Dynamic model and simulations of a PEM fuel cell for residential applications

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Abstract. The CO_2 levels present in the atmosphere are growing everyday, affecting consequently the global warming. One of the main reasons for this fact is due to the combustion of fossil fuels used in the electrical energy production in the stationary sector. Public awareness aims improved energy efficiency of the electricity generation systems, as well as new systems allowing the energy conservation and the decrease or even no emission of pollutant to the atmosphere.

Proton exchange membrane (PEM) fuel cells appear as devices capable of producing electricity with no pollutant emissions but only water.

This document presents a preliminary modeling of a PEM fuel cell stack based on the experimental curves obtained at a laboratory test. Not only the static model but the dynamic response of the stack will be estimated through different mathematical approximations. The purpose of the model is to design a tool suitable for predicting the fuel cell behaviour.

Key words

Proton exchange membrane (PEM) fuel cells, dynamic modelling, residential applications.

1. Introduction

Figure 1 shows that the world energy consumption is growing everyday. Some predictions present, in a medium term scenario, a total energy consumption near 1.900 millions of equivalent tons in 2030, as shown in Figure 2 extracted from [1].

For such demand and, consequently, energy consumption, CO_2 levels in the atmosphere are expected to increase along this period. Figure 3, extracted from [2], shows an estimation of this variation depending on the involved countries. Some regions like China, a developing country, could increase more than four times its emissions in 2030 when comparing with 1990.
On the other hand, eventhough renewables will increase during such period, solids, natural gas and even oil are not predicted to decrease in their consumption.

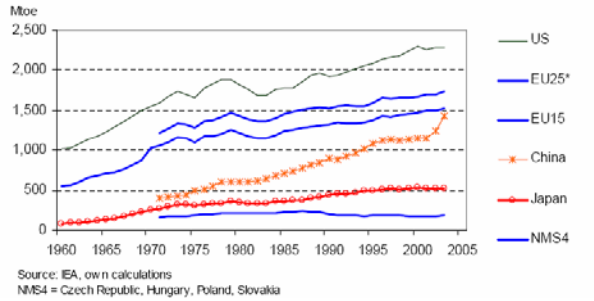

Figure 1. Total energy consumption.

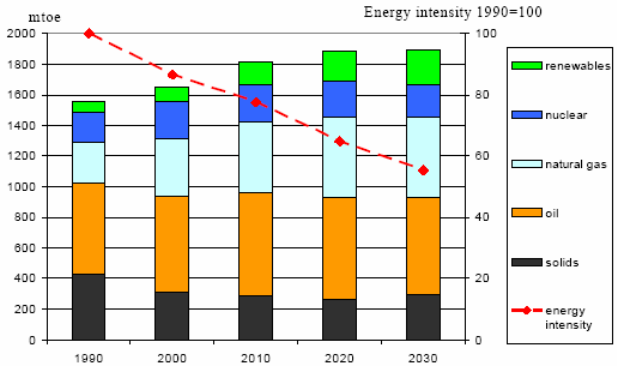

Figure 2. Total energy consumption by fuel and energy intensity.

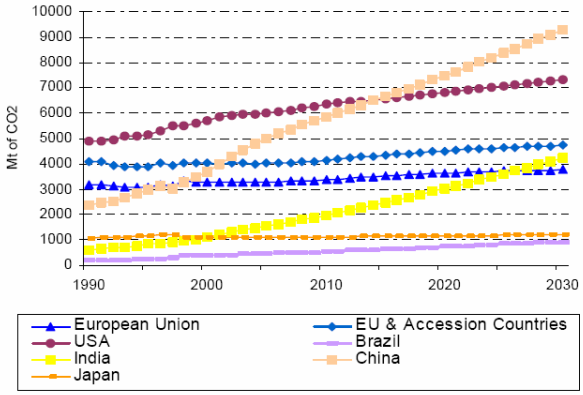

Figure 3. World CO_2 emissions.

Within this possible scenario, proton exchange membrane (PEM) fuel cells appear as devices capable of producing electricity without pollutant emissions. This type of fuel cell, characterised by its operating temperature, below 100 ºC, presents the following advantages:

- High efficiency in the electricity production (no Carnot limitation)
- Low emission to the atmosphere (zero emissions in case of operating with pure hydrogen)
- No noise (no moving parts)
- Modularity
- Flexibility

The basis of this technology lies in the electrochemical reactions produced in the anode and cathode sides of an individual cell. Both sides are in contact with an electrolyte layer, as it is shown in Figure 4, extracted from [3]. The fuel oxides in the anode side giving some electrons to the cathode side that is reduced producing water.

