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DYNAMIC MODELING AND SIMULATION OF AN OPTIMIZED PROTON EXCHANGE MEMBRANE FUEL CELL SYSTEM

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ABSTRACT

Hydrogen and fuel cells are widely regarded as the key to energy solutions for the 21st century. These technologies will contribute significantly to a reduction in environmental impact, enhanced energy security and development of new energy industries. Fuel cells operating with hydrogen have the potential to contribute to the transition for a future sustainable energy system with low-CO_2 emissions.

In this paper a dynamic PEM fuel cell model, implemented in Matlab/Simulink, is presented. In order to estimate the PEM fuel cell model parameters, an optimization based approach is used. The optimization is carried out using the Simulated Annealing (SA) algorithm. This optimization process evolves converging to a minimum of the objective function. The flexibility and robustness of SA as a global search method are extremely important advantages of this method.

A good agreement between experimental and simulated results is observed. This optimized PEM fuel cell model can significantly help designers of fuel cell systems by providing a tool to perform accurate design and consequently to improve system efficiency.

NOMENCLATURE

A	cell active area (cm2)
C	equivalent electrical capacitance (F)
E_{Nernst}	thermodynamic potential
Jn	no-load current density (A/cm2)
Jmax	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)
R_C	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

INTRODUCTION

Fuel cells are generally considered as a clean, efficient and silent technology that can produce electricity and heat from fossil fuels, biofuels as well as hydrogen produced from renewable energy sources such as wind energy and solar energy. The expectations for the commercial introduction of fuel cells in a large scale in transports and stationary applications have not yet been realized.

The fact is that fuels cells are still expensive, require hydrogen-rich fuel, have shorter lifetimes than current grid-connected power technologies (for example PEM fuel cells are unreliable past 2000 hrs), involve high system complexity and a lack of fuel infrastructure. Thus, they are not used for grid connected systems except in certain niche applications where their secondary benefits (such as low noise) outweigh the high cost.

Nevertheless, research and development efforts put into the fuel cells technologies combined with their enormous potentialities have made them very attractive candidates for applications in automotive and stationary applications as well, particularly the PEM fuel cells.

However, performance of PEM fuel cells is known to be influenced by many parameters, such as operating temperature, pressure and discharge current. In order to improve fuel cell performances, it is essential to understand these parametric effects on fuel cell operation. To understand and improve the performance of PEMFCs, researchers have developed several mathematical models to explain the behavior of potential variation with the discharge current [1] – [3].

The 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 [4]. The models can also provide detailed data that are frequently unavailable from experiments within an operating fuel cell system.

Fuel cell models require physical parameters that manufactures usually do not provide. Therefore, an accurate parameter extraction procedure must be developed in order to obtain reliable simulations results.

Following this objective an optimization approach is proposed in the present study. The optimization is carried out using the Simulated Annealing (SA) algorithm, which evolves converging to a minimum of an objective function that minimizes the error between experimental and simulation results.

FUEL CELL TYPES AND OPERATION

Whereas the 19th Century was the century of the steam engine and, the 20th Century was the century of the internal combustion engine; it is likely that the 21st Century will be the century of the fuel cell systems and hydrogen economy [5].

Full cells are now on the verge of being introduced commercially, revolutionizing the way we presently produce power. Fuel cells can use hydrogen as a fuel, offering the prospect of supplying the world with clean, sustainable electrical power.

The integrated energy system of the future would combine large and small fuel cells for domestic and decentralized heat and electricity power generation with local (or more extended) hydrogen supply networks that would also be used to fuel conventional (internal combustion) or fuel-cell vehicles [5].

There are several different types of fuel cells, most often categorized by the type of electrolyte present. Four of the more common fuel cells are proton exchange membrane fuel cells (PEMFC), phosphoric acid fuel cells (PAFC), molten carbonate fuel cells (MCFC), and solid oxide fuel cells (SOFC). The PEMFC is probably the most well known fuel cell and shows promise for applications in the medium power range.

