFC), whose technologies are among the most mature. These fuel cell technologies have been in use since the mid-1960s by NASA in the Apollo program. The process of AFC has been revisited in order to define the characteristics of the current operation of the baseline for the development of future technologies in the AFC that can take advantage of advances in alkaline water electrolyzers. The purpose is to advance a design that connects the actions of many devices in the AFC with AWE (Alkaline Water electrolyzer). According to the Betty et al., [7] work a good performance can be achieved by AFC while temperatures around  $70^\circ\text{C}$ . The model we developed predicts an ideal temperature of  $80^\circ\text{C}$ .

According to previous work, the major problems in a fuel cell  $H_2$ - $O_2$  are the production of water and heat that undermine the proper behavior of the cell. That is why we have developed a one-dimensional transient model for this type of battery, resulting mathematical equations Nernst-Planck Fick and conservation of mass, which will be solved by numerical methods, making varying different criteria such as the current density, the weight percentage of KOH, the temperature of the hydrogen input of the fuel cell, the temperature inside the fuel cell and the specific mass flow of the steam. The simulation model will allow us to choose the optimal solution of the operation of the fuel cell every time.

### Alkaline Fuel Cell AFC

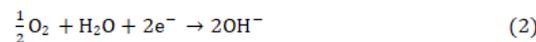
Alkaline fuel cells are developed in the early 60s to power the Apollo spacecraft. They use an electrolyte liquid, usually potassium hydroxide (KOH), which has the advantage of accelerating the reduction of oxygen. However, they work properly only when the use of pure hydrogen and oxygen. Indeed, when using air or reformed hydrogen, carbon dioxide content in the latter reacts with the KOH electrolyte and form the potassium carbonate, which reduces the mobility of ions [4].



**Figure 1:** Schematic diagram of the AFC.

This fuel cell has the advantage of using a variety of catalysts and presents the best performance of all fuel cells. The catalysts are usually a combination of nickel and a metal such as aluminum inactive to reduce the overall manufacturing cost of this technology. For the bipolar plates, metallic magnesium or graphite compounds is used [8]. The pattern of the electrodes is given in (Figure 1) for a fuel cell H<sub>2</sub>-O<sub>2</sub>, the electrolyte is an aqueous potassium hydroxide solution. The electrodes consist of macro-pores and micro-pores between the gas chambers (chamber hydrogen and oxygen chamber) of the electrolyte.

Each electrode consists of two parts: a gas filled macro-porous and micro-porous another, supposed very thin, and filled with the electrolytic solution. The electrochemical reactions take place in the micro-porous area. To represent the electrodes, the single pore model is used. This model assumes that the electrode is formed of a number of uniform and parallel cylindrical pores. The reactions taking place at the anode and cathode.



The overall reaction is:



## Development of the Mathematical Model

### Region of the Electrode

#### Law of FICK

For alkaline fuel cell one mole of water is formed at the anode for each mole of hydrogen consumed by the reaction. Steady-state mass transfer is defined as a process of equimolar diffusion against the current. For a binary gas mixture at low pressure and at constant temperature, the diffusion through the electrode is substantially independent of the composition of the mixture. Considering the constant molar concentration of the mixture through the thickness of the macro-pore region of the anode in the steady state, the mass of water vapor is carried by the given corrected Fick law, the correction factor being the porosity  $\epsilon$  electrode [9].

$$m_{\text{H}_2\text{O}} = \frac{\epsilon D_{\text{H}_2\text{O}-\text{H}_2} M_2 (P_K - P_V)}{tg RT} \quad (4)$$

#### Region of Electrolyte.

The model of the electrolytic solution. The cell is considered isolated at both ends in the x direction and at both ends in the y direction. The temperature inside the cell is maintained constant by a control system, so the fuel cell operates isothermally.

#### Nernst -Planck equation

The flow of "i" species flow, subjected to a gradient of concentration and potential can be written; [10]

$$J_i = -D_i \nabla c_i - c_i \mu_i \nabla \Phi + c_i v \quad (5)$$

This formula is valid for an isothermal system consisting of "n" neutral or ionized species.

From the equation above, it is easy to obtain the NERNST-PLANK formula- applying to a K<sup>+</sup> and OH<sup>-</sup> ions binary system [11].

$$J^+ = -D^+ \nabla C^+ - C^+ \frac{FD^+}{RT} \nabla \Phi + VC^+ \quad (6)$$

$$J^- = -D^- \nabla C^- + C^- \frac{FD^-}{RT} \nabla \Phi + VC^- \quad (7)$$

Knowing that the current density “i” is expressed by:

$$i = F(J^+ - J^-) \quad (8)$$

The electro-neutrality condition of one mole KOH frees one mole of  $OH^-$  and one mole of  $K^+$

$$[KOH] = [OH^-] = [K^+] = C^- = C^+ = C_1$$

$$\frac{i}{F} = C_{ste} \Rightarrow \operatorname{div} \frac{i}{F} = 0$$

$$J^+ = (1 - t) \frac{i}{F} - D \nabla C_1 + VC_1 \quad (9)$$

$$J^- = -t \frac{i}{F} - D \nabla C_1 + VC_1 \quad (10)$$

Index 1 denotes the solute KOH.

$$D = \frac{2D^+D^-}{D^+ + D^-}, \quad t = \frac{D^-}{D^- + D^+} \quad (11)$$

### Matter Outcome on Solute KOH

The equation of continuity applied to solute transient can be written as; [12]

$$\frac{\partial c_1}{\partial t} = (-\nabla J_1 + \delta i) \quad (12)$$

With  $\delta i$ : speed of the electrochemical reaction.

