An Electrochemical-Based Fuel-Cell Model Suitable for Electrical Engineering Automation Approach

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***Abstract*—This paper presents a dynamic electrochemical model for representation, simulation, and evaluation of performance of small size generation systems emphasizing particularly proton exchange membrane fuel-cell (PEMFC) stacks. The results of the model are used to predict the output voltage, efficiency, and power of FCs as a function of the actual load current and of the constructive and operational parameters of the cells. Partial and total load insertion and rejection tests were accomplished to evaluate the dynamic response of the studied models. The results guarantee a better analytical performance of these models with respect to former ones with a consequent reduction in time and costs of projects using FCs as the primary source of energy. Additionally, this electrochemical model was tested for the SR-12 Modular PEM Generator, a stack rated at 500 W, manufactured by Avista Laboratories, for the Ballard Mark V FC and for the BCS 500-W stack.**

***Index Terms*—Automation, control, fuel cells (FCs), modeling and simulation.**

I. Introduction

NONPOLLUTING energy generation and other environmental issues have been driving during the last few years an increasing demand for new energy conversion technologies. Within such perspective, fuel cell (FC) systems have been showing up as a promising alternative due their high efficiency, low aggression to the environment, excellent dynamic response, and superior reliability and durability in space, automotive, and stationary applications. In particular, proton exchange membrane FCs (PEMFCs) are considered great alternatives for distributed sources of energy. PEMFCs produce water as by-product waste, operating at low temperatures and allowing fast startup. PEMFCs use a solid polymer as the electrolyte, reducing construction, transportation, and safety concerns.

An FC produces electrochemical power due to the passage of a rich gas in hydrogen through an anode and in oxygen (or air) through a cathode, with an electrolyte between the anode and cathode to enable the exchange of electrical charges (ions). The ion flow through the electrolyte produces an electrical current in an external circuit or load.

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Any hydrocarbon material, in principle, can be used as fuel independent on being gas, liquid, or solid. However, these materials have to pass through a reformer to liberate the hydrogen of the carbon. Natural gas, for example, is reformed through vapor and high temperatures. A similar process, called gasification, is applied to coal, biomass, and to a wide range of hydrocarbon residues [9].

Under normal operation, a simple FC typically produces 0.5–0.9 V. For use in energy generation systems, where a relatively high power is needed, several cells are connected in series, arranging a stack that can supply hundreds of kilowatts. It is expected that in near future commercially available products will be rated at the megawatt range.

There is a need for a reliable mathematical model. Such model can allow the evaluation of the PEMFC dynamic performance for small-size electrical energy generation systems, reducing cost and time along the design stage and tests. Such need motivated us to conduct an electrochemical modeling to determine the open-circuit voltage and the voltage drops of the cells for each operating point. In power generation systems, the dynamic response is extremely important for the planner of control and management systems, especially when there is injection of energy into the grid. Therefore, special attention should be given to the dynamic response of the FC.

Different models of PEMFCs are available in the literature [1], [2]. In [3], a dynamical model for the PEMFC is presented, but it is more suitable for electrochemical purposes than for electrical engineering. For example, when considering the injection of FC energy into the grid, the generation control system should decide which amount of power the FC will supply to the grid, as a function of the load demand. For this, the dynamic response of the FC, considering the viewpoint of energy systems, should be compatible with the fast variations of a random load curve. Recently, this subject has caught the attention of many authors [4]–[8]. For example, in [4][1] is presented a dynamical model using PSpice, which is adequate for circuit simulation, including power electronics. In [8], is presented a very simplified electrical model, which is used to derive a fuzzy control system for a boost dc/dc converter.

Taking these aspects into consideration, this paper presents a model that predicts the FC stack performance against situations commonly encountered in electrical power generation systems, like insertion and rejection of loads, efficiency, and power characteristics. Using the present dynamical model, it is also possible to develop several control techniques for the operation of

[1]Slides of [4] are available at http://www.nfcrc.uci.edu/UFFC/PowerElectronics/PDFs/20_Famouri.pdf

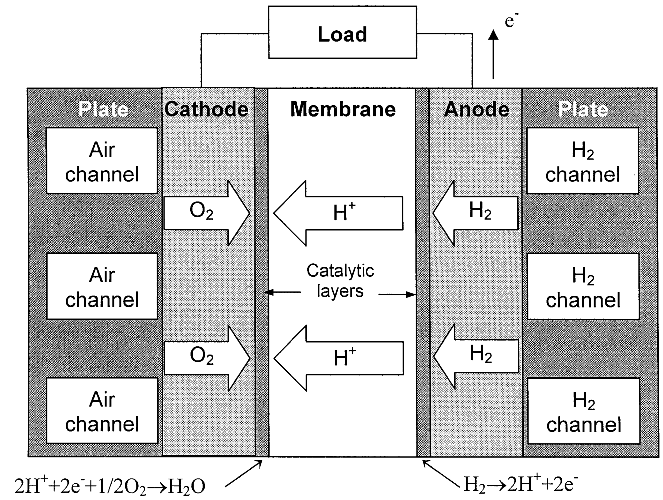

Fig. 1. Basic PEMFC operation.

the PEMFC, such as Fuzzy Logic Control and Hill Climbing Control (HCC) [5]. The model is well adapted for PEM cells and it incorporates the essential physical and electrochemical processes that happen in the cells along its operation. For practical evaluation, the parameters of a Mark V cell, manufactured by the Canadian company Ballard, Burnaby, BC, are used, whose operation and data are well known in the literature, allowing the comparison of the simulation results with practical tests. Also, as examples applied to FC stacks, there are sections dedicated to obtain the electrochemical model for the following stacks: 1) SR-12 Modular PEM Generator, manufactured by the American company Avista Laboratories [10], at a rated power of 500 W and 2) BCS 500 W stack, manufactured by the American company BCS Technology Inc. [11], also at a rated power of 500 W.