TABLE 1
CHARACTERISTICS OF FUEL CELL TYPES

	PEMFC	PAFC	MCFC	SOFC
Electrolyte	Membrane Polymer	Phosphoric Acid	Molten Mixture	Ceramic
Catalyst	Platinum	Platinum	Nickel	Perovskites
Temperature Operation	50- 80º C	150-200º C	≈650º C	800-1000º C
Output Power Range	50-250KW	< 200 KW	10KW-2MW	< 100KW
Efficiency	40-50%	40-80%	60-80%	~60%
Electrolyte	Membrane Polymer	Phosphoric Acid	Molten Mixture	Ceramic

Because of its efficiency and relatively low operating temperature range, the PEMFC is ideal for residential applications and is the chosen fuel cell for the system under study.

The PEMFC is especially attractive for automotive applications due to its higher power density (power per fuel cell active area) and lower operating temperature compared to other types of fuel cells.

The modeling and optimization of the PEMFC system carried out in this paper is aimed at achieving better fuel cell system designs.

Although fuel cell technology development requires a complex multidisciplinary effort, the basic concept of fuel cell operation is very simple. A fuel cell is an electrochemical device that converts chemical energy typically from hydrogen, directly into electrical energy. Similar to a battery, a fuel cell consists of two electrodes (anode and cathode) and an electrolyte. A basic scheme for a single cell is shown in Figure 1.

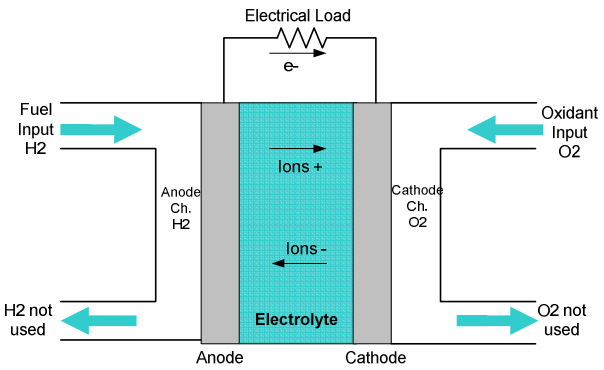

Figure 1 - Scheme of a single cell.

The electrochemical reactions involved in the process can be described such that in the anode side diatomic hydrogen is circulated through the anode channel in the separation plates and therefore, distributed across the PEM and catalysts by the microporous Gas Diffusion Layer. When the hydrogen gets near activation sites in the catalyst and transfer sites on the PEM, the molecules break up to single atoms and the hydrogen nuclei attach to the PEM. The electrons (e-) left behind attach to the conductive plate and are directed to an external circuit to produce power. As the fuel cell produces power, some of the water from the cathode side permeates to the anode side increasing the efficiency of the proton transfer to the PEM. This reaction can be represented by the equation:

$$H_2 \rightarrow 2H^+ + 2e^- \tag{1}$$

In the cathode side, heated, humidified air containing diatomic oxygen is distributed across the PEM and catalysts through the channels in the separation plates and microporous Gas Diffusion Layer. When the oxygen gets near activation sites in the catalyst, the molecules break up to single atoms. Electrons return from the external circuit and the cathode separation plate and the hydrogen protons (H+) are pulled from the PEM. Two electrons, two protons and an oxygen atom form a water molecule with release of excess heat. This reaction can be represented by the equation:

$$2H^+ + \tfrac{1}{2}O_2 + 2e \rightarrow H_2O \tag{2}$$

The overall reaction is represented by the equation:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \tag{3}$$

MODELLING OF THE PEMFC SYSTEM

An electrical equivalent circuit can be used to model the fuel cell dynamical behavior [4, [6], as represented in Figure 2. Equations (4) and (5) represent the fuel cell stack static electrochemical behavior.