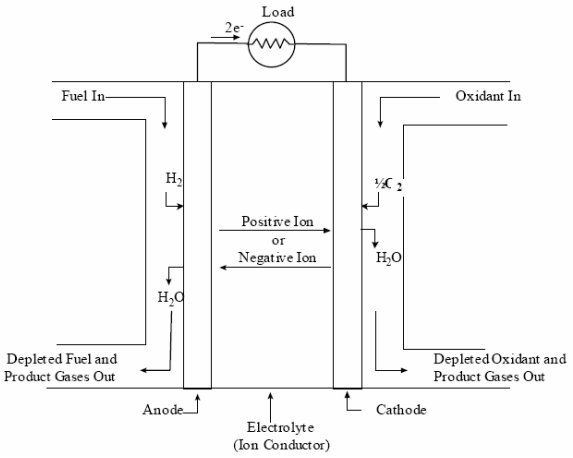

Figure 4. Schematic of an individual Fuel Cell

The scope of the work presented within this document cover the development of a preliminary modelling of a PEM fuel cell stack based on the experimental curves obtained at a laboratory test bench.

The paper content is described as follows. First, a more complex model, which is currently being implemented, is described. Then, the description of the main laboratory set up is presented. Finally, the measured data for that preliminary model and the main conclusions are included.

2. Accurate model equations

There are many studies related to fuel cell modelling with different complexities, due to fact that each individual fuel cell component interacts with others in a complex way, involving not only electrical but chemical and thermodynamic processes described by non linear equations [4].

The voltage output of the fuel cell could be determined from the following analysis:

1. Gas diffusion in the electrodes (described by Stefa-Maxwell, in order to determine the effective partial pressures of H_2 and O_2):

$$\nabla x_i = \frac{RT}{P}\sum_{j=1}^{N}\frac{x_i N_j - x_j N_i}{D_{i,j}} \quad (1)$$

Where x_i represents mole fractions of species *i*, as well as N_i represents superficial gas flux of species *i* [mol/(m^2*s)].

2. Material conservation equations (instantaneous change in the effective partial pressures of hydrogen and oxygen, described through the ideal equations)

$$\frac{V_a}{RT}\frac{dp^*_{H_2}}{dt} = M_{H_2,in} - M_{H_2,out} - \frac{i}{2F} \quad (2)$$

$$\frac{V_c}{RT}\frac{dp^*_{O_2}}{dt} = M_{O_2,in} - M_{O_2,out} - \frac{i}{4F} \quad (3)$$

Where V_i is the voltage drop of type *i* (in volts), p_i is the partial pressure of species *i* (in pascal), *Mi* is the mole flow rate of species *i* (in mol per second), *F* is the Faraday constant as well as *R* is the gas constant.

3. Nernst equation are used to calculate the reversible potential:

$$Ecell = Eo,cell + \frac{RT}{2F}\ln\left[p^*_{H_2}\cdot(p^*_{O_2})^{0.5}\right] \quad (4)$$

Where *Eo,cell* is a function of temperature and can be expressed as follows:

$$Ecell = E^0o,cell - K_E\left[T - 298\right] \quad (5)$$

$E^0_{0,cell}$ is the standard reference potential state, 298 K and 1 atm pressure, and k_E is an empirical constant (volts per Kelvin).

The output voltage of the fuel cell stack could be calculated taking into account the following losses: activation voltage drop, ohmic voltage drop and concentration voltage drop:

$$Vout = Ncell * Vcell = E - V_{act} - V_{ohm} - V_{conc} \quad (6)$$

Where activation losses can be expressed as follow:

$$V_{act} = \eta_o + (t - 298) * a + T * b * \ln(I) \quad (7)$$

With η_o, *a* and *b* being empirical constants.

Ohmic losses can be expressed as follows:

$$V_{ohm} = I * R_{ohm} \quad (8)$$

$$R_{ohm} = R_{ohm,o} + k_{RI} * I - k_{RT} * T \quad (9)$$

With $R_{ohm,0}$ K_{RI} and K_{RT} being empirical constants

And finally, concentration losses can be expressed as:

$$V_{conc} = -\frac{RT}{zF}\ln(1-\frac{I}{I_{\lim it}}) \quad (10)$$

Where I_{limit} is the limitation current and z is the number of participating electrons.

4. Double-layer charging effect. The model could include the effect of the capacity, C, created between the layers, which can store electrical energy and behave like a super capacitor.

5. Energy balance of the Thermodynamics. This balance would take into account the increase or decrease of the fuel cell temperature during transients and should be calculated from the energy obtained after computing the chemical reaction, the electrical output power, the sensible and latent heat absorbed during the process and the heat loss.

