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# Effect of fuel thermo physic parameters on electrical and energetic performances of fuel cell

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**ABSTRACT**

For the operation of a fuel cell, pure hydrogen gives the best results in terms of performance . But the choice of fuel does depend only on the fuel; there are other factors to be considered. In addition to the availability for the user through a distribution network, it is necessary to take into account the flow of energy from wells to the wheel and the technical problems of production, transport and storage of this fuel. Storing hydrogen on vehicle board is essentially limited by the volume and the weight assigned to the tank. Add to this, practical aspects of use and safety. This work gives a comparison of the thermodynamic properties of hydrogen pile and with alcohols fuels (methanol, ethanol) directly in a temperature range varying from 298.15 to 1273.15 K and a pressure varying from 1 to 10 atm and a molar concentration of oxygen ranging from 0.21 to 1.

***Nomenclature***

**m** : The number of carbon in alcohol; **m=1** For methanol **m=2** for ethanol ; $\Delta C_{P1}$ , $\Delta C_{P2}$ et $\Delta C_{P3}$: Specific heats; **R =8,315 J/mol.K**; The perfect gas constant. ; $P_i$ : The Partial Pressure; $\Delta H_r$ : Is the enthalpy of the reaction; $\Delta S_r$ : Is the entropy of the reaction; $L_v$(water) : Latent heat of water vaporization; $L_v$(Alcohol) : Latent heat of vaporization of alcohol; **Teb(a)** : The boiling temperature of the alcohol ; **n** : The number of electrons exchanged: **n=2** for hydrogen ; **n=6** for methanol (m=1) ; **n=12** for ethanol (m=2) ; **F** : faraday's constant ; P : The operating pressure of the FC

## 1. Introduction

The energy crisis and rising levels of pollution are major problems in the worldwide. New, renewable and clean sources of energy must therefore be considered. The fuel cell (FC) occupies a very important place in this field [1].

A fuel cell is a device that converts released chemical energy into a reaction directly into electrical energy [2]. It is composed of two electrodes (anode and cathode) separated by an electrolyte layer which allows the transfer of ions between the electrodes to loop the electrical circuit. Intensive research has been carried out on the electro-oxidation of methanol and ethanol at standard temperature; But very few studies have been interested in this phenomenon at higher temperatures [3].

In this work we tried to compare some thermodynamic and electric properties of fuel cells (FC) fed with hydrogen, methanol or ethanol; these properties are electromotive force (EMF), efficiency and energy density, the design and operating principles. The models of FC are explained in this article as well as the results of the simulations obtained by (Matlab v 7.5).

## 2. The Global Reaction taking place in a FC

The equations explaining the principle of the production of electricity from a chemical reaction:

*2.1. The Global Reaction taking place in a Hydrogen Cell*

On the anode side, hydrogen is decomposed into proton and electron [4].

$$\boldsymbol{H_2 \rightarrow 2H^+ + 2e^-} \qquad \textbf{(1)}$$

On the cathode side, the protons recombine with electrons and are oxidized to give water [5].

$$\boldsymbol{\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O} \qquad \textbf{(2)}$$

The overall chemical reaction takes the following form:

$$\boldsymbol{H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O}(\mathrm{l}) \qquad \textbf{(3)}$$

*2.2. The Global Reaction taking place in an Alcohol Stack*

The overall reaction in a fuel cell fed with an alcohol stack at standard temperature is given by the following reaction [6]:

$$\boldsymbol{C_mH_{2m+1}OH + (2m-1)H_2O \rightarrow 6mH^+ + 6me^- + mCO_2} \qquad \textbf{(4)}$$

$$\boldsymbol{\frac{3}{2}mO_2 + 6mH^+ + 6ne^- \rightarrow (3m)H_2O} \qquad \textbf{(5)}$$

$$\boldsymbol{C_mH_{2m+1}OH + \frac{3}{2}mO_2 \rightarrow mCO_2 + (3m)H_2O} \qquad \textbf{(6)}$$

## 3. Calculate the energy of Gibbs

Some thermodynamic and electrical properties of a chemical reaction:

The Gibb's energy corresponding to this reaction can be calculated using the following formula:

$$\boldsymbol{\Delta G_r = \Delta H_r - T\Delta S_r} \qquad \textbf{(7)}$$

The reaction enthalpy and entropy as a function of temperature are calculated using the Kirchhoff and Hess relations [7] .