For a single cell, the output voltage can be defined as the result of the following expression [6] - [8]:

$$V_{FC} = E_{Nernst} - V_{act} - V_{Ohmic} - V_{con} \tag{4}$$

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

$$V_s = n \times V_{FC}\ H_2 \rightarrow 2H^+ + 2e^- \tag{5}$$

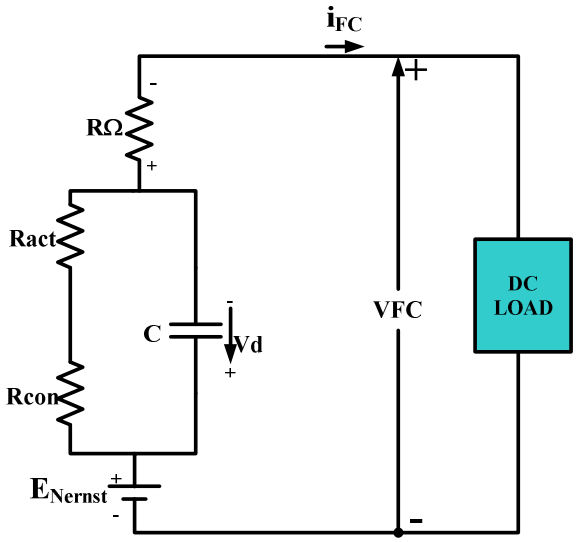

Figure 2 – Electrical equivalent circuit of PEM fuel cell dynamical model.

In Eq. (4), E_{Nernst} is the thermodynamic potential of the cell and it represents its reversible voltage; Vact is the voltage drop due to the activation of the anode and cathode (also known as activation overpotential); Vohmic 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 Vcon 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). But 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 Eq. (1) 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 Eq. (4) are presented and modeled 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 [6].

$$E_{Nernst} = 1.229 - 0.85\times10^{-3}\times(T - 298.15) + \\ + 4.31\times10^{-5}\times T\times\left[\ln(P_{H2}) + \frac{1}{2}\ln(P_{O2})\right] \tag{6}$$

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

Where ξ1, ξ3, and ξ4 are constant parameters and ξ2 is given by;

$$\xi 2 = 0.00286 + 0.0002 \times \ln A + \left(4.3.10^{-5}\right) \times \ln C_{H2} \quad (8)$$

$$V_{ohmic} = i_{FC}\ \left(R_M + R_C\right) \quad (9)$$

$$V_{con} = -B \times \ln\left(1 - \frac{J}{J_{\max}}\right) \quad (10)$$

$$C_{O_2} = \frac{P_{O2}}{5.08 \times 10^6 \times e^{-\left(\frac{498}{T}\right)}} \quad (11)$$

where, P_{H2} and P_{O2} are partial pressures (atm) of hydrogen and oxygen, respectively. T is the cell absolute Kelvin temperature.

The cell operating current is i_{FC} (A) and CO_2 is the concentration of oxygen in the catalytic interface of the cathode (mol/cm3). The ξi (i = 1,...4) and ψ represent the parametric coefficients for each cell model [9] - [11]. R_M is the equivalent membrane resistance to proton conduction. RC 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 [6]:

$$R_M = \frac{\rho_M \times l}{A} \quad (12)$$

where ρ_M is the membrane specific resistivity (Ω.cm) obtained by:

$$\rho_M = \frac{181.6\left[1 + 0.03 \times \left(\frac{i_{FC}}{A}\right) + 0.062 \times \left(\frac{T}{303}\right)^2 \times \left(\frac{i_{FC}}{A}\right)^{2.5}\right]}{\left[\psi - 0.634 - 3 \times \left(\frac{i_{FC}}{A}\right)\right] \times \exp\left[4.18 \times \left(\frac{T - 303}{T}\right)\right]} \quad (13)$$

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 Figure 3, the dynamical equation of the model is represented by:

$$\frac{dV_d}{dt} = \left(\frac{1}{C} \times i_{FC}\right) - \left(\frac{1}{\tau} \times V_d\right) \quad (14)$$

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:

$$\tau = C \times Ra = C \times \left(R_{act} + R_{con}\right) = C \times \left(\frac{V_{act} + V_{con}}{i_{FC}}\right) \quad (15)$$

where, Ra is an equivalent resistance.

