# Simulation of PEMFC performance

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**Résumé** - *A partir des travaux scientifiques dédiés à la modélisation des piles à combustible (PAC), il apparaît que les approches de modélisation diffèrent d'un auteur à un autre, mais finalement prétendent à l'estimation des performances, en puissance électrique, de la PAC via l'évaluation des courbes de polarisation et de puissance, puissance développée en fonction de la densité de courant. Deux approches existent pour l'estimation des performances des piles à combustibles. La première approche inclut les modèles mécanistes, qui visent à simuler le transfert de masse de chaleur et les phénomènes électrochimiques dans la PAC. La deuxième approche inclut les modèles qui sont basés sur les équations semi empiriques, et qui sont appliquées pour prévoir l'effet de différents paramètres d'entrée sur les caractéristiques courant – tension de la PAC, sans examiner en détail les phénomènes physiques et électrochimiques impliqués dans l'opération d'oxydoréduction. Nous présentons une description d'un modèle à la base d'une expression aboutit de la tension délivrée par la PAC.*

**Abstract** - *Throughout literature, there are two approaches to estimate fuel cells (FC) performance, by the evaluation of polarization curve. One includes, physical modelling of heat and mass transfer with electrochemical phenomena; the second is based on semi-empirical equation used in order to analysis the effect of different physical perturbation on the polarization curve and consider FC as a black box. The aim of this study is to present a simple but enhanced and accurate expression of PEMFC output voltage. The model includes operative conditions, current density and geometric parameter of the FC.*

**Keywords**: Hydrogen - Fuel cells - Proton Exchange Membrane - Butler-Volmer equation - Computer Simulation - Electrochemical Model - Over potential.

## 1. INTRODUCTION

A detailed analysis of models that describes PEMFC over potential [1, 2, 7, 10, 12, 13], allow to elaborate an enhanced expression to compute FC voltage output according to current density and FC geometry.

## 2. PEMFC OUTPUT VOLTAGE

The steady-state cell voltage is calculated by subtracting catalytic and resistive losses from the reversible electrochemical cell voltage as follows [1, 12]:

$$E_{cell} = E_{rev} - \eta_{anode} - \eta_{cathode} - \eta_{ohmic} - \eta_{int\,erface} \qquad (1)$$

The reversible cell potential $E_{rev}$ can be found from well-known thermodynamic data:

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$$E_{rev} = 1.2291 - 8.4517 \times 10^{-4} (T - 298.15) + 4.3080 \times 10^{-5} T \times (\ln p_{H_2} + 0.5 \ln p_{O_2}) \quad (2)$$

$p_{O_2}$, $p_{H_2}$, partials pressures of respectively hydrogen and oxygen at the catalysis interface, atm.

In PEMFC the dominant factor is the ohmic losses, due to the resistance of the wiring and the resistance of the imperfect electrodes. In most cases, the ohmic drop or the ohmic over potential is given by:

$$\eta_{ohm}^{proton} = - I \times R^{proton} \quad (3)$$

$R^{proton}$ : Proton membrane resistance, ohm

Modeling overpotential caused by the interaction of different phases, solid and gas interface between electrode and membrane, is complex and depend on many parameter, thus we adopt a simplified empirical equation proposed by Kim *et al.* [15]:

$$\eta_{interface} = m \exp (n \times J) \quad (4)$$

With $\underline{n} = 8$ and
For $T \geq 312.15$

$$m = 1.1 \times 10^{-4} - 1.2 \times 10^{-6} (T - 273.15) \quad (5)$$

For $T < 312.15$

$$m = 3.3 \times 10^{-3} - 8.2 \times 10^{-5} (T - 273.15) \quad (6)$$

The equation for over potential, deduced from Butler-Volmer approach, is used for the electrodes in general form:

$$n_k = \frac{R T}{\alpha_k F} \times \sinh^{-1} \left[ \frac{1}{2} \left( \frac{J_k / J_{k,0}}{1 - J_k / J_{k,L}} \right) \right] \quad (7)$$

$n_k$ : Overpotential for the element $k$, V
$\alpha_k$ : Symmetry factor for the element $k$
$J_k$ : Current density for the element $k$, A/m²
$J_{k,0}$ : Exchange Current density for the element $k$, A/m²
$J_{k,L}$ : Reference current density for the element $k$, A/m²
$F$ : Faraday's constant, C mol$^{-1}$
$k$ : anode, cathode

The symmetry factor is direct implication of oxidation in the anode $\alpha_{anode} = 0.5$ and reduction for the cathode $\alpha_{cathode} = 1$

## 2.1 Expression for the current density

The process considered in this paper is assumed at steady state conditions, thus the overall current density that runs through the different elements is the same, J considered for the membrane cross section:

$$J = -\sigma_{PEM} \times \frac{d\phi}{dx} \tag{8}$$

$\sigma_{PEM}$, the ionic conductivity of the solid membrane, S/m

$\phi$, the electrical potential of the membrane, V

$x$, the linear direction along the electrolysis cell beginning at the anode electrode, m

The membrane of the PEMFC, exhibit a resistance to the movement of hydrogen proton, this cause the apparition of the over potential across the membrane. Researchers conclude an easily compressive relation between the ionic conductivity, the degree of humidification, temperature and the membrane thickness [16].