Assumptions have been made:

- The oxidation reaction of the alcohol is complete.
- At standard temperature, alcohol and water are in the liquid state.
- The field of study varies from 298.15 to 1273.15 K.

3.1. Hydrogen cell

In the case of hydrogen, the temperature range will have two domains separated by the boiling temperature of the water.

$$\boldsymbol{\Delta H_r = \Delta H^0_{298} + \int_{298}^{373} \Delta C_{P1} dT - L_v(\textbf{eau}) + \int_{373}^{1273} \Delta C_{P2} dT} \qquad \textbf{(8)}$$

$$\boldsymbol{\Delta S_r = \Delta S^0_{298} + \int_{298}^{373} \frac{\Delta C_{P1}}{T} dT - \frac{L_v(\textbf{eau})}{373} + \int_{373}^{1273} \frac{\Delta C_{P2}}{T} dT} \qquad \textbf{(9)}$$

$$\boldsymbol{\Delta C_{P1} = C_p(H_2O, l) - C_p(H_2, g) - \frac{1}{2} C_p(O_2, g)} \qquad \textbf{(10)}$$

$$\boldsymbol{\Delta C_{P2} = C_p(H_2O, g) - C_p(H_2, g) - \frac{1}{2} C_p(O_2, g)} \qquad \textbf{(11)}$$

*3.2 Alcohol cell*

$$\boldsymbol{\Delta H_r = \Delta H^0_{298} + \int_{298}^{Teb(a)} \Delta C_{P1} dT + L_v(\textbf{alcool}) + \int_{Teb(a)}^{373} \Delta C_{P2} dT - L_v(\textbf{eau}) + \int_{373}^{1273} \Delta C_{P3} dT} \qquad \textbf{(12)}$$

$$\boldsymbol{\Delta S_r = \Delta S^0_{298} + \int_{298}^{Teb(a)} \frac{\Delta C_{P1}}{T} dT + \frac{L_v(\textbf{alcool})}{Teb(a)} + \int_{Teb(a)}^{373} \frac{\Delta C_{P2}}{T} dT - \frac{L_v(\textbf{eau})}{373} + \int_{373}^{1273} \frac{\Delta C_{P3}}{T} dT} \qquad \textbf{(13)}$$

$$\boldsymbol{\Delta C_{P1} = 3mC_p(H_2O, l) + mC_p(CO_2, g) - \frac{3}{2} mC_p(O_2, g) - C_p(C_mH_{2m+1}OH, l)} \qquad \textbf{(14)}$$

$$\boldsymbol{\Delta C_{P2} = 3mC_p(H_2O, l) + mC_p(CO_2, g) - \frac{3}{2} mC_p(O_2, g) - C_p(C_mH_{2m+1}OH, g)} \qquad \textbf{(15)}$$

$$\boldsymbol{\Delta C_{P3} = 3mC_p(H_2O, g) + mC_p(CO_2, g) - \frac{3}{2} mC_p(O_2, g) - C_p(C_mH_{2m+1}OH, g)} \qquad \textbf{(16)}$$

## 4. Calculation of the fuel cell electromotive force

The standard electromotive force provided by the stack is given by the following formula:

$$E = \Delta G_r / nF \qquad \textbf{(17)}$$

## 5. Calculation of the theoretical fuel cell reversible efficiency

The theoretical reversible yield [8] is given by the following equation:

$$\eta_r = \Delta G_r / \Delta H_r \qquad \textbf{(18)}$$

## 6. The influence of pressure on the electromotive force

The Gibbs free energy variations depend not only on the temperature but also on the gases pressure through Nernst's law [9]:

$$\Delta G = \Delta G^0 - RT\ln\left(P_{H_2} P_{O_2}^{\frac{1}{2}} \Big/ P_{H_2O}\right) \quad \text{J/mol} \qquad \textbf{(19)}$$