Including the dynamic behavior represented by Eq. (14), the resulting fuel cell voltage is then defined by:

$$V_{FC} = E_{Nernst} - V_{Ohmic} - V_d \quad (16)$$

The electrical output of the cell can be linked to any load, with no restriction related to the load type since the power supplied by the stack is enough to feed it.

The load can 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 (A/cm) is defined by the expression:

$$J = \frac{i_{FC}}{A} \quad (17)$$

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

$$P_{FC} = i_{FC} \times V_{FC} \quad (18)$$

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

$$\eta = \mu_f \times \frac{V_{FC}}{1{,}48} \quad (19)$$

where μ_f 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.

OPTIMIZATION OF THE PEMFC MODEL

The dynamical model of the PEM fuel cell system presented in previous section requires the definition of several parameters: A- cell active area (cm2), l- membrane thickness (μm), RC- 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) and C- equivalent to electrical capacitance (F). These parameters are estimated by an optimization process. To solve the optimization problem, the Simulated Annealing (SA) optimization algorithm was used [10], [11].

The implementation of the annealing strategy as shown in Figure 3 is very simple and requires definition of some parameters:

1) Initial population (initial guess);
2) Initial temperature (T0);
3) Perturbation mechanism – a method to create new trial vector of values for parameters;
4) Objective function – a scalar equation to measure the goodness of each trial vector;
5) Cooling schedule (s) – a method that controls how temperature decreases. Note that temperature must be large enough to move off a local minimum but small enough not to move off a global minimum;
6) Terminating criterion – a method to control termination of algorithm. It could be a maximum number of iterations, a minimum temperature, a minimum value of objective (cost) function, or a combination of three.

Considering an initial set of parameters, the PEM fuel cell model compares simulated and experimental waveforms, producing an error value (objective function). Then, parameters are varied and simulation is re-executed to produce new waveforms. This is again compared with measured data and optimization continues accordingly. Once parameters have converged to give a minimum error, optimization process stops and the optimal set of model parameters for the PEMFC are obtained.

Table 2 below lists the initial set of parameters given by [8] and correspondent optimum values obtained for the stacks.

The optimum set of parameters given by the optimization algorithm was obtained with the following conditions: initial temperature is 15°K, number of iterations is 500 and the cooling rate temperature is 0.97.

Therefore, these optimum parameters will be used to characterize the performance of the PEMFC system.

The model allows at getting the all parameters within analytical formulation of any fuel cell. In consequence, fuel cell performance characteristics are well described as they are carried out through a methodology that simultaneously calibrates the model.