II. Basic FC Operation

A PEMFC converts the chemical energy of a fuel, just as the hydrogen (H_2), and an oxydizer, just as the oxygen (O_2), in electrical energy. The outline of a typical PEMFC is illustrated in Fig. 1 [3]. On one side of the cell, referred to as the anode, the fuel is supplied under certain pressure. The fuel for this model is the pure gas H_2, although other compositions of gases can be used. In these cases, the hydrogen concentration should be determined in the mixture. The fuel spreads through the electrode until it reaches the catalytic layer of the anode where it reacts to form protons and electrons, as shown below in the reaction

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

The protons are transferred through the electrolyte (solid membrane) to the catalytic layer of the cathode. On the other side of the cell, the oxydizer flows through the channels of the plate and it spreads through the electrode until it reaches the catalytic layer of the cathode. The oxydizer used in this model is air or O_2. The oxygen is consumed with the protons and electrons and the product, liquid water, is produced with residual heat on the surface of the catalytic particles. The electrochemical reaction that happens in the cathode is

$$\frac{2\mathrm{H}^+ + 2\mathrm{e}^- + 1}{2\mathrm{O}_2 \rightarrow \mathrm{H_2O} + \mathrm{heat}}. \tag{2}$$

Then, the full physical–chemical FC reaction is

$$\frac{\mathrm{H}_2 + 1}{2\mathrm{O}_2 \rightarrow +\mathrm{H_2O} + \mathrm{heat} + \mathrm{electrical\ energy}}. \tag{3}$$

III. Model Formulation

The output voltage of a single cell can be defined as the result of the following expression [1], [3], [9]:

$$V_{\mathrm{FC}} = E_{\mathrm{Nernst}} - V_{\mathrm{act}} - V_{\mathrm{ohmic}} - V_{\mathrm{con}}. \tag{4}$$

In the equation above, 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), a measure of the voltage drop associated with the electrodes; 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 overpotential). There is another voltage drop associated with the internal currents and/or the fuel crossover [9]. This voltage drop is considered in the model, using a fixed current density even at no-load operation (represented by J_n). The first term of (4) represents the FC open-circuit voltage (without load), while the last three 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) is discussed and modeled separately in the sections that follow. Also, the following sections show the dynamic behavior of FCs and the equations for electrical power generation.

A. Cell Reversible Voltage

The reversible voltage of the cell (E_{Nernst}) is the potential of the cell obtained in an open circuit thermodynamic balance (without load). In this model, E_{Nernst} is calculated starting from a modified version of the equation of Nernst, with an extra term to take into account changes in the temperature with respect to the standard reference temperature, 25 °C [1]. This is given by

$$E_{\mathrm{Nernst}} = \frac{\Delta G}{2 \cdot F} + \frac{\Delta S}{2 \cdot F}(T - T_{\mathrm{ref}}) + \frac{R \cdot T}{2 \cdot F} \cdot \left[\ln(P_{\mathrm{H_2}}) + \frac{1}{2}\ln(P_{\mathrm{O_2}})\right] \tag{5}$$

where ΔG is the change in the free Gibbs energy (J/mol); F is the constant of Faraday (96.487 C); ΔS is the change of the entropy (J/mol); R is the universal constant of the gases (8.314 J/K·mol); while $P_{\mathrm{H_2}}$ and $P_{\mathrm{O_2}}$ are the partial pressures of hydrogen and oxygen (atm), respectively. Variable T denotes the cell operation temperature (K) and T_{ref} the reference temperature. Using the standard pressure and temperature (SPT) values for ΔG, ΔS and T_{ref}, (5) can be simplified to [1]

$$E_{\mathrm{Nernst}} = 1.229 - 0.85.10^{-3} \cdot (T - 298.15) + 4.31.10^{-5} \cdot T \cdot \left[\ln(P_{\mathrm{H}_2}) + \frac{1}{2}\ln(P_{\mathrm{O}_2})\right]. \quad (6)$$

It has to be noted that membrane temperature and gases partial pressures change with cell current: with increasing current, partial pressure of hydrogen or oxygen decreases, whereas temperature increases.

B. Activation Voltage Drop

As shown in [1], the activation overpotential, including anode and cathode, can be calculated by

$$V_{\mathrm{act}} = -[\xi_1 + \xi_2 \cdot T + \xi_3 \cdot T \cdot \ln(C_{\mathrm{O}_2}) + \xi_4 \cdot T \cdot \ln(i_{\mathrm{FC}})] \quad (7)$$

where i_{FC} is the cell operating current (A), and the ξ's represent parametric coefficients for each cell model, whose values are defined based on theoretical equations with kinetic, thermodynamic, and electrochemical foundations [1]. C_{O_2} is the concentration of oxygen in the catalytic interface of the cathode $(\mathrm{mol/cm}^3)$, determined by

$$C_{\mathrm{O}_2} = \frac{P_{\mathrm{O}_2}}{5.08.10^6 \cdot e^{(-498/T)}}. \quad (8)$$

C. Ohmic Voltage Drop

The ohmic voltage drop results from the resistance to the electrons transfer through the collecting plates and carbon electrodes, and the resistance to the protons transfer through the solid membrane. In this model, a general expression for resistance is defined to include all the important parameters of the membrane. The equivalent resistance of the membrane is calculated by

$$R_M = \frac{\rho_M \cdot \ell}{A} \quad (9)$$

where ρ_M is the specific resistivity of the membrane for the electron flow (Ω·cm), A is the cell active area (cm^2) and ℓ is the thickness of the membrane (cm), which serves as the electrolyte of the cell.