And  $\delta i = 0$  because the reaction produces as much as it consumes  $OH^-$  ions.

Then combining it with a molar flow of equations on the solute is obtained:

$$\frac{\partial C_1}{\partial t} = D \nabla^2 C_1 - \nabla VC_1 \quad (13)$$

Where as in a concentration gradient along an axis perpendicular to the surface of the electrode in the y direction, and then passing to the mass concentration can be written

$$\frac{\partial \rho_1}{\partial t} = \frac{\partial^2 \rho_1}{\partial y^2} - \frac{\partial (V \rho_1)}{\partial y} \quad (14)$$

The passage of two moles of electrons through the cell uses two moles of  $OH^-$  ions and two moles of water to the anode against the cathode produces two moles of  $OH^-$  and consumes one mole of water. If i amperes per unit electrode surface flow in the cell, the average

flow of volume related to this unit area of anode and cathode are expressed as follows:

$$V_a = \left(2r - \frac{m_{2a}}{M_2}\right) v_{2a} - 2rv_{-,a} \quad (15)$$

$$V_c = \left(r + \frac{m_{2c}}{M_2}\right) v_{2a} - 2rv_{-,c} \quad (16)$$

$r = \frac{i}{2F}$ : Number of moles of water produced per unit of time and area.

$m_{2a}$ ,  $m_{2c}$ : mass of water evaporated at the anode and at the cathode per unit of time and area.  $v_{2a}$ ,  $v_{2c}$ : partial molar water respectively to the anode and cathode volume.  $v_{-,a}$ ,  $v_{-,c}$ : partial molar OH<sup>-</sup> ions respectively to the volumes to the cathode and anode.  $M_2$ : molecular weight of water.

A difference between  $V_a$  and  $V_c$  leads to an increase in the volume of electrolyte solution equal to:

$$\rho_1[V_a - V_c] = \rho_1\Delta v \quad (17)$$

This increase is according to the y-axis. In introducing in equation (14), we can write:

$$\frac{\partial \rho_1}{\partial t} = D \frac{\partial^2 \rho_1}{\partial y^2} - V \frac{\partial(\rho_1)}{\partial y} \quad (18)$$

### Equation of the distribution of the water density

By solving the equation (18), we must ensure that in the calculations, the following relation is always verified.

To 1 mole of KOH- H<sub>2</sub>O solution:

$$\rho_1 \frac{v_1}{M_1} + \rho_2 \frac{v_2}{M_2} = 1 \quad (19)$$

### Boundary conditions

They are the following:

At the anode

$$D \frac{\partial \rho_1}{\partial y} = 2rM_1(1 - t) + \rho_1 V_a \quad (20)$$

At the cathode

$$D \frac{\partial \rho_1}{\partial y} = 2rM_1(1 - t) + \rho_1 V_c \quad (21)$$

To solve numerically [13, 14] the equation of diffusion-convection:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial y^2} - V \frac{\partial \rho}{\partial y} \quad (22)$$

## Calculation of Parameters

### Diffusion Coefficient

For the calculation of the diffusion coefficients in electrolytic solutions, there are formulations established in the case of diluted solutions. To extend the use of these formulas in concentrated solutions are introduced into these equations simple methods of empirical correction. We propose a simple formula of correction for the effect of temperature:

### Case of liquids

The diffusion coefficient is given by the Wilke, Chang and Tyn Calus formula [15]:

$$\frac{D_{AB} \mu}{T} = \frac{D_{AB}^0 \mu_0}{T^0} = \text{Cste} \quad (23)$$

$$D_{AB} = D_{AB}^0 \frac{T}{334 \mu} \quad (24)$$

Along With:

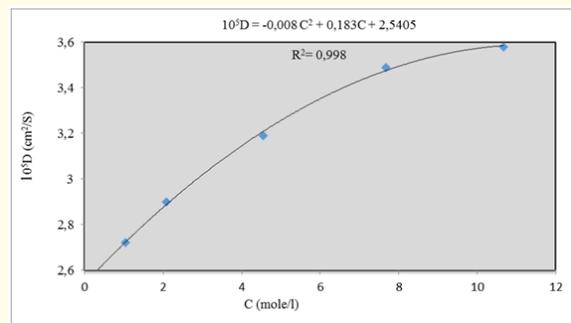
$D_{AB}$ : the diffusion coefficient of the solute in the solution at the temperature T.

$D_{AB}^0$ : the diffusion coefficient at 25 °C.

T: absolute temperature.

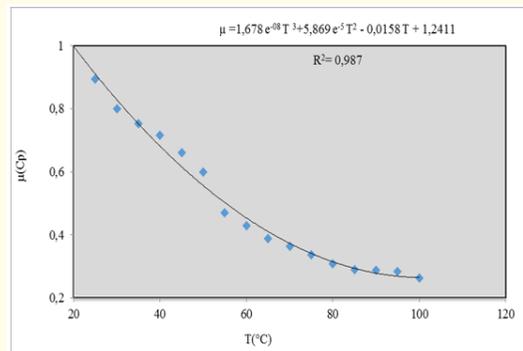
$\mu$ : viscosity of the solvent in centipoises.