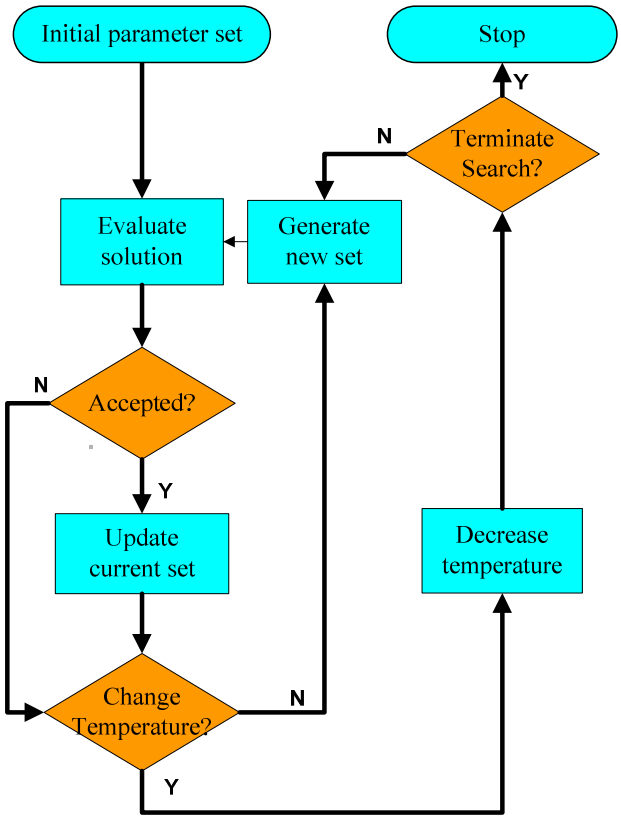

Figure 3 – Flowchart representation of the annealing algorithm.

TABLE 2
INITIAL AND OPTIMAL STACK PARAMETERS

Parameter	Initial Value	Optimum Value
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 (8)	Equation (8)
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

EXPERIMENTAL SETUP

A proton exchange membrane fuel cell system GenCore™ 5B48 from Plug Power [12] was used in order to validate the model presented above. This system is designed to provide quality backup DC electric power for critical service DC bus applications. Both provide a positive output nominal voltage of +48Vdc (range from +42 to +60 Vdc), 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 ±1.5 to 1.8 psi.

Hydrogen and oxygen pressures are very important conditions in the performance of the PEMFC. The hydrogen pressure considered for the identification of parameters was 1.6psi=0.108864 atm and the oxygen pressure was 1atm.

A detailed view of the Plug Power system is presented in Figure 4.

Figure 4 – Plug Power GenCore™ Fuel Cell System.

ANALISYS AND DISCUSSION OF RESULTS

For characterization of the performance of the PEMFC, some tests had been made with the GenCore™5B48 system. The experimental results provided can be observed in figures below. These experimental results are also compared with the simulated, with validated the system model developed in Matlab and Simulink software.

In Figure 5 and Figure 6, 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, V_{act}, 2) the voltage drop resulting from the resistances of the conduction of protons through the solid electrolyte and the electrons through its path, V_{ohmic}, and 3) the voltage drop resulting from the decrease in the concentration of the oxygen and hydrogen, V_{con} .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 6 is in accordance with the information provided by the manufacturer. For 126.9 A of demanded load, the stack provides 5360W of power.

Figures 7 and 8 show the efficiency of the system and the hydrogen consumption, respectively. The typical PEMFC 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 7 is in this range. The minimum and maximum values are 45.15 and 55.94, respectively.

Similarly of the stack power, it is verified that the hydrogen consumption, presented in Figure 8, is proportional to the power demanded for the load.

A comparison between simulation and experimental results was made for several variables for the validation of the developed model.

In Figures 9 and 10 the fuel cell stack voltage is shown before and after optimization. Similarly, Figure 11 corresponds to the stack power after optimization. These figures clearly illustrate the efficiency of the optimization algorithm used.

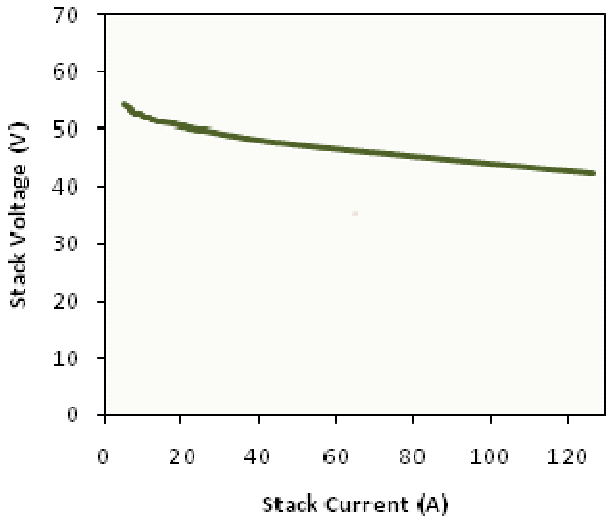

Figure 5 – Experimental PEMFC V-I characteristic.