This complex model taking into account all the physical processes involved in the fuel cell stack is being developed in order to precisely asses the fuel cell behaviour both in steady-state and transients.

3. Laboratory set up

A simplified scheme of the whole system involved in the tested PEM fuel cell is presented in Figure 5. It can be observed that hydrogen and oxygen supplied to the stack are recirculated while water produced is recuperated in two water tanks (water/gas separators at the anode and cathode outputs). Different parameters as pressure and temperature of the stack, as well as the state of different actuators (pumps and valves, mainly) and the voltage and the current at the output of the stack are measured and recorded by the control unit. A DC/DC converter is used to adequate the voltage at the output of the stack to the voltage required by the load.

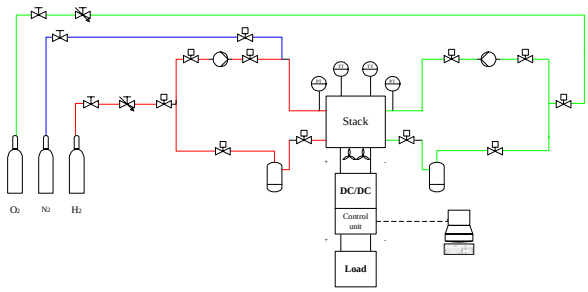

Figure 5. Schematic of the system

On the other hand, the main fuel cell data are presented in Table 1.

Table 1. Fuel cell specifications.

Rated voltage (V)	16
Rated current (A)	15.5
Maximum power (W)	250
Number of cells	20
Operating temperature (ºC)	< 70
Operating pressures (bar)	1

4. Statistic model

Some measurements have been acquired in order to adjust the stationary behaviour of the stack to its characteristic curve. A constant increase of the current demand, 1A/s, in the range of 2 A to 20 A was applied to measure the output stack voltage, output stack power and the average stack temperature. In the same way, a constant decrease within the same current range and current gradient was applied to obtain the reverse curves. A constant hydrogen flow rate of 130 Nl/h were introduced into the stack. The results are presented in figures 7 to 9..

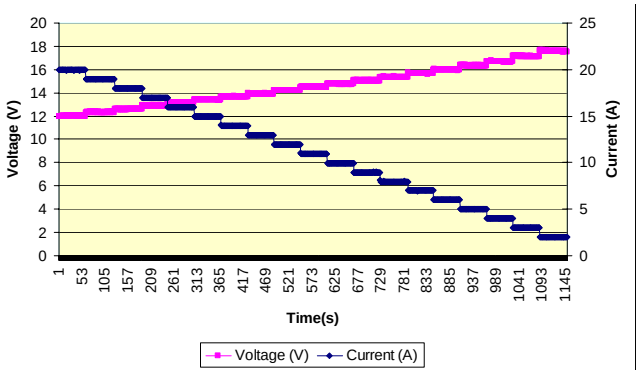

Figure 6. Voltage and Current, run down operation.

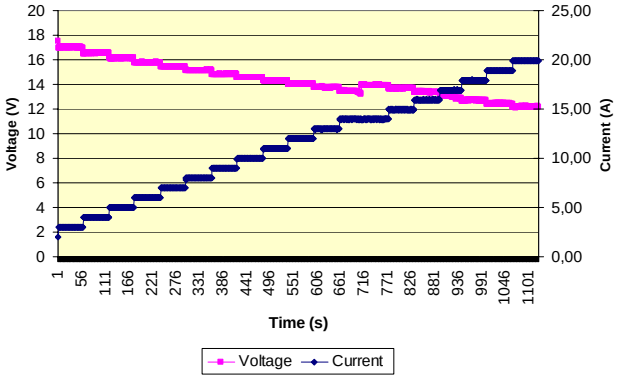

Figure 7. Voltage and current, run up operation

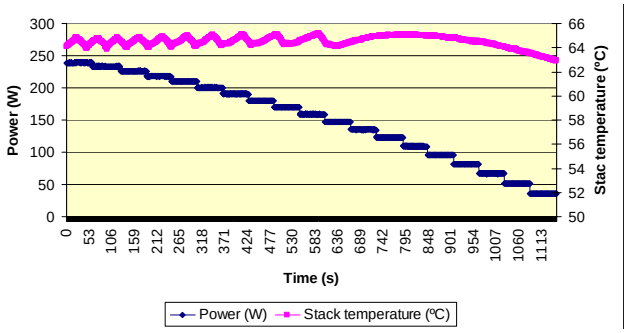

Figure 8. Power and temperature, run down operation.