The membrane of the Nafion type considered in this work is a registered trademark of Dupont and broadly used in PEMFC. Dupont uses the following product designations to denote the thickness of the Nafion membranes:

$$\text{Nafion 117}: 7\ \text{mil}\ (\ell = 178\ \mu\text{m});$$
$$\text{Nafion 115}: 5\ \text{mil}\ (\ell = 127\ \mu\text{m});$$
$$\text{Nafion 112}: 2\ \text{mil}\ (\ell = 51\ \mu\text{m}).$$

The following numeric expression for the resistivity of the Nafion membranes is used [1]:

$$\rho_M = \frac{181.6 \cdot \left[1 + 0.03 \cdot \left(\frac{i_{\mathrm{FC}}}{A}\right) + 0.062 \cdot \left(\frac{T}{303}\right)^2 \left(\frac{i_{\mathrm{FC}}}{A}\right)^{2.5}\right]}{\left[\psi - 0.634 - 3 \cdot \left(\frac{i_{\mathrm{FC}}}{A}\right)\right] \cdot \exp\left[4.18 \cdot \left(\frac{T-303}{T}\right)\right]} \quad (10)$$

where the term $181.6/(\psi - 0.634)$ is the specific resistivity (Ω·cm) at no current and at 30 °C; the exponential term in the denominator is the temperature factor correction if the cell is not at 30 °C. The parameter ψ is an adjustable parameter with a possible maximum value of 23. This parameter is influenced by the preparation procedure of the membrane and it is a function of relative humidity and stoichiometry relation of the anode gas. It may have a value order of 14 under the ideal condition of 100% relative humidity. There are also reported values in the order of 22 and 23 under oversaturated conditions.

Using the value of (9) for the membrane resistance, the following expression determines the ohmic voltage drop:

$$V_{\mathrm{ohmic}} = i_{\mathrm{FC}} \cdot (R_M + R_C) \quad (11)$$

where R_C represents the resistance to the transfer of protons through the membrane, usually considered constant.

D. Concentration Or Mass Transport Voltage Drop

The mass transport affects the concentrations of hydrogen and oxygen. This, in turn, causes a decrease of the partial pressures of these gases. Reduction in the pressures of oxygen and hydrogen depend on the electrical current and on the physical characteristics of the system. To determine an equation for this voltage drop, a maximum current density is defined, $J_{\max}$, under which the fuel is being used at the same rate of the maximum supply speed. The current density cannot surpass this limit because the fuel cannot be supplied at a larger rate. Typical values for $J_{\max}$ are in the range of 500–1500 mA/cm^2.

Thus, the voltage drop due to the mass transport can be determined by

$$V_{\mathrm{con}} = -B \cdot \ln\left(1 - \frac{J}{J_{\max}}\right) \quad (12)$$

where $B(V)$ is a parametric coefficient, which depends on the cell and its operation state, and J represents the actual current density of the cell $(\mathrm{A/cm}^2)$.

E. Dynamics of the Cell

In FCs a phenomenon known as "charge double layer" exists. This phenomenon is of extreme importance for the understanding of the cell dynamics: whenever two differently charged materials are in contact there is a charge accumulation on their surfaces or a load transfer from one to the other. The charge layer on the interface electrode/electrolyte (or close to the interface) acts as a storage of electrical charges and energy and, in this way, it behaves as an electrical capacitor. If the voltage changes, there will be some time for the charge (and the associated current) to vanish (if the voltage increases) or to increase (if the voltage decreases). Such a delay affects the activation and concentration potentials. It is important to point out that the ohmic overpotential is not affected, since it is linearly related to the cell current through Ohm's Law. Thus, a change in the current causes an immediate change in the ohmic voltage drop.

In this way, it can be considered that a first-order delay exists in the activation and concentration voltages. The time constant $\tau(s)$ associated with this delay is the product

$$\tau = C \cdot R_a \quad (13)$$

where C represents the equivalent capacitance (F) of the system and R_a the equivalent resistance (Ω). The value of the capac-