Wearing the diffusion coefficient D as a function of the concentration C, we obtain a polynomial form of relationship between D to C (Figure 2).



**Figure 2:** Change KOH diffusion coefficient in a potassium hydroxide solution at 25°C.

We proceed in the same way, using the data in Table to establish a relationship between the viscosity of the water and the temperature (Figure 3).



**Figure 3:** Variation of the viscosity of water as a function of temperature.

### Case of gas

In the gas phase, there are quite complex relationships giving diffusivity. In practice, it often happens that we know the diffusion coefficient of a gas at a temperature  $T_1$  and pressure  $P_1$  data. To have the same diffusion coefficient at a temperature  $T_2$  and at a desired pressure  $P_2$ , we can use the following equation:

$$\frac{D_1}{D_2} = \left( \frac{T_1}{T_2} \right)^{1.5} \frac{P_2}{P_1} \quad (25)$$

$D_1$  is the diffusion coefficient of the gas at the temperature  $T_1$  and the pressure  $P_1$ ,  $D_2$  than the same gas at temperature  $T_2$  and pressure  $P_2$ .

In the case of binary mixtures of hydrogen-steam and oxygen- steam Gililand [9] gives the relationship as:

$$D_{H_2}^{H_2O} = \frac{0,0043 T^{1.5} \sqrt{\frac{1}{M_{H_2}} + \frac{1}{M_{H_2O}}}}{P \left[ \left( \frac{1}{V_{H_2}} \right)^{0.33} + \left( \frac{1}{V_{H_2O}} \right)^{0.33} \right]^2} = 1,21 \text{ cm}^2/\text{s} \quad (26)$$

$$D_{O_2}^{H_2O} = \frac{0,0043 T^{1.5} \sqrt{\frac{1}{M_{O_2}} + \frac{1}{M_{H_2O}}}}{P \left[ \left( \frac{1}{V_{O_2}} \right)^{0.33} + \left( \frac{1}{V_{H_2O}} \right)^{0.33} \right]^2} = 0,351 \text{ cm}^2/\text{s} \quad (27)$$

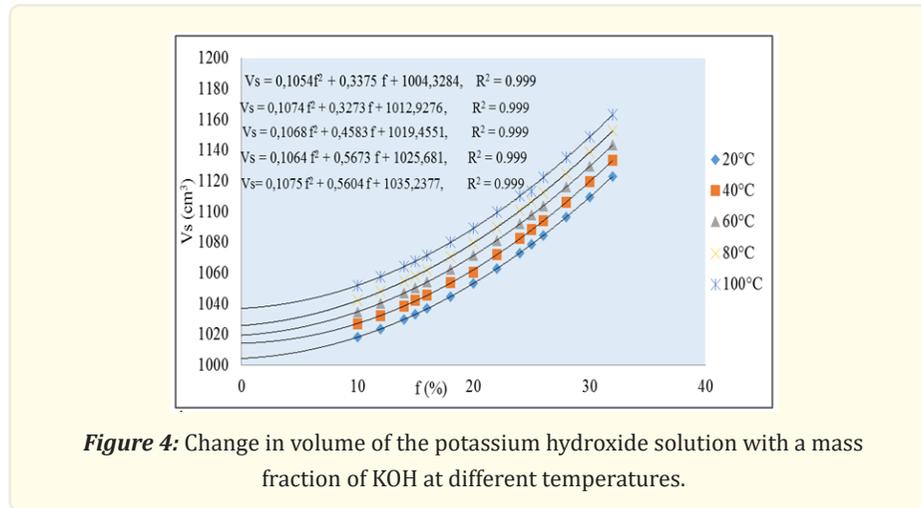
### Volume of the Electrolytic Solution

The mass fraction  $f$  of KOH electrolyte is expressed by taking a mass of 1000 g water.

$$V_s = \frac{1000 f}{\rho_s(1 - f)} \quad (28)$$

This last equation shows that  $V_s$  depends on the mass fraction of KOH and the density of the solution that it is a function of temperature and composition.

Figure 4 gives the values of the density of the potassium hydroxide solution at different values of temperatures and composition.



**Figure 4:** Change in volume of the potassium hydroxide solution with a mass fraction of KOH at different temperatures.

Figure 4. Change in volume of the potassium hydroxide solution with a mass fraction of KOH at different temperatures.

These correlations are of the form:

$$V_s = V_0 + V_1 f + V_2 f^2 \quad (29)$$

For the volume of the solution to a temperature and composition data is plotted the coefficients  $V_0$ ,  $V_1$  and  $V_2$  according to the temperatures and the corresponding correlations are given.

The volume of the potassium hydroxide solution will be in the form:

$$V_s = V_0(T) + V_1(T)f + V_2(T) f^2 \quad (30)$$

$V_0(T)$ ,  $V_1(T)$  and  $V_2(T)$  are a function of temperature only.

