PARAMETERS OPTIMIZATION OF A PEM FUEL CELL MODEL THROUGH A RANDOM-SEARCH TECHNIQUE

M. T. Outeiro [(1)], R. Chibante [(2)], A. S. Carvalho [(3)], A.T. de Almeida [(3)]

[(1)] Department of Electrical Engineering, Institute of Engineering of Coimbra, 3030-119 Coimbra, Portugal
[(2)] Department of Mathematics, Institute of Engineering of Porto, 4200-072 Porto, Portugal
[(3)] Department of Electrical Engineering and Computers, Engineering Faculty of Oporto University, 4200-465 Porto, Portugal
[(4)] Department of Electrical Engineering and Computers, Faculty of Science and Technology, Coimbra University, 3030-290 Coimbra, Portugal,

This paper presents an optimization based procedure to extract parameters of a PEM fuel cell model implemented in Matlab/Simulink.
Parameter optimization is based on a random-search technique which is carried out using the Simulated Annealing algorithm (SA).
Based in experimental data SA produces changes in parameter values in order to minimize the error between experimental and simulated results.
The performance of the PEM fuel cell is characterized thorough experimental tests, as well as the comparison between simulation and experimental results analysed for several variables which validate the developed model.
The main contribution of this study is related to the useful information about model parameters which enables prototype-less design of the fuel cell systems through accurate simulations.

Keywords: **Optimization, Proton Exchange Membrane Fuel Cell, Simulated Annealing.**

Nomenclature

A	cell active area (cm2)
B	constant (V)
C	equivalent electrical capacitance (F)
E_{Nernst}	thermodynamic potential
J_n	no-load current density (A/cm2)
J_{max}	maximum current density (A/cm2)
l	membrane thickness (μm)
n	number of cells in stack
PO_2	oxygen partial pressure (atm)
PH_2	hydrogen partial pressure (atm)
RC	contact resistance (Ω)
T	cell operating temperature (K)
V_{act}	activation voltage drop (V)
V_{ohmic}	ohmic voltage drop (V)
V_{con}	concentration voltage (V)
ξi , ψ	parametric coefficients

1. Introduction

Fuel cells are emerging as a highly promising alternative to the conventional power generation systems due to their high efficiency, lower environmental impact, reliability, compactness, modularity, quiet operation and fuel flexibility. They will not only supply clean renewable energy to millions of users, but will also help reduce the dependence on oil and contribute to the planet sustainability [1]-[2].
The expectations for the commercial introduction of fuel cells in a large scale in transports and stationary applications have not yet been realized. They are still expensive, require hydrogen-rich fuel, have shorter lifetimes than current grid-connected power technologies, involve high system complexity and a lack of fuel infrastructure. Nevertheless, research and development efforts put into the fuel cells technologies combined with their enormous potentialities have made them very attractive candidates for automotive and stationary applications as well, particularly the PEM fuel cells [3]-[4].
To understand and improve the performance of PEM fuel cells, researchers have developed several mathematical models. Mathematical models are very important because they can provide general trends as well as quantitative measures of relative changes in performance for the device as model parameters are varied [5]-[11]. Mathematical models can also provide detailed data that are frequently unavailable from experiments within an operating fuel cell system.
The models are characterized by a set of parameters that must be precisely identified in order to achieve accurate simulation results. With a global search method of optimization coupled to the PEM fuel cell model, an optimum set of parameters is achieved.
Therefore, the purpose of this paper is to accurate useful information about the parameters that must be considered in order to get the optimum performance of the PEM fuel cell. The optimization is based on a random-search technique which is carried out using the Simulated Annealing algorithm (SA) [12].