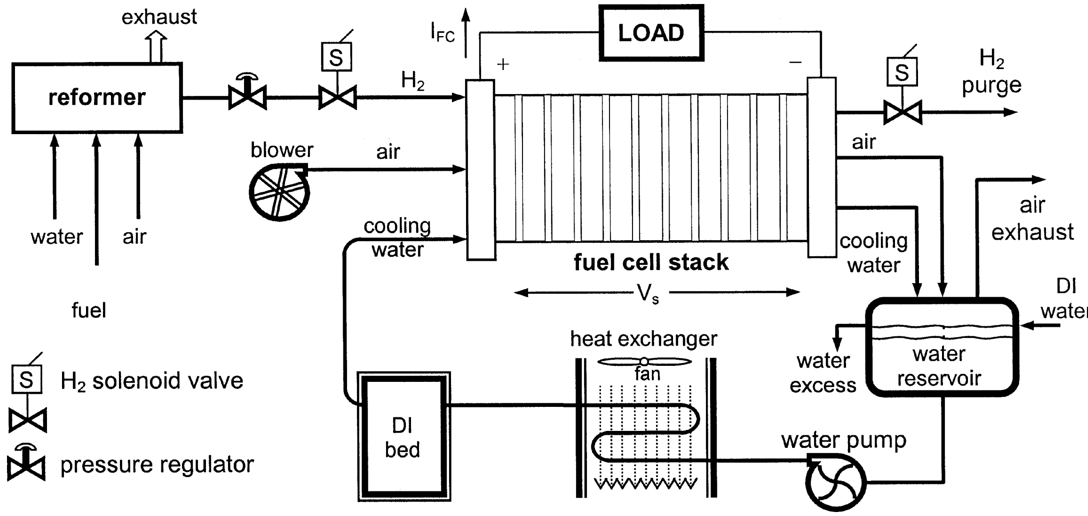

Fig. 2. Generation system with PEMFC stacks.

itance is of some few farads. The resistance R_a is determined from the cell output current and the calculated activation and concentration voltages. In this way, these voltages will change dynamically with the current, until they reach their new steady-stated values. Then, R_a is obtained from

$$R_a = \frac{V_{\text{act}} + V_{\text{con}}}{i_{\text{FC}}}. \tag{14}$$

In broad terms, the capacitive effect assures the good dynamic performance of the cell, since the voltage moves smoothly to a new value in response to a change in the current demand.

F. Power Generation

An electrical energy generation system using a stack of PEMFCs can be represented according to Fig. 2, which shows the stack with the feeding of hydrogen, oxygen (air), and water for refrigeration, as well as its output products, hot water and electricity. V_s represents the stack output voltage, which is obtained from the multiplication of the FC voltage and the number of cells. The reformer is also represented, to obtain hydrogen starting from a fuel with hydrocarbon. The amount of components of the system will depend, mainly, on the total power of the stack.

The electrical output of energy of the cell is linked to a certain load, represented in the diagram of Fig. 2 as a generic load. There is no restriction related to the load type, since the power supplied by the stack is enough to feed it. For example, in systems used to inject energy into the grid, the load can represent a boost dc/dc converter, followed by a dc/ac converter, linked to the grid through a transformer. In isolated systems it can represent a purely resistive load (heating) or a resistive–inductive load (motor), for example. In any case, the density of current of the cell $J(\text{A/cm}^2)$ is defined by the following expression:

$$J = \frac{i_{\text{FC}}}{A}. \tag{15}$$

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

$$P_{\text{FC}} = V_{\text{FC}} \cdot i_{\text{FC}} \tag{16}$$

where V_{FC} is the cell output voltage for each operating condition, (4), and P_{FC} is the output power, in watts.

With a liquid state subproduct, the FC efficiency can be determined from the equation [9]

$$\eta = \mu_f \cdot \frac{V_{\text{FC}}}{1.48} \tag{17}$$

where μ_f is the fuel utilization coefficient, generally in the range of 95%, and 1.48 V represents the maximum voltage that can be obtained using the higher heating value (HHV) for the hydrogen enthalpy. Fuel utilization is assumed to be constant, which is valid where the FC has a hydrogen flow rate control. In this case, the hydrogen is supplied according to the load current.

IV. Simulation Results

A. Model Validation

For validation of the model, one single cell, model Ballard Mark V, was simulated, which was fed with gases H_2 and O_2, using the membrane Nafion 117. The parameters used for this simulation are presented in Table I. Also, Sections V and VI present results for two stack models that confirm the model results.

It should be made a proviso related to the parameters of the cells and of the model. The main proposal of this model is to supply the characteristics of the system operation in a more precisely possible way, allowing the development and improvement of electrical energy generation systems using this new and highly promising technology. However, there is a series of parameters involved in this model, some of them empiric and others difficult to determine. For the simulations that follow, the parameters were mainly obtained in the literature and the results fully agree with those presented in the literature. With development of the technology, more precise parameters, easier to determine, will be obtained, due to the great and growing worldwide interest in the subject. For the current situation, a model that can be used as a block in the construction of simulators of generation systems using PEMFC, with reasonable results and good dynamic response, comes as a quite interesting and

TABLE I
PARAMETERS OF THE BALLARD MARK V FUEL CELL

Param.	Value	Param.	Value
T	343 K	ξ_1	-0.948
A	50.6 cm^2	ξ_2	$0.00286+0.0002.\ln A+(4.3.10^{-5}).\ln c_{H_2}$
	178 μm	ξ_3	$7.6.10^{-5}$
P_{H_2}	1 atm	ξ_4	$-1.93.10^{-4}$
P_{O_2}	1 atm	ψ	23
B	0.016 V	J_{max}	1500 mA/cm^2
R_C	0.0003 Ω	J_n	1.2 mA/cm^2

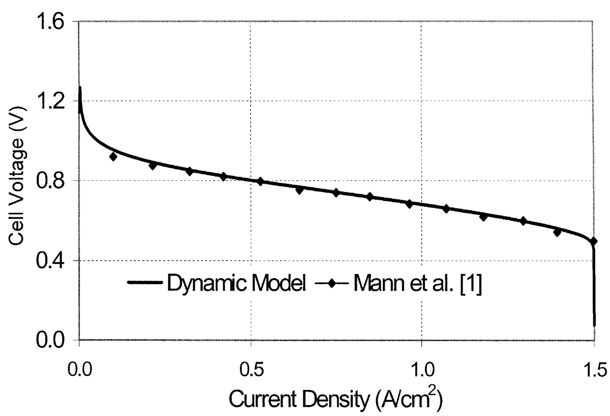

Fig. 3. Ballard PEMFC polarization curve.