From the graphs drawn the relationship between the coefficients  $V_0$ ,  $V_1$ ,  $V_2$  and temperature are given in the following equations:

$$V_0 = 0,3729 T + 997,1544 \quad R^2 = 0,999 \quad (31)$$

$$V_1 = 0,0034 T + 0,2444 \quad R^2 = 0,908 \quad (32)$$

$$V_2 = 1,6 \cdot 10^{-5} T + 0,105 \quad R^2 = 0,45 \quad (33)$$

The volume of an aqueous solution containing  $n_1$  moles of solute and 1000g of water can be expressed by:

$$V_s = 55.55 V_2 + n_1 V_1 \quad (34)$$

$V_1$  and  $V_2$  represent the partial molar volumes of the solute and water

Where:

$$n_1 = \frac{m_1}{M_1} \quad (35)$$

Where :  $M_1$  is the molar mass of the solute, relations (28) and (35) allow us to write:

$$n_1 = \frac{1000 f}{M_1(1-f)} \quad (36)$$

$$f = \frac{n_1}{n_1 + \frac{1000}{M_1}} \quad (37)$$

### Partial molar volume of OH<sup>-</sup> ions

To calculate the partial molar volume of the OH<sup>-</sup> ions in aqueous potassium hydroxide solution, it is assumed that:

$$V_1 = V_{K^+} + V_{OH^-} \quad (39)$$

Where  $V_{K^+}$  and  $V_{OH^-}$  designate the molar volumes of K<sup>+</sup> and OH<sup>-</sup> ions in solution and that the partial molar volumes of the ionic species vary in the same way with the temperature and concentration.

Knowing that at the temperature of 298.1 K we have:

$$V_{K^+} = 8.0 \frac{\text{cm}^3}{\text{mol}} \quad (40)$$

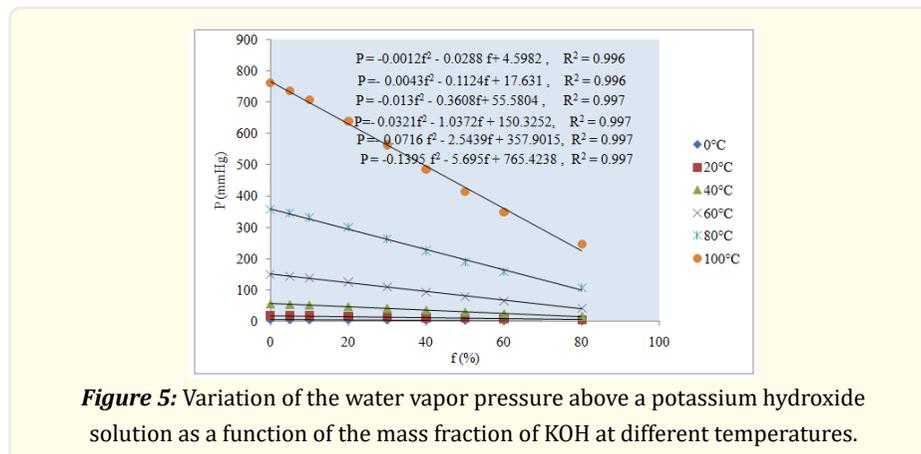
$$V_{OH^-} = 1.4 \text{ cm}^3/\text{mol} \quad (41)$$

$$\text{Alors } \frac{V_{K^+}}{V_{OH^-}} = 5.714 \quad (42)$$

The relations (39) and (42) give:

$$V_{OH^-} = 0,1406 V_1 \quad (43)$$

By converting the concentrations of weight percentage, the pressure is plotted as a function of the percentage for different temperatures (Figure 5). We get the following type of relationships: Where P is the water vapor pressure above the potassium and  $P_0$ ,  $P_1$  and  $P_2$  are constants. The same condition was done in the case of volumes; we carry  $P_0$ ,  $P_1$  and  $P_2$  according to the temperatures.



**Figure 5:** Variation of the water vapor pressure above a potassium hydroxide solution as a function of the mass fraction of KOH at different temperatures.

From the graphs drawn the relationship between the coefficients  $P_0$ ,  $P_1$  and  $P_2$  and temperature gives the following equations:

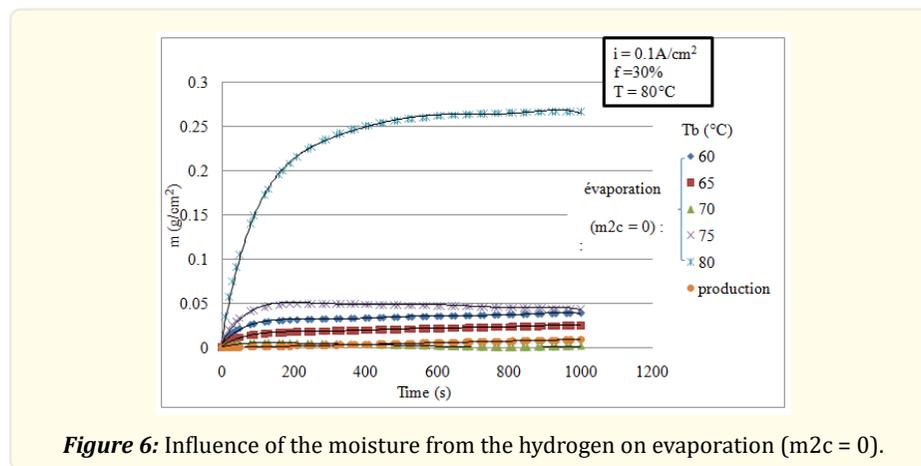
$$P_0 = 0,0012 T^3 - 0,0628 T^2 + 1,8104 T + 2,653 \quad R^2 = 0,999 \quad (44)$$

$$P_1 = -9,96 \cdot 10^{-6} T^3 + 5,846 \cdot 10^{-4} T^2 - 0,0155 T - 0,0102 \quad R^2 = 0,999 \quad (45)$$

$$P_2 = -1,667 \cdot 10^{-7} T^3 + 5,036 \cdot 10^{-6} T^2 - 2,205 \cdot 10^{-4} T - 0,0011 \quad R^2 = 0,999 \quad (46)$$