The local ionic conductivity, $\sigma_{PEM}$, has been correlated empirically as a function of temperature and the water content, according to the correlation of Neubrand cited by Ramousse [17].

$$\sigma_{PEM}[S/m] = \exp\left[-E_{A,m}\left(\frac{1}{T} - \frac{1}{353}\right)\right] \times$$
$$\left(0.0013 \times \lambda^3(x) + 0.029 \times \lambda^2(x) + 0.2658 \times \lambda(x)\right) \tag{9}$$

$$E_{A,m} = 1183 + 2640 \exp\left(-0.6\,\lambda(x)\right) \tag{10}$$

$\lambda$, the water content, in the case of Nafion membrane, this is the number of water molecules per sulfonate group ($mol_{H_2O}/mol_{SO^{3-}}$), $E_{A,m}$ is the energy activation of the membrane (J mol$^{-1}$). The water content, $\lambda$, at location $x$ (from the anode electrode), can be expressed linearly with the empirical equation [16] as:

$$\lambda(x) = \lambda_c + (\lambda_a - \lambda_c)\frac{x}{L_{PEM}} \tag{11}$$

$\lambda_a$, $\lambda_c$ the water contents at the anode-membrane and cathode-membrane interface respectively and $L_{PEM}$ membrane thickness, m.

The enhanced expression for current density is deduced from the current density $J*$ considered for the effective catalytic cross section within the electrode compartment:

$$J_{k,0} = \gamma_{M-k} \times J_{k,0}^* \tag{12}$$

$J_{k,0}^*$: Exchange current density per PEMFC membrane cross section, [A/m²]; $J_{k,0}$: Exchange current per PEMFC effective catalytic cross section within the electrode compartment, [A/m²]; $\gamma_{M-k}$: Roughness coefficient; $k$: anode, cathode.

The roughness coefficient $\gamma_{M-k}$, allows to account for the geometrical deviation of the electrodes [7]:

$$\gamma_{M-k} = \frac{\text{Electrode active surface}}{\text{FC cross section}} \qquad (13)$$

## 2.2 Polarization curve of the PEMFC

Combining preceding equations, the electrochemical model is used to simulate the voltage of the PEMFC. The numerical parameters used are from data published in the literature, summarized in **Table 1**.

**Table 1**: PEMFC characteristics

| Paramètre | Valeur | Ref. |
|-----------|--------|------|
| Roughness coefficient | 0.5 | [13] |
| Nafion membrane thickness | $0.23 \times 10^{-3}$ m | [13] |
| PEMFC Cross section | 50 cm$^3$ | [13] |

The membrane type is Nafion 117. Pressure of hydrogen and oxygen uniformly and equally set to $pH_2 = pO_2$. For the temperature range is chosen between 30 ° C and 80 ° C.

**Table 2**: Temperature and pressure used

| Parameter | Value |
|-----------|-------|
| $pH_2$ , $pO_2$ (atm) | 1 atm, 2 atm, 5 atm |
| T (°C) | 30 °C, 50 °C, 80 °C |

## 2.3 Simulation of the PEMFC voltage, power density and efficiency

The polarization curves, power density and overall efficiency of a PEMFC are shown in Figure 1 and 2.
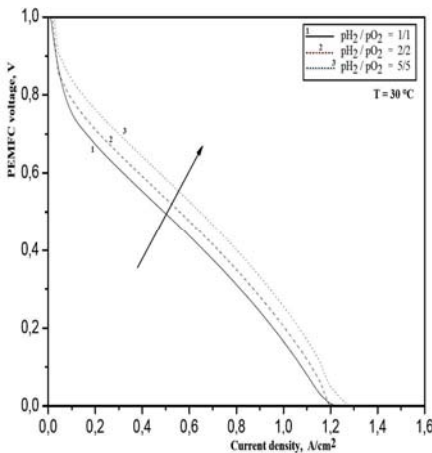


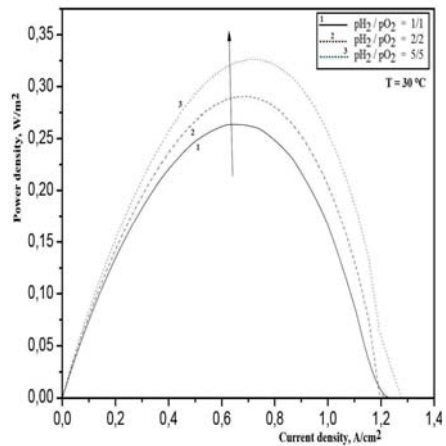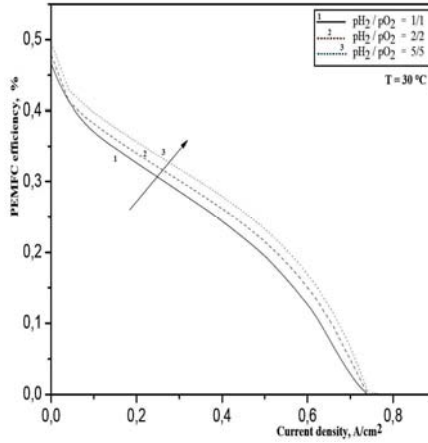Fig. 1: Voltage vs pressure          Fig. 2: Power density vs pressure