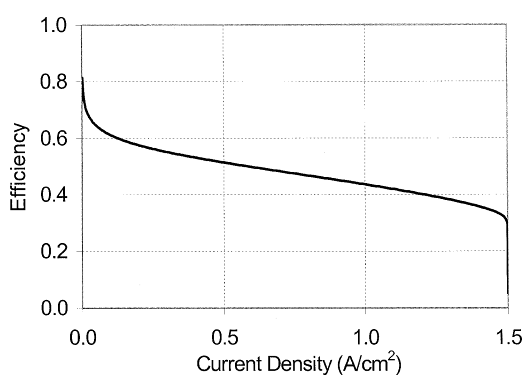

Fig. 4. Ballard PEMFC efficiency.

up-to-date option, which can benefit planners and researchers of the subject.

The cell polarization curve represents the FC output voltage as a function of the current density in steady state. The result obtained with the simulation is presented in Fig. 3, which also shows the practical test results presented in [1]. The simulation results show good agreement with the experimental ones. For current density values above 0.1 A/cm^2 and below 1.3 A/cm^2 the absolute error was less than 3%. This figure is completely acceptable taking into account the difficulty of finding the right values for the different model parameters.

The resulting PEMFC efficiency is represented in Fig. 4, while Fig. 5 represents the cell power density. The efficiency shown in Fig. 4 is related to the chemical conversion. As can be observed, there is a value for the efficiency, even when the output power is zero. This can be explained by considering that the cell voltage presents a value, even in this condition. Therefore, using (17), the conversion efficiency will be different from zero.

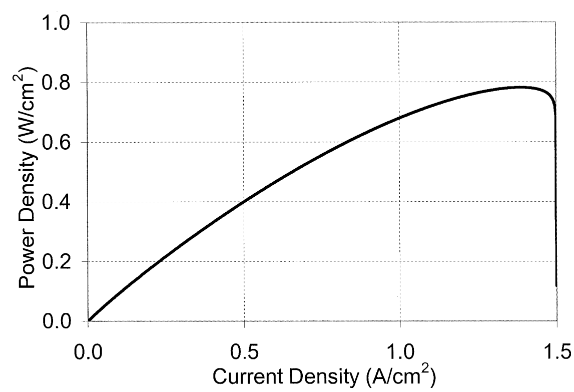

Fig. 5. Ballard PEMFC power density.

From the presented data, it can be observed that the cell voltage and efficiency present higher values for low current densities and power densities. On the other hand, for higher values of power, the efficiency and the voltage present smaller values. Therefore, when the designer of the control system wants to find the best operation point for the cell, he/she must take into account efficiency and voltage levels suitable for the application. Operating the cell in a constant current (which means constant power and voltage) is a good starting point.

It is also important to note that one cannot work with a very high voltage (and, consequently, high efficiency) because the possible output power would be very much reduced, meaning that the cell should be overestimated for this case. One cannot also operate the cell with a very high output current, because, in this case, the cell output voltage and efficiency would be very much reduced, and in addition, the useful life of the cell would be decreased. A compromise should be established between the demand of the load and the power supplied by the cell. The control algorithm should decide when the FC assumes the demanded load, even when this is too high, or when it should just supply part of the load power, to not cause temporary or permanent damage to the cell.

Through the use of this model, the action of an FC can be analyzed for certain practical conditions of load and, therefore, for developing the generation control algorithm.

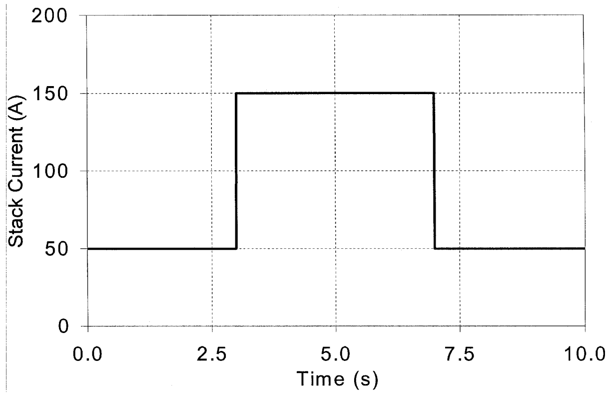

Fig. 6. Stack current for partial load insertion and rejection test.

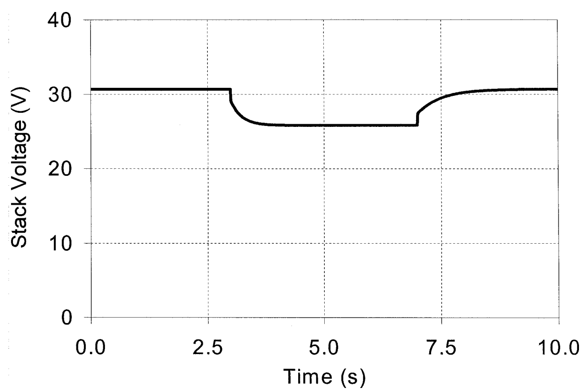

Fig. 7. Stack voltage for partial load insertion and rejection test.