2. PEM fuel cell description

The PEM fuel cell that is used in the present study is the GenCore® 5B48 model from Plug Power [14]. This system is designed to provide quality backup DC electric power for critical service DC bus applications. A positive output nominal voltage of +48Vdc is provided (Adjustable Voltage: +46 Vdc to +56Vdc), an operating current range of 0-109 Amps, as well as a continuous output power range of 0-5000W which can be used to supply the DC bus or to charge an existing battery bank. It has 63 cells, and a 99.95% hydrogen dry supply is necessary and the operation temperature range varies between +42°C and +56°C. Temperature operation is almost constant and equal to +55ºC in order to generate the electricity.
The GenCore® system is fuelled with hydrogen at an inlet pressure range of 64 to 96 psig. The hydrogen is however reduced from 80 psi to the range of ±1.2 to 1.8 psi.
The hydrogen pressure considered in the parameters optimization process was 1.6psi=0.108864 atm and the oxygen pressure was 1atm. Fuel Consumption: 36 slm at 3kW, 64 slm at 5kW
A detailed view of the Plug Power system is presented in Figure 1.

2.1 Stack Hydrogen and Air Subsystems

The fuel cell stack requires a constant flow of hydrogen and oxygen (from ambient air) in order to sustain the electrochemical reactions for the power required. Hydrogen is introduced from the HSM (or other hydrogen delivery option) into the Fuel Cell System and into the stack. However, not all hydrogen is consumed during its first pass through the stack, requiring a recirculation of some hydrogen. The stack hydrogen and air subsystems work to keep the required amount of fuel and oxygen running through the stack. Both subsystems have provisions to drain condensate from their gas streams. In the Exhaust Gas Recirculation (EGR) blower circulates unused hydrogen, inert gasses and water vapour from the anode exit to the anode inlet. Recirculation is required to prevent build up of liquid-phase water in the stack cell channels. The Exhaust Gas Recirculation (EGR) and Cathode Air Stack fittings have integral floats valves with condensate drain ports on the bottom to remove excess water.

2.1.1 Functions of the Air Subsystem

1) Deliver filtered and warmed Cathode Air to the Fuel Cell Stack for the chemical reaction.
2) Remove excess water from the Fuel Cells.
3) Accept non-fuel gasses from Exhaust Gas Recirculation (EGR) orifice for discharge.

2.1.2 Functions of the Hydrogen Subsystems

1) Deliver hydrogen to the fuel cell stack at the required pressure the chemical reaction.
2) Control hydrogen gas flow into the Fuel Cell System, and isolate it if necessary.
3) Recirculate exhaust gases to remove excess water and non-fuel gasses.

Figure 1 – Overview of the PEM GenCore™ fuel cell system.

2.2 Heating and Cooling Subsystem

It is important to keep the GenCore® fuel cell stack and system enclosure at the correct temperature.
This can mean heating the enclosure and stack during cold ambient temperature conditions; and cooling the stack during operation. Therefore, the functions concerning to the heating and cooling subsystems are:
1) Maintain stack coolant inlet temperature in the proper operating range during stack operation.
2) Maintain the FCS enclosure and stack temperature to >10 degrees Celsius.

3. PEM fuel cell Operation

Since each fuel cell can produce about 1Vdc, the GenCore® employs a stack of 63 such fuel cells to raise the output voltage. When stacked, machined holes in the fuel cells form headers that allow for the hydrogen, oxygen, and coolant to be distributed throughout the stack. The gasses and PEM are contained between two conductive plates that have flow channels on their faces to direct gas flow to, along the surface of, and from the PEM. The process

creates heat which is removed by coolant in channels on either side of the fuel cell.
In the Fuel Cell Stack heat and water are created as a result of the hydrogen and oxygen reaction.
Coolant is provided to the Stack where it flows between each cell. A thermostat at the top of the Coolant Outlet header directs coolant to the radiator when the temperature is high enough. Excess water falls to the bottom of the hydrogen and air headers where it is drained via float valves. Each cell's voltage is monitored by the control system, in conjunctions with fuel cell scanner cards. A basic scheme for a single cell is shown in Figure 2.

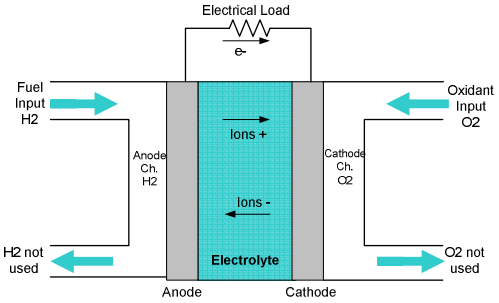

Figure 2 - Scheme of the reactions for a single cell.