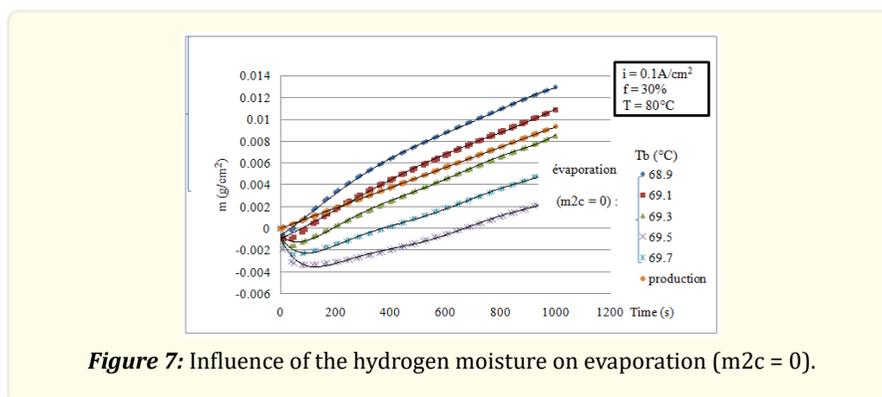
## Results and Discussion

The resolution of the balance equation (22) allows us to draw a number of curves that we present on Figures.6 to 7 In these figures, we will try to find the optimum conditions for operation of the cell such as, the current density ( $i$ ), the mass percentage of KOH in the potassium hydroxide solution ( $f$ ), the temperature of the hydrogen at the entrance of the cell ( $T_b$ ), the temperature inside the cell ( $T$ ) and the specific mass flow of water vapor through the cathode ( $m_{2c}$ ). But for now temperature of the fuel cell has set, which most authors have adopted, is that of 80°C. Then in a second time to refine our research we draw the first curve that covers a wide field of hydrogen inlet temperature in the cell.



**Figure 6:** Influence of the moisture from the hydrogen on evaporation ( $m_{2c} = 0$ ).

Figure 6 shows the evolution of the production and evaporation of water (through the anode) over time for different temperatures of hydrogen values to the input of the cell from 60 to 80°C. Curve generation and evaporation coinciding in the best way is that of the neighboring temperature  $T_b$  of 70°C consequently in the rest of our simulation we adopt this temperature and its immediate vicinity.

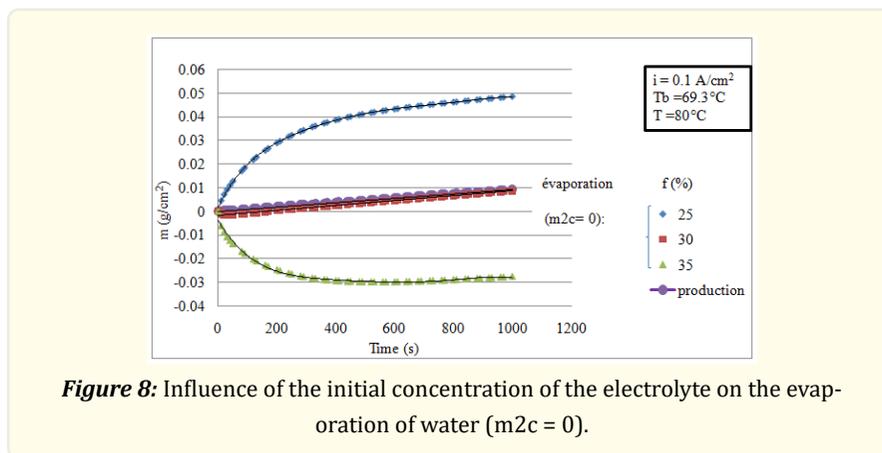


**Figure 7:** Influence of the hydrogen moisture on evaporation ( $m_{2c} = 0$ ).

From Figure 7 to Figure 10 we consider that there is no water vapor that passes through the cathode. Figure 7 shows the evolution of the production and evaporation of the water curve (through the anode) over time for different temperatures of hydrogen values to the input of the fuel cell. We may distinguish three cases: If the water production curve is above the evaporation curve, two possible cases may arise:

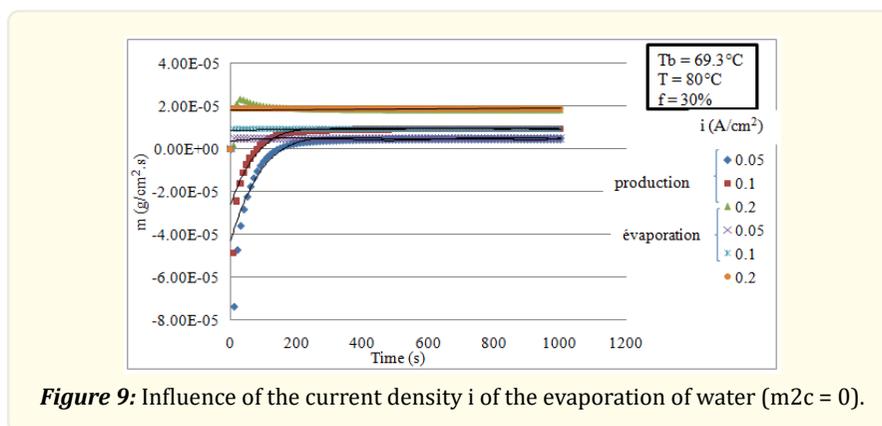
- The value of the amount of evaporated water is negative; in this case the water is transferred from the hydrogen to the cell.
- The value of the amount of evaporated water is positive: in this case the water produced is not completely evaporated.