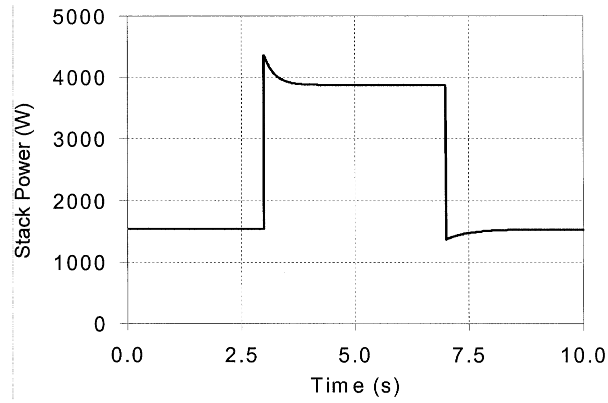

Fig. 8. Stack power for partial load insertion and rejection test.

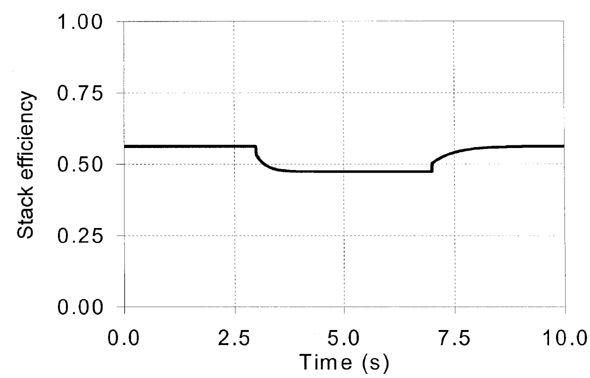

Fig. 9. Stack efficiency for partial load insertion and rejection test.

Several tests were run using the model discussed in this paper with both total and partial load insertion and rejection situations. The most expressive of these tests were the partial load insertion and rejection, as discussed below.

B. Partial Load Insertion and Rejection Tests

Results from the model for one single cell are extrapolated for an association in a series of FCs, resulting in an output voltage V_s that is the sum of the individual cell voltages. In the same way, it is possible to obtain the total stack output characteristic variables against the load current.

For the following results, the tests correspond to the use of a Ballard Mark V PEMFC stack, consisting of an association of 35 cells, with an active area for each cell of 232 cm^2, with a power of 5 kW at 960 mA/cm^2. The capacitor used to evaluate the dynamic response is of 3 F [9]. The other parameters are the same as those described in Table I. In agreement with the model described in Section III, the partial pressures of hydrogen and oxygen influence the resulting stack voltage. In the simulations that follow, air was used as the oxydizer and, then, the partial pressure of oxygen becomes 0.2095 atm [9].

Fig. 6 depicts the load current for test of a partial load insertion followed by load rejection. Initially, the stack supplies 50 A to the load; after 3 s of simulation, the current is increased to 150 A, and remains at this value until the simulation time reaches 7 s. Finally, the load current is decreased again to 50 A, until the end of the simulation ($t = 10$ s).

Fig. 7 presents the curve of the resulting voltage. It can be noticed that there is a response attenuated as much in the insertion as in the load rejection, as expected. The values of the voltage are 30.70 V before the load increase, 25.83 V during the load pulse and, again, 30.70 V when the current is decreased. These values are obtained after having ceased the transient regime. Fig. 8 presents the power response. A peak can be observed at the load insertion instant, with a maximum value of 4.36 kW. When the load is decreased, the power presents a minimum value of 1.37 kW. The power steady-state value is 1.53 kW for a current of 50 A and 3.87 kW for a current of 150 A.

The stack efficiency is shown in Fig. 9. The behavior is similar to the voltage, since these are directly related. The steady-state values for the efficiency are 56.2% for a current of 50 A and 47.3% for a current of 150 A. It can be noticed that there is a significant reduction in the efficiency for variations of the demanded current, which should be taken into consideration when one evaluates a certain system.

V. Modeling of an SR-12 Modular PEM Generator

The SR-12 Modular PEM Generator, manufactured by Avista Laboratories, is a modular FC stack, which has some characteristics adequate for use in electrical generation systems [10]. Recently, the Colorado School of Mines received one SR-12 Modular PEM Generator, with a rated power of 500 W. The data provided by Avista Laboratories for the SR-12 stack was used to match the model proposed in this paper. The procedure to obtain the parameters for this specific stack is as follows.

TABLE II
PARAMETERS OF THE SR-12 MODULAR PEM GENERATOR

Param.	Value	Param	Value
n	48	ξ_1	-0.948
T	323 K	ξ_2	$0.00286+0.0002.\ln A+(4.3.10^{-5}).\ln c_{H_2}$
A	62.5 cm^2	ξ_3	$7.22.10^{-5}$
	25 μm	ξ_4	$-1.0615.10^{-4}$
P_{H_2}	1.47628 atm	ψ	23
P_{O_2}	0.2095 atm	J_{max}	672 mA/cm^2
B	0.15 V	J_n	22 mA/cm^2
R_C	0.0003 Ω	I_{max}	42 A