The electrochemical reactions involved in the process can be described by the equations:

In the anode side:

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

In the cathode side:

$$2H^+ + \tfrac{1}{2}O_2 + 2e \rightarrow H_2O \quad (2)$$

The overall reaction in the cell:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad (3)$$

3.1 Mathematical Model

An electrical equivalent circuit can be used to model the fuel cell dynamical behavior [5]-[7] as represented in Figure 3. Equations (4) - (12) represent the fuel cell stack static electrochemical behavior related to this circuit.
For a single cell, the output voltage can be defined as the result of the following expression [5]-[7]:

$$V_{FC} = E_{Nernst} - V_{act} - V_{Ohmic} - V_{con} \quad (4)$$

For n cells connected in series, forming a stack, the voltage Vs can be calculated by:

$$V_s = n \times V_{FC} \quad (5)$$

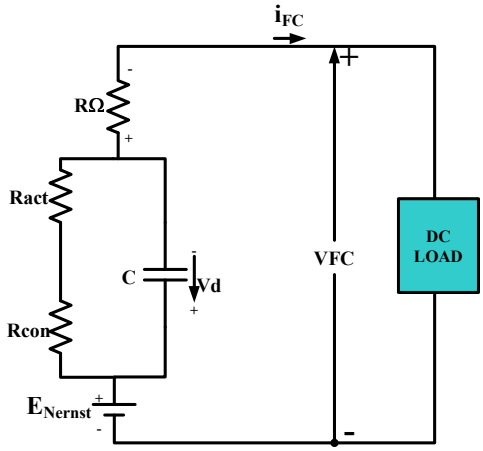

Figure 3 - Electrical equivalent circuit of fuel cell dynamical model.

In (4), E_{Nernst} is the thermodynamic potential of the cell and it represents its reversible voltage; V_{act} is the voltage drop due to the activation of the anode and cathode (also known as activation overpotential); V_{ohmic} is the ohmic voltage drop (also known as ohmic overpotential), a measure of the ohmic voltage drop resulting from the resistances of the conduction of protons through the solid electrolyte and the electrons through its path; and V_{con} represents the voltage drop resulting from the reduction in concentration of the reactants gases or, alternatively, from the transport of mass of oxygen and hydrogen (also known as concentration over potential). Additionally there is another voltage drop associated to the internal currents and the fuel crossover. This voltage drop is considered in the model using a fixed current density even at no-load operation (represented by Jn). The first term of (4) represents the fuel cell open circuit voltage, and the three last terms represent reductions in this voltage to supply the useful voltage across the cell electrodes, V_{FC}, for a certain operation current.
Each one of the terms of (4) are presented and modelled separately. Also, the dynamic behavior of fuel cells and the equations for electrical power generation and efficiency are shown. Each individual term is defined by [5]-[7].

$$E_{Nernst} = 1.229 - 0.85 \times 10^{-3} \times (T - 298.15) + 4.31 \times 10^{-5} \times T \times \left[\ln(P_{H2}) + \frac{1}{2}\ln(P_{O2}) \right] \quad (6)$$

$$V_{act} = -[\xi 1 + \xi 2 \times T + + \xi 3 \times T \times \ln(C_{O2}) + \xi 4 \times T \times \ln(i_{FC})] \quad (7)$$

$$V_{ohmic} = i_{FC} \left(R_M + R_C\right) \quad (8)$$

$$V_{con} = -B \times \ln\left(1 - \frac{J}{J_{\max}}\right) \quad (9)$$

$$CO_2 = \frac{P_{O2}}{5.08 \times 10^6 \times e^{-\left(\frac{498}{T}\right)}} \quad (10)$$

where, PH2 and PO2 are partial pressures (atm) of hydrogen and oxygen, respectively. T is the cell absolute Kelvin temperature.
The cell operating current is iFC (A) and CO2 is the concentration of oxygen in the catalytic interface of the cathode (mol/cm3). The ξi (i = 1,...4) and □ represent the parametric coefficients for each cell model [5]-[7]. R_M is the equivalent membrane resistance to proton conduction. R_C is the equivalent contact resistance to electron conduction. Jmax is the maximum current density. B(V) is a constant dependent on the cell type and its operation state. J is the actual cell current density (A/cm2) including the permanent current density Jn.
The equivalent membrane resistance (R_M) can be calculated by [2]:

$$R_M = \frac{\rho_M \times \lambda}{A} \quad (11)$$

where ρ_M is the membrane specific resistivity (Ω.cm), A is the cell active area (cm2) and l is the thickness of the membrane (cm), which serves as the electrolyte of the cell. ρM is obtained by:

$$\rho_M = \frac{181.6\left[1 + 0.03 \times \left(\frac{i_{FC}}{A}\right) + 0.062 \times \left(\frac{T}{303}\right)^2 \times \left(\frac{i_{FC}}{A}\right)^{2.5}\right]}{\left[\psi - 0.634 - 3 \times \left(\frac{i_{FC}}{A}\right)\right] \times \exp\left[4.18 \times \left(\frac{T - 303}{T}\right)\right]} \quad (12)$$

3.1.1 Dynamics of the cell

To account the phenomenon known as "charge double layer" on which the interface electrode/electrolyte acts as storage of electrical charges and energy, represented by an electrical capacitor in the electrical equivalent circuit of Fig. 2, the dynamical equation of the model is represented by:

$$\frac{dV_d}{dt} = \left(\frac{1}{C} \times i_{FC}\right) - \left(\frac{1}{\tau} \times V_d\right) \quad (13)$$

where Vd represents the dynamical voltage across the equivalent capacitor (associated with Vact and Vcon); C is the equivalent electrical capacitance; and, τ is the fuel cell electrical time constant defined as:

$$\tau = C \times Ra = \\ = C \times \left(R_{act} + R_{con}\right) = \\ = C \times \left(\frac{V_{act} + V_{con}}{i_{FC}}\right) \quad (14)$$

where, Ra is an equivalent resistance.
Including the dynamic behavior represented by (13), the resulting fuel cell voltage is then defined by:

$$V_{FC} = E_{Nernst} - V_{Ohmic} - V_d \quad (15)$$

3.1.2 Power generation and efficiency

The electrical output of the cell can be linked to any load, with no restriction related to the load type if the power supplied by the stack is enough to feed it.
The load may be represented through a boost dc/dc converter, followed by a dc/ac converter and linked to the grid through a transformer if the system is used to inject energy into the grid. The load can be purely resistive or a resistive–inductive if the system is used in isolated form. In any case, the current density of the cell J - (A/cm) is defined by the expression:

$$J = \frac{i_{FC}}{A} \quad (16)$$

and the instantaneous electrical power supplied by the cell to the load can be determined by the equation:

$$P_{FC} = i_{FC} \times V_{FC} \quad (17)$$

where VFC is the cell output voltage for each operating condition and PFC is the output power (Watts). Finally, the FC efficiency - η can be determined by the equation [6]- [9]:

$$\eta = \mu_f \times \frac{V_{FC}}{1{,}48} \quad (18)$$

where μf is the fuel utilization coefficient, generally in the range of 95%, and 1.48V corresponds to the maximum voltage that can be obtained using the higher heating value for the hydrogen enthalpy.

4. Optimization method

The optimization of the parameters of the PEM fuel cell is an interesting challenge due to: i) the lack of an exact procedure for parameter identification and ii) the highly nonlinear optimization problem where the objective function is obtained using a mathematical model [13]. Nonlinear optimization involves the search for a minimum of a nonlinear objective function subject to nonlinear constraints.
Normally for these optimization problems there are multiple optima. Because of this difficulty, two different approaches have emerged in this area: 1) Local methods, which do not aim to obtain an absolute minimum, but can guarantee that local minimum is achieved and 2) global methods, which aim to obtain the absolute minimum of the function.