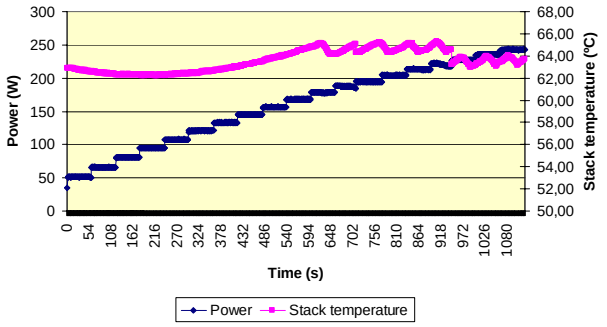

Figure 9. Power and temperature, run up operation.

On the other hand, Figure 10 shows some differences between the voltages in the run up and run down operation modes. This is the well-known hysteresis effect produced in the fuel cell due to temperature variation. Note that the cooling system of the stack tries to maintain the temperature within the range from 60ºC to 65ºC.

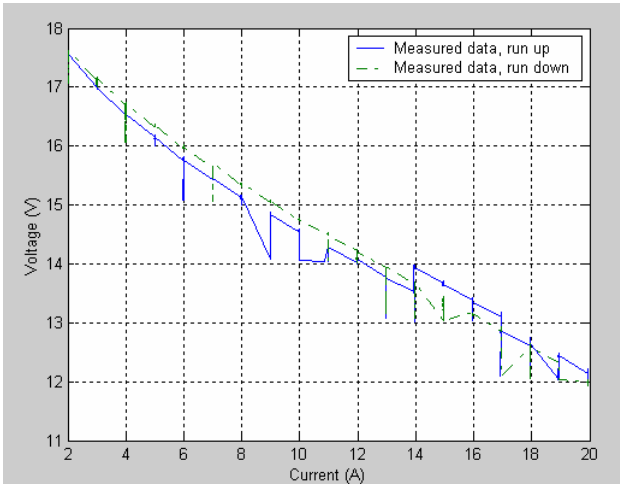

Figure 10. Voltage vs current.

The fuel cell stationary behaviour has been modelled as a polynomial function using the acquired current and voltage measurements:

$$V = 5 \cdot 10^{-4} I^3 + 0.016 I^2 - 0.5814 I + 18.5952 \quad (11)$$

Figure 11 represents the *V(I)* equation for both model and measured data. Some deviation occurs mainly in the right-hand part of the curve, around concentration losses.

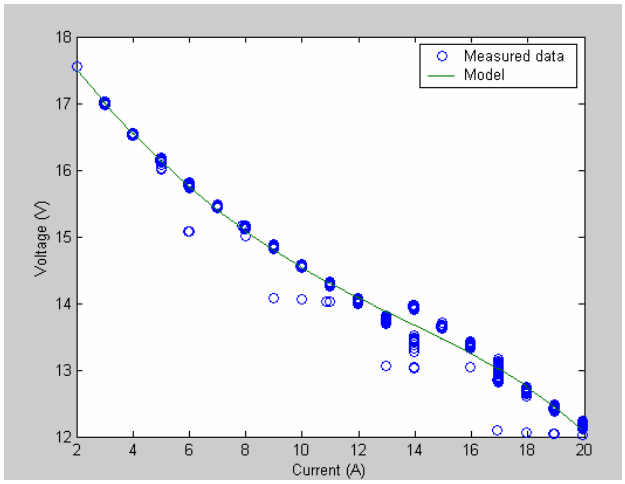

Figure 11. Voltage measured vs model

5. Dynamic model: transient response

This section is devoted to present some results of the dynamic behaviour of the tested PEM fuel cell stack. The transient response has been studied for different load current steps. Then, the voltage and power supplied by the fuel cell has been measured, being the results presented in figures 12 to14.