In both cases, there will be dilution of the electrolytic solution. If the water production curve lies below the evaporation curve, then it means that the water leaves the cell with greater quantity than that which is produced by the electrochemical reaction and there is therefore consequently increasing the concentration of the potassium hydroxide solution. If the curve of production and evaporation overlap, then the amount of water produced is equal to the amount of water evaporated. Finally, notice that the best operation is obtained for a temperature of the hydrogen gas of 69.3°C.



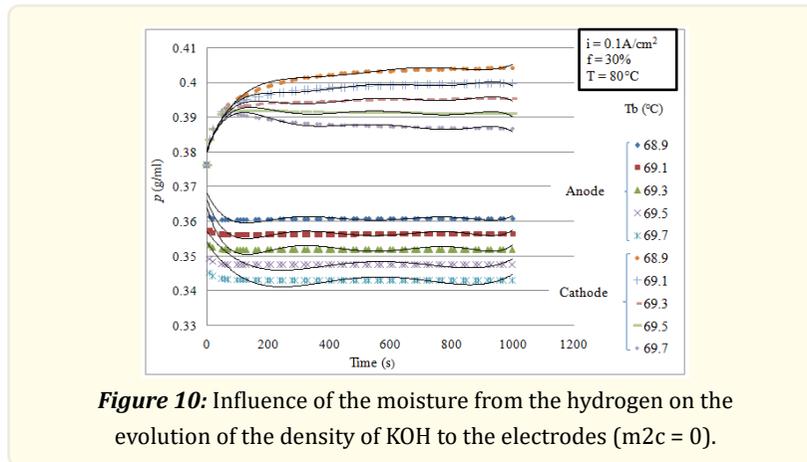
**Figure 8:** Influence of the initial concentration of the electrolyte on the evaporation of water ( $m_{2c} = 0$ ).

Figure 8 shows the influence of the initial concentration of the potassium hydroxide to the quantity of water produced and evaporated. It is noted that the optimum operation is given to a KOH mass percentage of 30%. For percentages below this value water diffuses into hydrogen and otherwise water will accumulate in the cell. This is due to the fact that the vapor pressure of water in the potassium hydroxide solution varies inversely with the concentration of KOH.



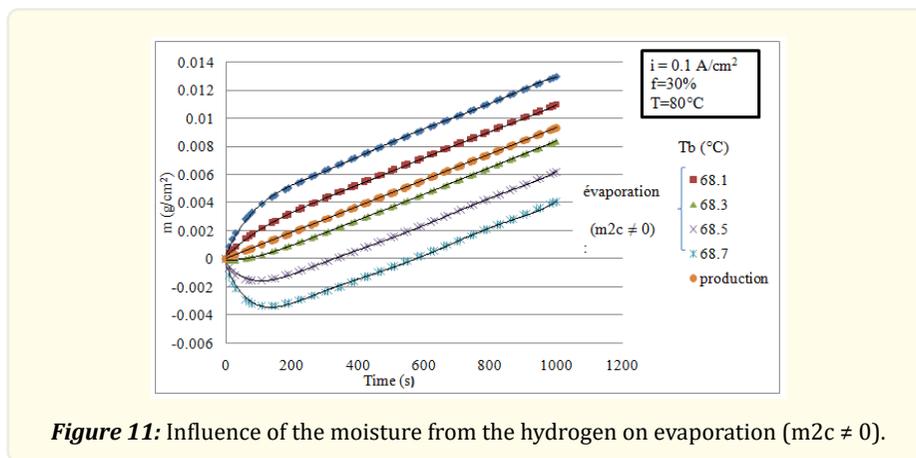
**Figure 9:** Influence of the current density  $i$  of the evaporation of water ( $m_{2c} = 0$ ).

Figure 9 shows the specific mass flow of the produced water and evaporated water over time for different current density values. In working conditions imposed, it is preferable to operate at  $0.1A / cm^2$  because the current density value introduces a transitional regime of relatively short duration during which the flow of water evaporated substantially varies as during the first's moments. In general we find that the charging current density does not influence much on the performance of the fuel cell.



**Figure 10:** Influence of the moisture from the hydrogen on the evolution of the density of KOH to the electrodes ( $m_{2c} = 0$ ).

Figure 10 shows the influence of the production and evaporation of the water on the density of KOH to the electrodes as a function of time for different values of temperatures of the hydrogen at the entrance of the fuel cell, we will be interested to the electrodes, because it is at this level where the electrochemical reactions take place. Thus the density of KOH to the electrodes is plotted as a function of time for different values of the temperature of the hydrogen to the inlet of the fuel cell. For a fixed gas temperature, KOH density decreases at the anode due to partial evaporation of the water produced and increases at the cathode as the water is consumed there. Increasing the temperature of the gas, the density drops because of the reduction of the diffusion phenomenon of the water vapor in the hydrogen.