4.1 Simulated Annealing (SA)

To solve the optimization problem presented in this work, the Simulated Annealing (SA) algorithm for Matlab [12] is used.
The SA algorithm is a random-search technique which exploits an analogy between the way in which a metal cools and freezes into a minimum energy crystalline structure (the annealing process) and the search for an optimum in a more general system.
A major advantage of SA is its ability to avoid becoming trapped in local minimum. The algorithm employs a random search which not only accepts changes that decrease the objective function f, but also some changes that increase it. The latter can be accepted with a probability p. Its flexibility and robustness as a global search method are also extremely important advantages of this method.
The model of the PEMFC system presented in the previous section requires the definition of the following parameters: A-cell active area (cm2), l- membrane thickness (μm), R_C-contact resistance(Ω), ξi(i=1,2,3,4) and ψ - parametric coefficients, Jn - no-load current density (A/cm2), Jmax - maximum current density (A/cm2), C - equivalent electrical capacitance (F).
These parameters needed to be estimated by the optimization process represented through the flowchart follow.

4.2 Optimum operating parameters

Table I lists the initial set of parameters given by [9] and the corresponding optimum solution. The optimum set of parameters given by the optimization algorithm is obtained with the following conditions: initial temperature – 15 ºK, number of iterations - 500, cooling rate temperature - 0.97.
Therefore, this section serves for the identification of the correct parameters to use in the dynamic PEMFC model which corresponds to the better conditions of PEMFC performance.

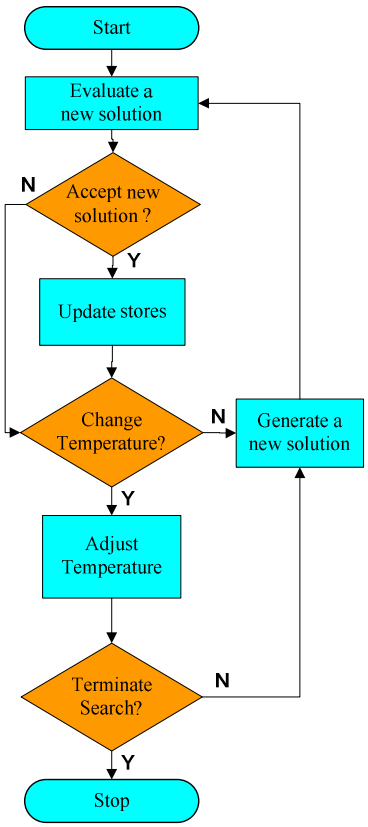

Table 1- Initial and optimal parameters.

PEM Parameter	*Initial Solution*	*Optimum Solution*
A	50.6	69.7 cm2
λ	178 μm	118 μm
B	0.0160 V	0.0171 V
RC	0.00030 Ω	0.00019 Ω
C	3.0 F	2.3 F
ξ1	-0.948	-0.475
ξ2	Equation *	Equation *
ξ3	7.6e-5	0
ξ4	-1.93e-4	-1.0 e-4
ψ	23.0	26.8
Jmax	1500mA/cm2	1600 A/cm2
Obj. Function	3.287284	2.620216

$*\,\xi 2 = 0.00286 + 0.0002 \times \ln A + \left(4.3.10^{-5}\right) \times \ln C_{H2}$

5. Results and discussion

The performance of the PEM fuel cell GenCore™5B48 is characterized thorough experimental tests. A comparison between simulation and experimental results was made for several variables for the validation of the developed model.

In Figure 4 and Figure 5, there are shown the stack voltage and stack power, respectively. The tests were made by a DC/AC power converter; a DC load current was applied for a period of 52,4min during 2,1min of step interval for each value of load from 5.15A to 126,9A.

As can be observed, the stack voltage decreases slightly with the increase of the stack current. This decrease on the stack voltage is due to: 1) the voltage drop associated with the activation of anode and cathode, Vact, 2) the voltage drop resulting from the resistances of the conduction of protons through the solid electrolyte and the electrons through its path, Vohmic, and 3) the voltage drop resulting from the decrease in the concentration of the oxygen and hydrogen, Vcon .The stack voltage decays from 54.26 to 42.17 V for this stack.

This characteristic of the stack is also referred to as the polarization curve of the stack.

The stack power presented in Figure 5 is in accordance with the information provided by the manufacturer. For 126.9 A of demanded load, the stack provides 5360W of power.