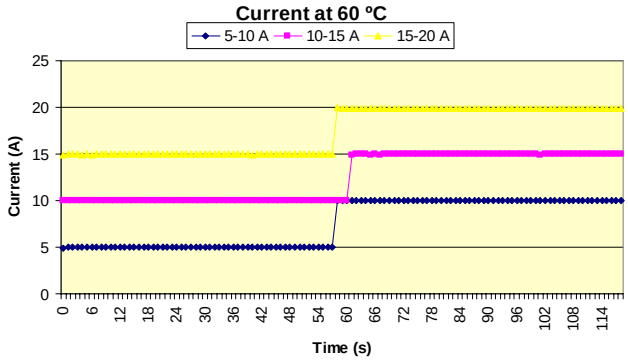

Figure 12. Current steps applied to the stack

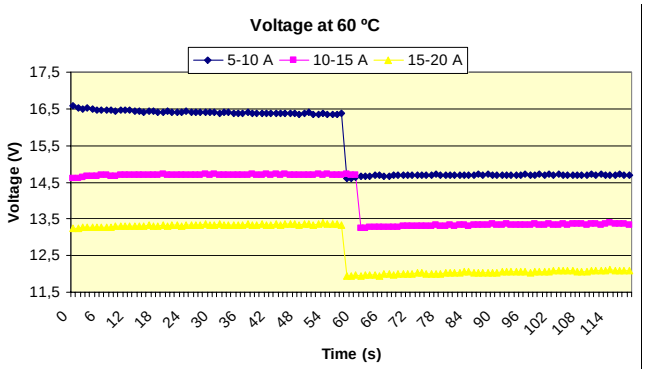

Figure 13. Voltage response at different current steps

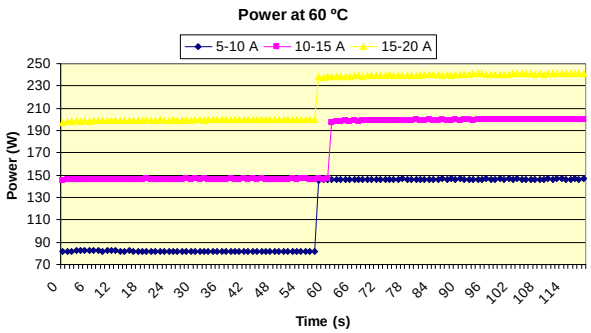

Figure 14. Power supplied for the stack at different current steps

In case of a load current step the output voltage of the fuel cell reacts with a similar step but in the opposite direction. The dynamic behaviour of the voltage during this transient response can be modelled as a first order RC circuit [5], where the voltage can be expressed as:

$$V(t) = V_i - R\Delta I \exp(-t/\tau_1) \qquad (12)$$

where V_i is the initial output voltage and R, C the characteristic electrical parameters representing the fuel cell.

After analysing the time constant, τ_1, of the circuit from the transient response curves shown in Fig. 14, the resistance and the capacitance can be calculated as:

$$R = \frac{\Delta V}{\Delta I \exp(-1)} \qquad (13)$$

$$C = \frac{\tau_1}{R} \qquad (14)$$

Table 2 shows the obtained results for the different load current step changes tested in the laboratory.

Table 2.- Dynamic model parameters: τ_1

Current step (A)	τ_1 (s)	R (Ohm)	C (F)
5-10	0,63	0,609	1,033
10-15	0,63	0,500	1,259
15-20	0,63	0,470	1,323

After this first transient response, the fuel cell slightly increases the output voltage. This second part of the transient voltage curve can be modelled as an exponential of the form:

$$V(t) = V_o + \Delta I(1 - \exp(-t/\tau_2)) \qquad (15)$$

where V_o is the final voltage after the first transient, and $\Delta V = V_n - V_o$, being V_n the new steady-state value of the output voltage.

The time constant τ_2 depends on the time the reactants react to the new current value demanded by the stack. As a consequence, this parameter depends on the initial current value and other parameters such as temperature. Table 3 presents these values for the three applied load current steps.

Table 3. Dynamic model parameters: τ_2

Current step (A)	τ_2 (s)	V_o (V)	V_n (V)
5-10	11	15,25	14,70
10-15	22	14,30	13,34
15-20	25	12,46	12,05

6. Conclusion

A simplified model for a 250 W PEM fuel cell stack has been developed taking into account a polynomial approximation for its steady state and an equivalent R-C circuit for its transient response.

The study of the steady-state response of the PEM fuel cell reveals that a good approximation has been performed because of the good agreement of the experimental and theoretical values. However, slight discrepancies can be found in the current range corresponding to concentration losses. On the other hand, dynamic tests have been carried out by applying load current step changes. The results points out the two different parts of the output voltage curve, both dominated by a first order dynamical equation.

In spite of the results presented in this paper, some deeper analysis has been started in order to take into account a more accurate representation of the physical phenomena involved in the PEM fuel cell stack. Nernst voltages and the effects of activation losses, ohmic losses and concentration losses have to be modelled. In addition the inclusion in the model of the operation temperature is a critical point to work in. The model on course will be extended for higher power stacks, allowing further developments. In fact, these models are relevant to successfully design the power conditioning units for converting the DC electricity produced by the fuel cell to the requirements of the load, in case of isolated applications, or even the electric public supply, in case of stationary electric energy generation.

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