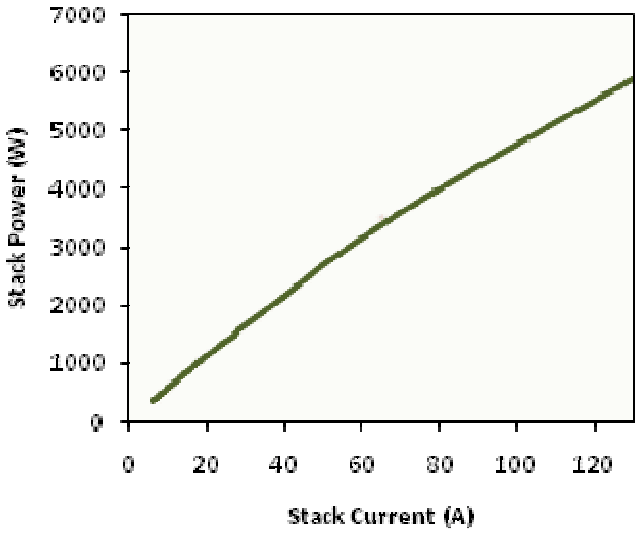

Figure 6 – Experimental stack power.

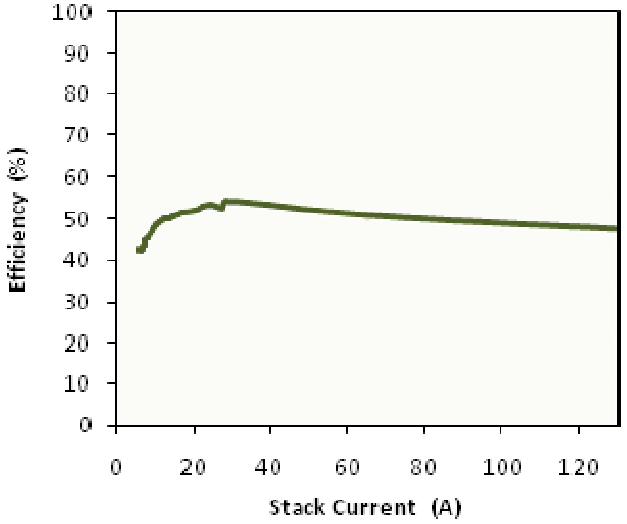

Figure 7 – Experimental efficiency.

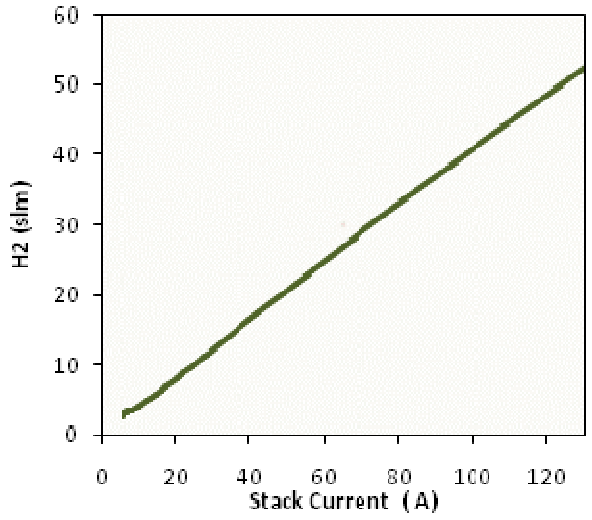

Figure 8 – Experimental hydrogen consumption.