Fig. 3: Overall efficiency vs pressure

It is observed that the efficiency of the cell increases with increasing pressure and temperature. With increasing temperature the activation losses are reduced and mass transfer is enhanced, resulting in a reduction in cell resistance and increase performance [13].

There is also the displacement of the polarization curve towards higher current densities by increasing the temperature; this is due to the increase of the conductivity of the membrane with increasing temperature.

Also, Figure 5 shows that the maximum power density shifts to higher current densities with increasing temperature as a result of reduced ohmic losses [13].
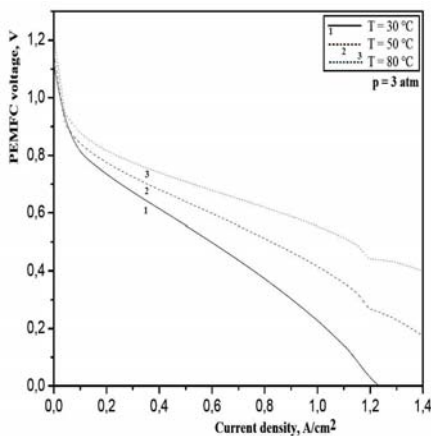
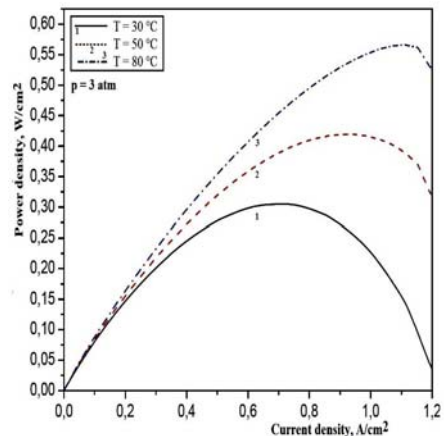

Fig. 4: Voltage vs temperature


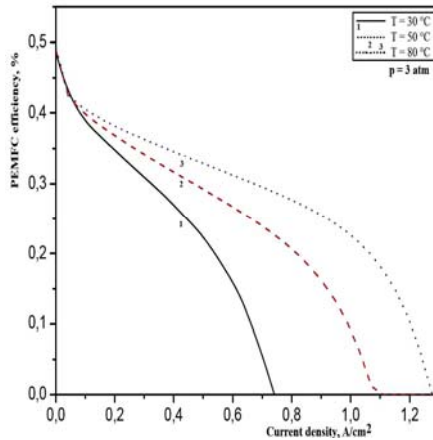
Fig. 5: Power density vs temperature

Fig. 6: Overall efficiency vs temperature

Figures 3 and 6 show that the performance of the PEMFC is improving with increasing pressure, this can be explained by the Nernst equation. All the polarization curves shift positively with increasing pressure.

Another reason for the improved performance is the increase of partial pressure of reactive gas with increasing operating pressure. The maximum power density evolves positively with increasing pressure as the rate of chemical reaction is proportional to the partial pressure of hydrogen and oxygen.

Thus, the effect of increasing pressure is more important when using air. Indeed, higher pressures can forces hydrogen and oxygen to be in close contact with the electrolyte. This pressure sensitivity is most pronounced around the region of high current densities.

It is interesting to note, by comparing Figure 2 and 5 that the maximum power corresponds to a fairly strong current. At the maximum point, the internal resistance of the cell is equal to the electrical resistance of the external circuit. However, efficiency is declining in the region of strong currents, it is imperative to find a compromise between high power and high efficiency.

## 3. CONCLUSION

The model for estimating PEMFC electrical power performance, is based on the description and modelling of over potential. The expression developed, is valid for a large interval of current density and involves factors related to the geometric design of PEMFC. The shape of theoretical curves obtained corroborates published data which is added value and qualitatively, the model shows a clear advantage in the region of low current densities.

The observations are consistent with the fact that the performance of the PEMFC is improving with increasing pressure, and all the curves of polarization varies positively. The maximum power density evolves positively with increasing pressure because as the rate of chemical reaction is proportional to the partial pressure of hydrogen and oxygen.

It is interesting to note that the maximum power corresponds to a fairly strong current. However, efficiency is declining in the region of strong currents, it is imperative to find a compromise between high power and high efficiency.

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