We thus obtain for the vacuum tension the expression of the Nernst's law:

$$E = E^0 + \frac{RT}{nF}\ln\left(P_{H_2} P_{O_2}^{\frac{1}{2}} \Big/ P_{H_2O}\right) \qquad \textbf{(20)}$$

If P is the operating pressure of the battery, the gases pressures can be referenced with respect to this pressure:

$$a_i = P_i / P \qquad \textbf{(21)}$$

$$P_{H_2} = a_{H_2} P \qquad \textbf{(22)}$$

$$P_{O_2} = a_{O_2} P \qquad \textbf{(23)}$$

$$P_{H_2O} = a_{H_2O} P \qquad \textbf{(24)}$$

Where $a_{H_2}$ is equal to 1 if pure hydrogen is used and where $a_{O_2}$ is close to 0.21 if air is used. For liquid water, the term $a_{H_2O}$ is equal to 1.
We then obtain:

$$E = E^0 + \frac{RT}{nF}\ln\left(a_{H_2} a_{O_2}^{\frac{1}{2}} \Big/ a_{H_2O}\right) + \frac{RT}{2nF}\ln(P) \qquad \textbf{(25)}$$

## 7. The influence of the oxygen molar concentration on the electromotive force

$$E = E^0 + \frac{RT}{nF}\ln\left(a_{H_2} P^{\frac{1}{2}} / a_{H_2O}\right) + \frac{RT}{2nF}\ln(a_{O_2}) \qquad \textbf{(26)}$$

## 9. The energy density

The energy density allows reporting the energy produced by the cell to the molar mass of the fuel [10]:

$$W = -\Delta G_r^0 / (3600 \times M) \qquad \textbf{(27)}$$

## 9. Application and evaluation of results

Figure 1 shows that the use of pure oxygen rather than air increases the EMF. The shape of the EMF curve of the two alcohols and hydrogen forms an almost horizontal plateau and then increases slightly with the increase in the molar concentration of oxygen. The standard temperature of the EMF of hydrogen is higher than that of the alcohols and remains higher during the whole studied interval.

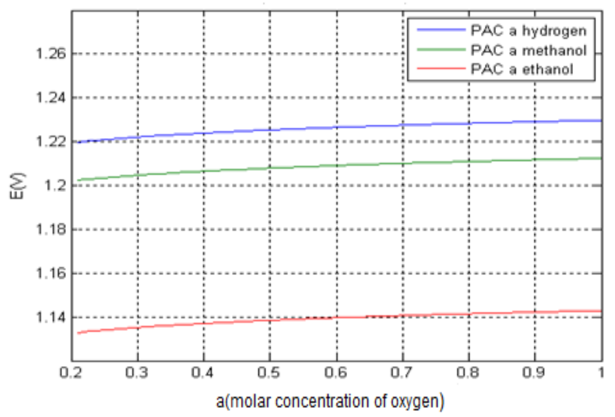


**Figure 1** : Influence of the molar concentration of oxygen on the EMF (T = 298K P = 1atm)

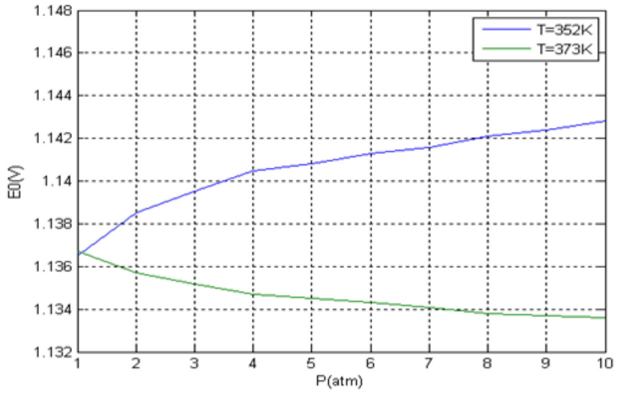


**Figure 2 :** The pressure effect on EMF of Ethanol FC at boiling temperature (T=352K et T=373K)

The curves in Figure 2 show that the EMF supplied by the CAP increases with increasing pressure and The shape of the EMF standard ethanol curve increases with increasing pressure during ethanol boiling (352K) and decreases during boiling water (373K).