1) Initially, it is necessary to obtain the basic information from the manufacturer's data sheet [10]. In this case, the information provided was: a) number of cells n equals 48; b) hydrogen pressure: 1.476 28 atm; c) oxygen pressure: 0.2095 atm (air at atmospheric pressure); and d) normal operation temperature: 50 °C.
2) Avista Laboratories kindly allowed access to the polarization curve for this generator. From these data, it was possible to obtain: a) maximum current: 42 A and b) open-circuit voltage: 41.7 V. Avista Laboratories also provided information about the membrane thickness $\ell = 25\ \mu$m and the membrane active area $A = 62.5$ cm^2.
3) Initially, the values for the electrochemical parameters ξ_i and Ψ are considered to be the same as the ones used for the Mark V FC (Table I).
4) The maximum current density can be calculated using (15), for maximum current and membrane active area, resulting in a maximum current density $J_{\max}$ of 0.672 A/cm^2.
5) Now, it is necessary to obtain the equivalent current density for the internal currents/fuel crossover (J_n) and the B parameter, used in the calculation of the concentration overpotential (12). In order to obtain J_n, it is necessary to run the program and verify the open-circuit stack voltage. The value chosen for J_n is the one that makes the resulting simulated open-circuit voltage approximately equal to the manufacturer's data. For the SR-12 PEM Modular Generator, $J_n = 22$ mA/cm^2. It can be noted that this value is relatively high, when compared to other FCs [9].
6) The next step is to obtain the value of B (used in (12)). First, one has to make a first guess for B (for example, 0.016 V). This value must be played in a way that the last part of the voltage characteristic has approximately the same behavior as the manufacturer's one. For the SR-12 stack, this value is again high, $B = 0.15$ V.
7) As a last step, the parameters ξ_i need to be adjusted for this model. Using the same parameters as those used for the Mark V FC, the activation voltage drop is too large, (7). For the SR-12 generator, the parametric coefficients ξ_3 and ξ_4 were decreased to their new values: $\xi_3 = 7.22.10^{-5}$ and $\xi_4 = -1.0615.10^{-4}$.

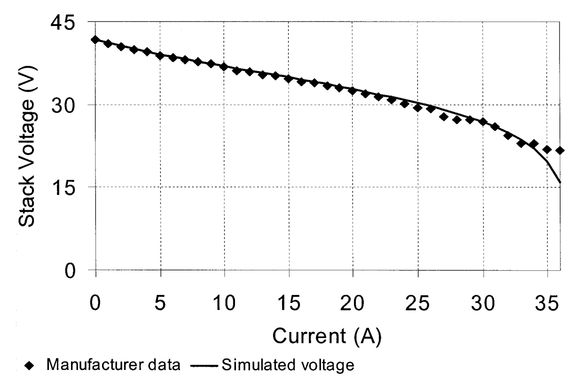

Fig. 10. Avista SR-12 PEM polarization curve.

Using the procedure and data presented above, Table II shows the parameters set for the Avista SR-12 Modular PEM Generator.

Using the data presented in Table II, Fig. 10 shows the results for the polarization curve. The simulated curve presents a good agreement whit the manufacturer's data. It should be said that this Avista FC system is a proof-of-concept and the final industrial performance may surpass such characteristics.

The graph of Fig. 10 shows a maximum current of 36 A, while the maximum current used to model this stack was 42 A. This difference exists because it has been considered that the stack can operate at a current higher than the specified current, once the membrane temperature is kept below 50 °C through the cooling system. This can be done, for example, by increasing the supply of cooling air or by using water as an auxiliary cooling fluid. This also explains why the curve does not decay quickly when the current reaches its maximum value.

Another important point is that, at the beginning of the curve, there is no noticeable voltage decrease. This is because the stack has a low activation voltage drop. In this way, to have an acceptable response for the model, the parametric coefficients ξ_3 and ξ_4 were decreased, to represent this low activation voltage drop.

VI. MODELING OF A BCS 500 W STACK

To show the versatility of the electrochemical model presented in this paper, this section shows a model valid for another

TABLE III
PARAMETERS OF THE 500-W BCS STACK

Param.	Value	Param.	Value
n	32	ξ_1	-0.948
T	333 K	ξ_2	$0.00286+0.0002.\ln A+(4.3.10^{-5}).\ln c_{H_2}$
A	64 cm^2	ξ_3	$7{,}6.10^{-5}$
	178 µm	ξ_4	$-1{,}93.10^{-4}$
P_{H_2}	1 atm	ψ	23
P_{O_2}	0.2095 atm	J_{max}	469 mA/cm^2
B	0,016 V	J_n	3 mA/cm^2
R_C	0.0003 Ω	I_{max}	30 A

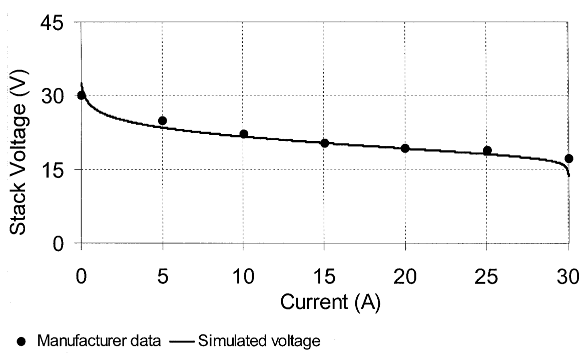

Fig. 11. 500-W BCS stack polarization curve.

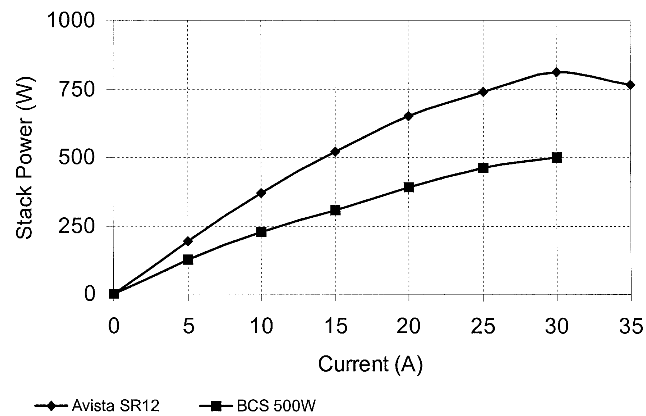

Fig. 12. Comparison between the power of the Avista SR 12 and of the 500-W BCS stacks.