**Figure 11:** Influence of the moisture from the hydrogen on evaporation ( $m_{2c} \neq 0$ ).

In Figures 11 to 14, it is considered that there is the water vapor which passes through the cathode. Figure 11 shows the evolution of the production and evaporation of the water curve (through the anode and the cathode) over time for different hydrogen temperature values at the entry of the fuel cell. Curve of production and evaporation are superimposed, hence the amount of water produced is equal to the amount of water evaporated. Finally, it will be noted that the best operation is obtained by a temperature of the hydrogen gas of  $68.3^\circ C$ .

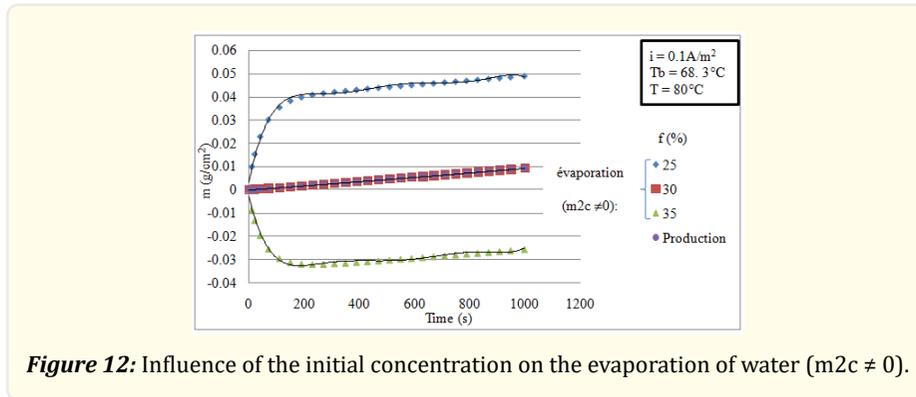


Figure 12: Influence of the initial concentration on the evaporation of water ( $m_{2c} \neq 0$ ).

Figure 12 shows the influence of the initial concentration of the potassium hydroxide to the quantity of water produced and evaporated. It is noted that the optimum operation is given to a KOH mass percentage of 30%. For percentages below this value was water which diffuses into hydrogen and otherwise water will accumulate in the cell. This is due to the fact that the vapor pressure of water in the potassium hydroxide solution varies inversely with the concentration of KOH.

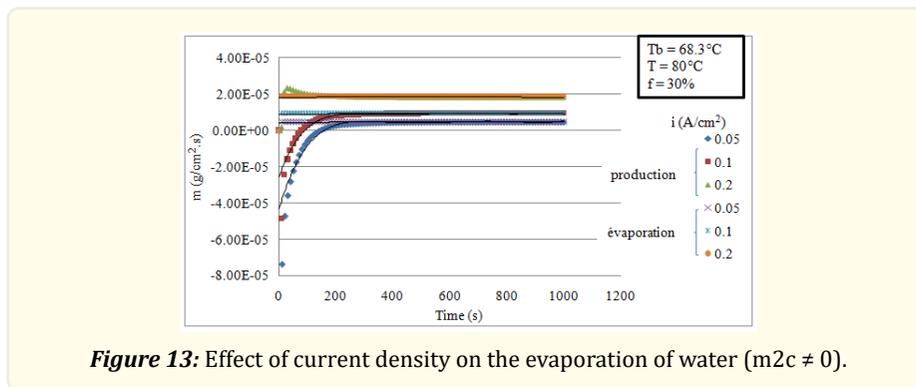


Figure 13: Effect of current density on the evaporation of water ( $m_{2c} \neq 0$ ).

In Figure 13 is shown the specific mass flow of the produced water and evaporated over time for different current density values. In working conditions imposed, it is preferable to operate at 0.1 A / cm<sup>2</sup> because the current density value introduces a transitional regime of relatively short duration during which the flow of water evaporated does not vary significantly only during the first moments.

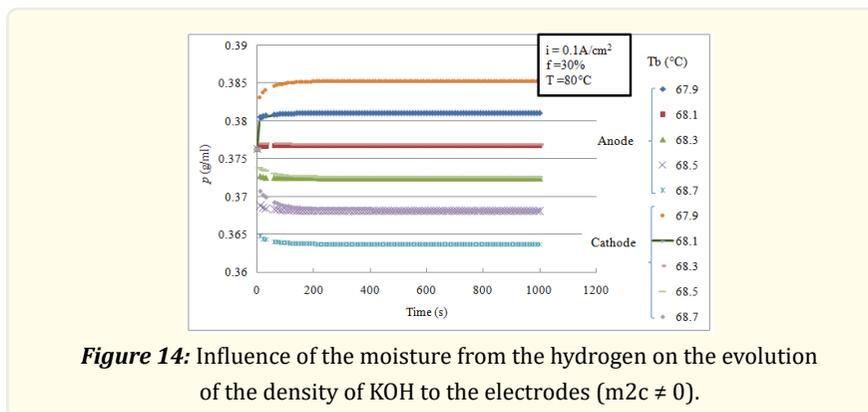


Figure 14: Influence of the moisture from the hydrogen on the evolution of the density of KOH to the electrodes ( $m_{2c} \neq 0$ ).