Figures 6 and 7 show the efficiency of the system and the hydrogen consumption, respectively. The typical PEM fuel cell efficiency related to the chemical conversion is normally in the range of 40-50%. The efficiency for this stack, as can be seen in Figure 6 is in this range. The minimum and maximum values are 45.15 and 55.94, respectively.

In Figures 8 and 9 the fuel cell stack voltage is shown before and after optimization. Similarly, Figure 10 corresponds to the stack power after optimization. These figures clearly illustrate the efficiency of the optimization algorithm used.

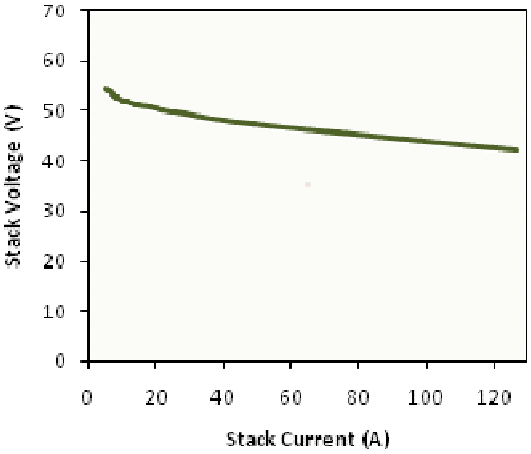

Figure 4 - Experimental PEMFC V-I characteristic.

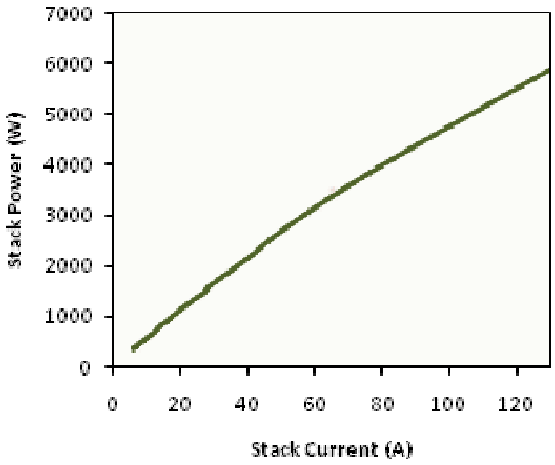

Figure 5 - Experimental stack power.

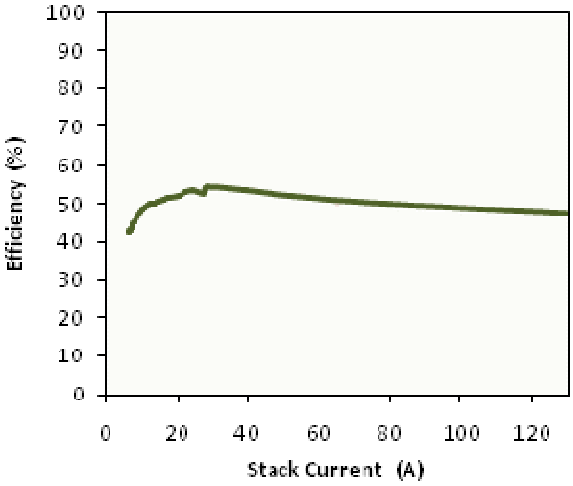

Figure 6 - Experimental efficiency.

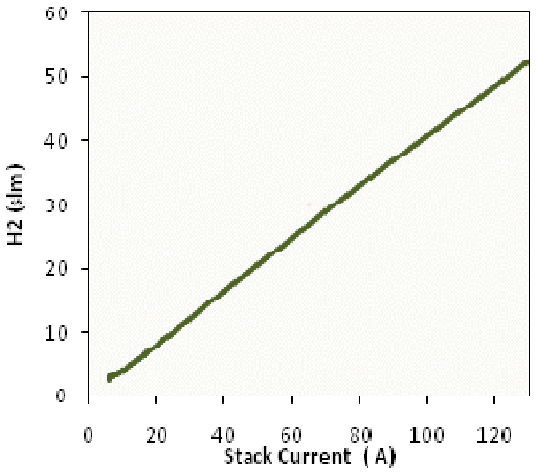

Figure 7 - Experimental hydrogen consumption.