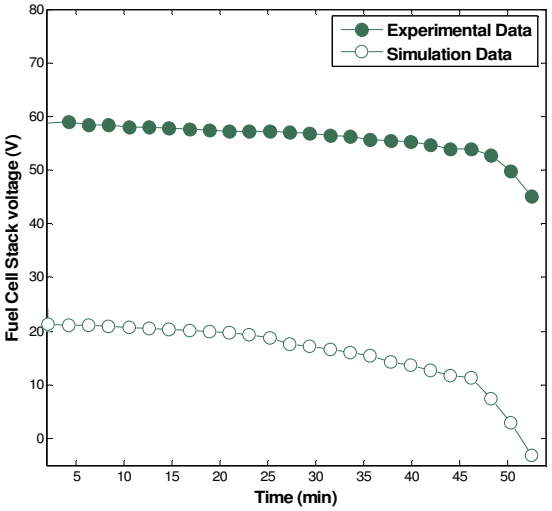

Figure 9 – Fuel cell stack voltage before optimization.

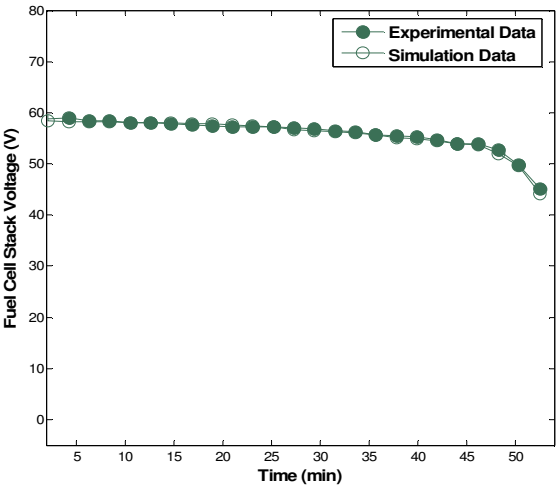

Figure 10 – Fuel cell stack voltage after optimization.

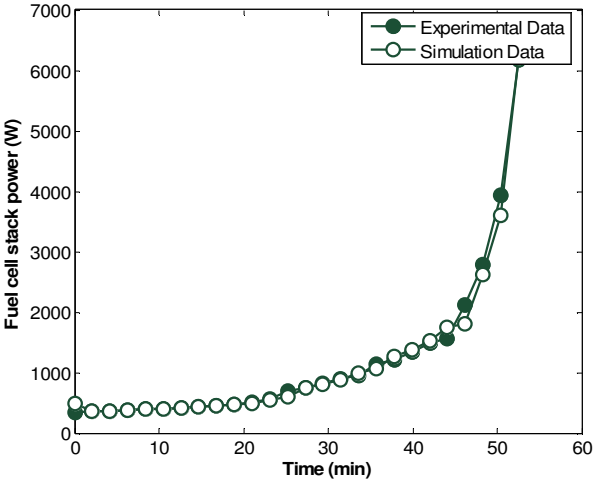

Figure 11 – Fuel cell stack power after optimization.

CONCLUSIONS

Performance of PEM fuel cells is known to be influenced by many parameters, such as operating temperature, pressure and discharge current. In order to improve fuel cell performances, it is essential to understand these parametric effects on fuel cell operation.

Fuel cell models require physical parameters that manufactures usually do not provide. Therefore, an accurate parameter extraction procedure must be developed in order to obtain reliable simulations results.

Following this objective, a new optimization method for accurate model of Proton Exchange Membrane Fuel Cell (PEMFC) systems is presented in this paper.

The method adopted in order to determine the optimum set of these parameters is SA algorithm, which proves to be well adapted to satisfy this goal of a fast convergence to establish right values for the cell parameters.

The optimized results show a good agreement between experimental and simulated waveforms.

As a result, the model allows at getting the all parameters within analytical formulation of any fuel cell. In consequence, fuel cell performance characteristics are well described as they are carried out through a methodology that simultaneously calibrates the model.

It can be used as a block in the construction of simulators or generation systems using fuel cells with good dynamic response.

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