FC stack: a 500 W PEM stack, manufactured by the American Company BCS Technologies [11]. For this stack, the parameters set is presented in Table III and its polarization curve is shown in Fig. 11. This figure presents the manufacturer data and the simulation results [11]. Again, good accuracy of the results can be observed.

Fig. 12 presents a comparison of the stack power between the SR 12 Modular PEM Generator and the BCS 500 W. The rated power for these two stacks are the same (the rated power of the BCS model is up to 200 W under air cooling only and 500 W under water circulation), but the curves presented in Fig. 12 show that for a certain current value the corresponding SR 12 stack power is greater than that of the BCS 500 stack power. This means that for the SR 12 it is possible to obtain more power than rated, as stated in Section V and used to obtain the model for this stack.

VII. CONCLUSION

In this paper most of the parameters used in PEM FCs were taken into account to obtain their realistic dynamic model. The model discussed in this paper was used to conduct a performance analysis of PEMFC stacks in conditions similar to those commonly encountered in small-size energy generation systems, such as load insertion and load rejection. However, it must be said that a model that reproduces the characteristics of FCs with a high degree of precision, as a function of the stack load current, is still a challenge.

The results obtained for FCs from different manufacturers agree with the results presented in the current literature on FCs, for the cell polarization curve, thus validating the model presented here as a block that can be used in the modeling of any complete power generating system. Also, tests at load variation suggest the possibility of use of algorithms such as the HCC for load power control. With this model, the HCC and other algorithms can be debugged and tested in the laboratory, with neither playing nor expending hydrogen, not putting at risk the cell and load integrities, besides having readily available all models and sizes of cells whose parameters are available.

The partial and total load insertion and rejection tests demonstrated that the FC output voltage present a component directly related to the load current, known as the ohmic overpotential. This varies instantly with the variation of the current. There are, still, two other components: the activation and the concentration overpotential, that are responsible for the attenuation of the voltage variation as a function of the current variation through the cell. Such dynamic voltage variation has significant reflexes on the supplied power, as this could cause power peaks, as discussed by other authors.

The characteristics outlined in this paper should be taken into account during the design stage of FC energy generation systems. It would permit one to conclude the need for other sources of energy necessary to attenuate the effects of the abrupt variations of power, since these could damage the cells temporarily or permanently.

For injection of energy into the grid and driving larger loads, this power characteristic imposes the use of power converters to elevate and to control the voltage across the cell terminals and the power supplied to the load.

Using a simple procedure and data obtained from the manufacturer and from the literature, it is possible to obtain a model for an FC stack, whose resulting characteristic is similar to the real system. For example, the results obtained for the SR-12 PEM Modular Generator, for the Ballard Mark V, and for the 500 W BCS stack presented good agreement with their manufacturer's data. In this way, the model for these stacks could be used to analyze the behavior of actual stacks in FC generation systems.

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REFERENCES

[1] R. F. Mann, J. C. Amphlett, M. A. I. Hooper, H. M. Jensen, B. A. Peppley, and P. R. Roberge, "Development and application of a generalized steady-state electrochemical model for a PEM fuel cell," *J. Power Sources*, vol. 86, pp. 173–180, 2000.

[2] J. J. Baschuck and X. Li, "Modeling of polymer electrolyte membrane fuel cells with variable degrees of water flooding," *J. Power Sources*, vol. 86, pp. 181–196, 2000.

[3] J. C. Amphlett, R. F. Mann, B. A. Peppley, P. R. Roberge, and A. Rodrigues, "A model predicting transient responses of proton exchange membrane fuel cells," *J. Power Sources*, vol. 61, pp. 183–188, 1996.

[4] P. Famouri and R. Gemmen, "PEM fuel cell electric circuit model," presented at the Power Electronics for Fuel Cells Workshop, Nat. Fuel Cells Res. Center, Univ. California, Irvine, CA, Aug. 8–9, 2002.

[5] F. A. Farret, J. R. Gomes, and A. S. Padilha, "Comparison of the hill climbing methods used in micro powerplants," in *Proc. IEEE INDUSCON 2000*, Porto Alegre, Brazil, pp. 756–760.

[6] J. Padullés, G. W. Ault, and J. R. McDonald, "An integrated SOFC plant dynamic model for power systems simulation," *J. Power Sources*, vol. 86, pp. 495–500, 2000.

[7] D. Chu and R. Jiang, "Performance of polymer electrolyte membrane fuel cell (PEMFC) stacks—Part I. Evaluation and simulation of an air-breathing PEMFC stack," *J. Power Sources*, vol. 83, pp. 128–133, 1999.

[8] Y. Kim and S. Kim, "An electrical modeling and fuzzy logic control of a fuel cell generation system," *IEEE Trans. Energy Conversion*, vol. 14, pp. 239–244, June 1999.

[9] J. E. Larminie and A. Dicks, *Fuel Cell Systems Explained*. Chichester, U.K.: Wiley, 2000, pp. 308–308.

[10] *SR-12 Modular PEM Generator Operator's Manual, Last Revised 7/2000; Revision 0000*, Avista Laboratories, Spokane, WA, July 2000.

[11] "Data sheet of a 500 W fuel cell stack," BCS Technologies, Englewood, CO, 2001.

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