Figure 14 shows the influence of the production and evaporation of the water on the density of KOH to the electrodes as a function of time for different values of temperatures of the hydrogen at the entrance of the fuel cell, the curves of the current density of the anode and cathode superimposed. In fact, in this case, the water vapor pressure in the hydrogen and oxygen are initially equal. During operation of the fuel cell the consumption of water at the cathode causes a diffusion of water vapor from the oxygen chamber to the interior of the cell, while at the anode the water vapor diffuses to the hydrogen chamber.

## Conclusion

In the work that has been presented, we have developed a model that reflects the water transport phenomenon in a fuel cell. The proposed model combines the general laws of electrochemistry and mass transfer. For its development the following hypotheses were issued: unidimensional problem, using the model of single pore (uniform parallel pores and cylindrical), use of an amount of hydrogen in excess of what is consumed by the electrochemical reaction rate large enough to consider gas constant moisture between the input and the output, isothermal regime, linear speed profile, constant concentration of gas mixture through the electrodes, constant volume between the electrodes.

To solve the problem describing the model, we have established, with the help of correlations giving some parameters (diffusion coefficient, water vapor pressure in the potassium hydroxide solution and volume electrolyte solution) involved in the calculation.

The equation of the model is a nonlinear differential equation of second order; we opted for a digital resolution, after discretization of the problem based on the finite differences method.

After resolving the equation, we have drawn a number of graphs by varying several parameters (current density, moisture and gas initial concentration of potassium) to see their influence on the amount of water produced and evaporated in the cell. This study allowed us to define the optimal values of these parameters are the cell temperature  $T = 80^\circ\text{C}$ , hydrogen at the entrance  $T_b = 69.3^\circ\text{C}$ , KOH mass fraction  $f = 30\%$  and current density  $i = 0.1 \text{ A/cm}^2$ .

## Perspectives

In the immediate future, it would be interesting to create build an experimental device to test the degree of compatibility of this model with experience.

The major problem mounting this device will identify the materials of each element of the fuel cell which is a simple thing as the industrial secrecy surrounding the manufacture of such technology.

Then the optimal parameters that we are able to find through simulation should be checked such as hydrogen temperature at the entrance to the cell, the mass fraction of the KOH solution, the current density, temperature of the cell and the humidity of the hydrogen are actually transposable to experience.

However, there is one final aspect that could not explain of an AFC and more precisely at the electrodes or there is a dry area surrounding the hydrogen entry point that diminish over time and alters the function of the fuel cell by letting leakage of KOH gas. We believe this is due to the assumption that shows that the gas flow is large enough to be considered it moisture constant between the input and the output of the hydrogen. It encourages us to think complete the model of the electrolyte solution by a second bi-dimensional model of the hydrogen compartment because it is clear that there is pressure drop between the inlet and the outlet of the gas compartment and therefore the partial pressure of water vapor as well. But this will be mentioned in our following research.

## Nomenclature

$C_i$	Concentration of the species "i" (mole/ $\text{m}^3$ )
$D_{H_2O-H_2}$	Steam-hydrogen diffusion coefficient ( $\text{m}^2/\text{s}$ )

$D_i$	diffusion coefficient of the species "i" ( $m^2/s$ )
$D$	average diffusion coefficient ( $m^2/s$ )
$F$	Faraday constant (96500 c/mole)
$i$	current density ( $A/m^2$ )
$I$	Intensity (A)
$J_i$	molar flow of the species "i" (mole/ $m^2s$ )
$m_{H_2O}$	water mass flow evaporated through the electrode ( $Kg/m^2s$ )
$M_i$	molar mass of the species "i" (kg/mole)
$P^{\text{"V"}}$	Partial pressure of water vapor in the gas chamber (Pa)
$P^{\text{"K"}}$	partial pressure of water in the aqueous KOH solution (Pa)
$P_e$	Total pressure at the entrance (Pa)
$P_s$	Total pressure at the exit (Pa)
$R$	Constant of ideal gases (8,314 j /mole. K)
$T$	Temperature of the battery (K)
$tg$	Electrode Thickness (m)
$t$	Time (s)
$t^-$	transport number of $OH^-$ ion
$V$	Speed (m/s)
$V_a, V_c$	volume flow ( $m^3/m^2.s$ )
$f$	Mass fraction (%)
$m_i$	Mass of the species "i" (kg)
$V_s$	Volume of the electrolyte solution ( $m^3$ )
$v_i$	partial molar volumes of the species "i" ( $m^3/mole$ )
$n$	Number of moles (mole)
$r$	water production rate
$x$	Variable Position
$y$	Variable Position
1	KOH solute
2	$H_2O$ solvent
+	$K^+$ ions
-	$OH^-$ ions
$C_i$	Concentration of the species "i"
$D_{H_2O-H_2}$	Steam-hydrogen diffusion coefficient

### Greek letters

$\varepsilon$	Porosity of the electrode
$\mu$	electrochemical Mobility of species "i" ( $m^2/V.s$ )
$\Phi$	Electric potential (Volt)
$\rho$	Density of the gas mixture ( $kg/m^3$ )
$\rho_i$	Density of the species "i" ( $kg/m^3$ )
$\lambda$	Water content of the membrane

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