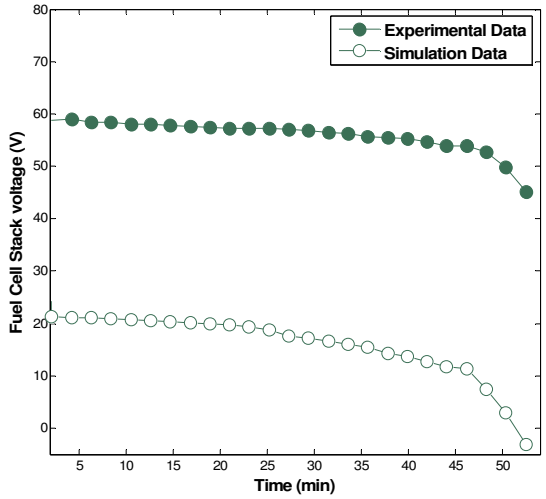

Figure 8- Fuel cell stack voltage before optimization

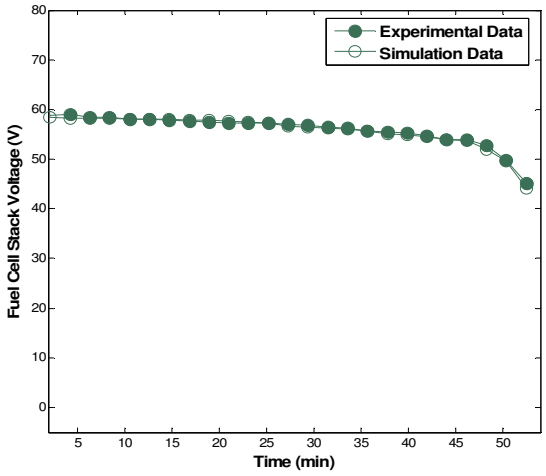

Figure 9 - Fuel cell stack voltage after optimization

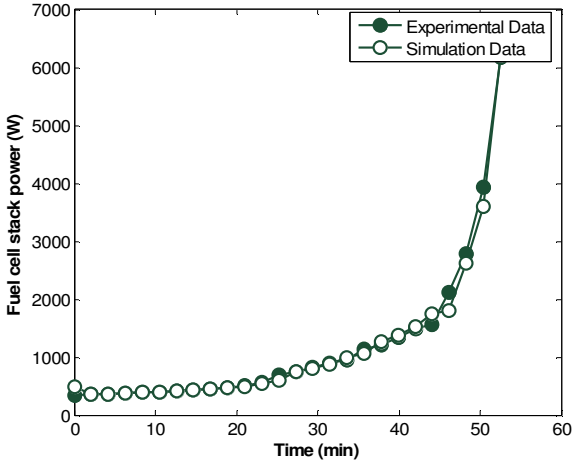

Figure 10- Fuel cell stack power after optimization

5. Conclusions

Efficient parameter extraction techniques are need for designers working with fuel cell model. Accurate simulations are only possible with the knowledge of correct model parameters.

It is show in this paper that an extraction based on a random-search technique produces excellent results.

The method adopted is the Simulated Annealing algorithm (SA), which evolves by converging to a minimum of an objective function.

Results show a good agreement between experimental and simulated waveforms.

The performance of the PEM fuel cell is also characterized thorough a set of experimental tests.

As a result, the model presented in this paper can be used as a block in the construction of simulators or generation systems using PEMFC with good dynamic responses.

Acknowledgments

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Author(s) address

M. T. Outeiro, Department of Electrical Engineering, Institute of Engineering of Coimbra, 3030-119 Coimbra, Portugal

R. Chibante, Department of Mathematics, Institute of Engineering of Porto, 4200-072 Porto, Portugal

A. S. Carvalho, Department of Electrical Engineering and Computers, Engineering Faculty of Oporto University, 4200-465 Porto, Portugal

A.T. de Almeida, Department of Electrical Engineering and Computers, Faculty of Science and Technology, Coimbra University, 3030-290 Coimbra,Portugal