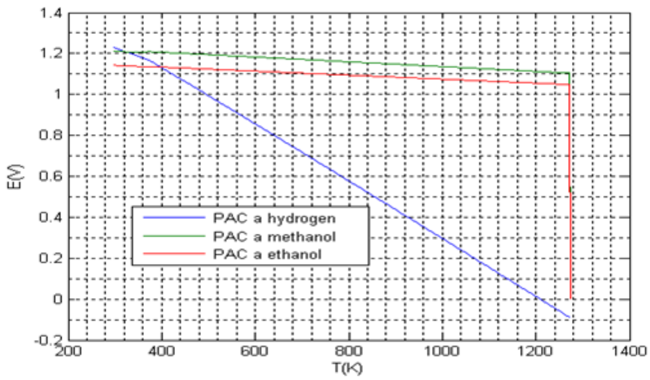


**Figure 3 : :** Effect of temperature on EMF of FC (pure Oxygen P=1atm)

The hydrogen fuel cell FEM is high at the standard temperature but decreases sharply with the temperature rise to around 0V at 1200 K. On the contrary, the FEM of the alcohols decreases slightly than that of the hydrogen cell and remains Greater than the latter throughout the studied interval.

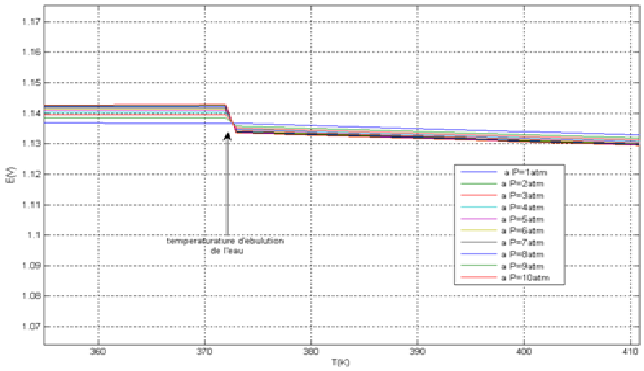


**Figure 4 :** Effect of the temperature on the EMF of ethanol FC for different pressure values (P=1atm et P=10atm)

The shape of the EMF ethanol curve forms a horizontal plateau to the boiling temperature of the water and then decreases slightly with the temperature variation for different pressure values.

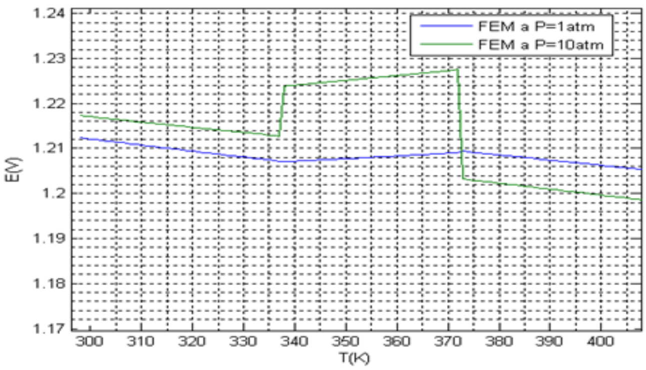


**Figure 5:** Effect of the temperature on the EMF of methanol FC for different pressure values (P=1atm et P=10atm pure oxygen)

The effect shows that the influence of the temperature on the methanol FEM is high at the boiling points (337K for methanol and 373K for water) when the pressure is higher.

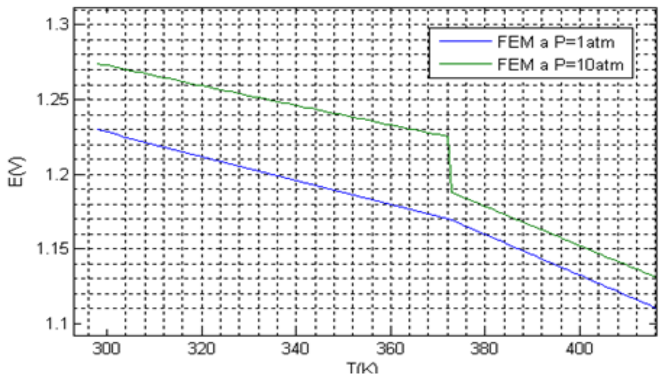


**Figure 6 :** Effect of the temperature of the EMF of hydrogen FC for different pressure values (P=1atm et P=10atm)

The pace shows that the influence of temperature on the hydrogen FEM is high at the boiling point (373K for water) when the pressure is higher.

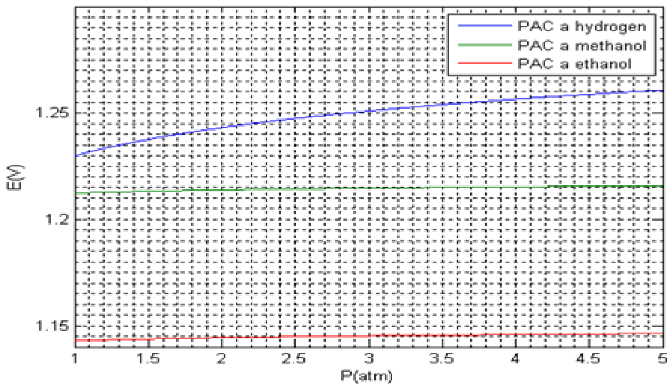


**Figure 7** : Effect of the pressure on the EMF of FC  (T=298K   pure oxygen pure)

The pace shows that the influence of the pressure on the hydrogen EMF is high, but on the contrary the alcohols FEM is slightly varied as that of the hydrogen cell with the pressure variation.

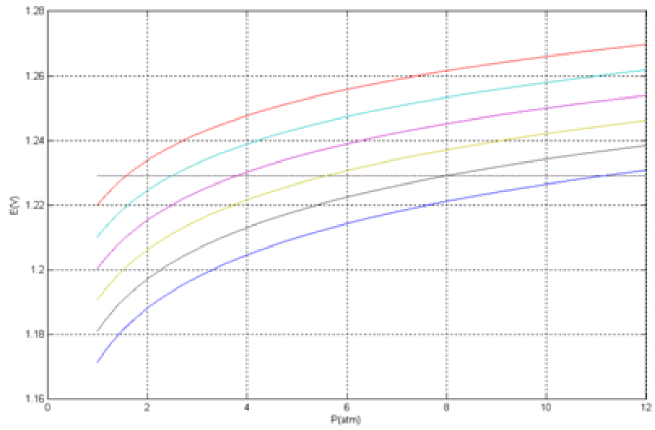


**Figure 8 :** The compensation pressure at different temperature values for FC with hydrogen (E = 1.23V)

Due to the increase in temperature, the hydrogen FEM decreases, and to compensate for the voltage drop the pressure must be increased.

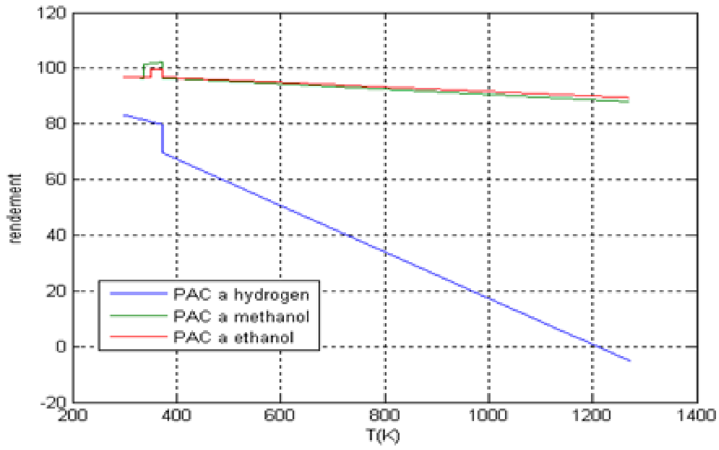


**Figure 9** : Influence of temperature on the reversible yield of FC (P = 1atm Pure Oxygen)

The efficiency of the hydrogen cell is high at standard temperature, but decreases sharply with the increase in temperature to around 0% around 1200 K. From the standard temperature, the yield of the alcohols is higher than that of the battery hydrogen, and remains higher than the latter throughout the interval studied. Among the alcohols, methanol gives a yield greater than unity in the range between the boiling temperatures of methanol and water.

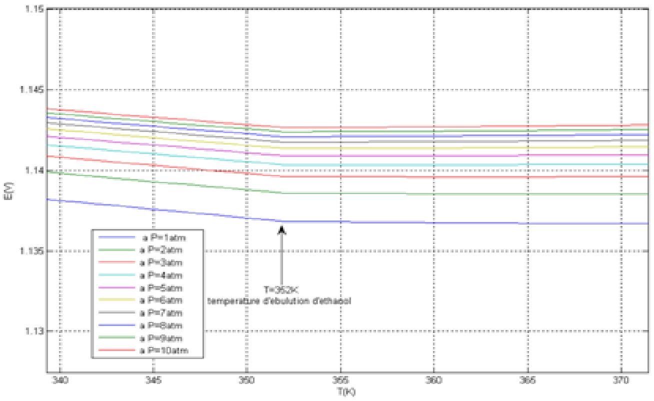


**Figure 10 :** Effect of the temperature on the EMF of ethanol FC for different pressure values (T=298K a T=370K)

The shape of the ethanol EMF curve decreases slightly with the change in temperature up to the boiling point of ethanol and then takes the form of a horizontal pavement for different pressure values.

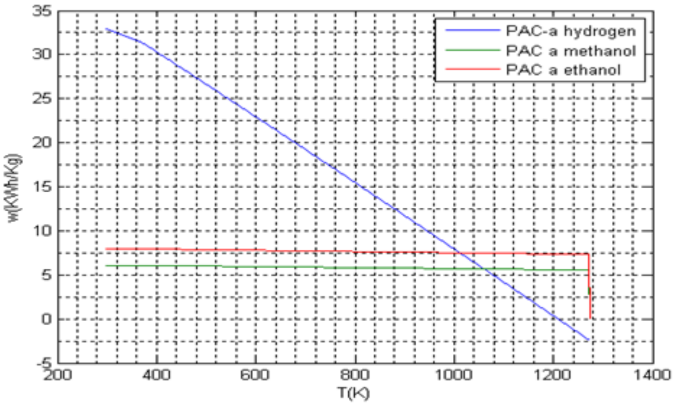


**Figure 11 :** Influence of temperature on the energy density of FC

The shape of the energy density curve of the studied two alcohols forms a horizontal plateau and then decreases slightly; nevertheless, it remains between 6-9 KWh/Kg throughout the interval studied. But the energy density of the hydrogen is more than five times higher than the alcohols at the standard temperature and then decreases more appreciably than for the alcohols with the increase of the temperature.

## 10. Conclusions

The results obtained show that:
- Alcohols are more efficient than hydrogen
- On the contrary, the energy density of hydrogen is more than three times higher than that of alcohols
- The EMF supplied by the hydrogen fuel cell is large, and that of the alcohols does not move too far
- Phase change for reagents leads to an increase in EMF.
- On the contrary, the phase change for the products leads to a decrease in the EMF

It would be premature to make a choice between one of these fuels on the basis of theoretical thermodynamic calculation only, a more thorough investigation is recommended, in particular a kinetic of the electro-oxidation of the different fuel, and tests on Batteries are required.

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