

# A method for the identification of solid oxide fuel cells using a Hammerstein model

Francisco Jurado\*

*University of Jaén, Department of Electrical Engineering, 23700 Alfonso X, no. 28, EPS Linares (Jaén), Spain*

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## Abstract

The complexity of the solid oxide fuel cell requires the use of very large computers. For this reason, models based on various engineering assumptions have been created so that the numerical calculations may be performed on small personal computers.

The Hammerstein models are special kinds of nonlinear systems where the nonlinear block is static and is followed by a linear system. This method is applied to model the static and dynamic characteristics of the solid oxide fuel cell.

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## 1. Introduction

The solid oxide fuel cell (SOFC) is viable for generating electricity from hydrocarbon fuels. The high operating temperature from 600–1000 °C allows internal reforming and promotes rapid kinetics with nonprecious materials. The high temperature of the SOFC, however, places stringent requirements on its materials.

Padullés et al. [1] develop a SOFC model which includes species dynamics, but it does not consider temperature dynamics. Hall and Colclaser [2] modeled a 3-kW SOFC but they did not take into account dynamics of the chemical species. Achenbach develops a mathematical model of a planar SOFC, which concentrates on effects of temperature changes on output voltage response [3]. Temperature dynamics is modeled in a three-dimensional (3D) vector space. The same author investigated the transient behavior of a stand-alone SOFC caused by a load change in Ref. [4]. It shows that the relaxation time of the output voltage is highly related to the effect of temperature dynamics.

The application of the autoregression with exogenous signal (ARX) identification algorithm to compute linear system models is presented in Ref. [5]. In this paper, the Hammerstein nonlinear system approach is used for identification of the nonlinear system model of SOFC.

The Hammerstein models are special kinds of nonlinear systems where the nonlinear block is static and is followed by a linear system. These models have applications in many engineering problems, and therefore, identification of Hammerstein models has been an active research area for many years. There exist a large number of research papers in the literature on the topics of Hammerstein model identifications.

Existing methods for Hammerstein model identification can be roughly divided into four categories: the iterative method [6,7], the over-parametrization method [8–11], the stochastic method [12–14] and the separable least-squares method [15]. In most cases, the structure of the nonlinearity is assumed to be known. Otherwise, identification becomes a structural estimation problem [16].

Due also to the particular parameterization used in Ref. [8], an extension of the results to the multiple input, multiple output (MIMO) setting does not seem to be straightforward. Gomez and Baeyens [17] proposed a noniterative algorithm for the identification of Hammerstein models, which, in

\* Tel.: +34 953 648518; fax: +34 953 648508.

E-mail address: [fjurado@ujaen.es](mailto:fjurado@ujaen.es).

### Nomenclature

$C_p^s$	heat capacity of the cell unit ( $\text{J (kg K)}^{-1}$ )
$E_o$	standard reversible cell potential (V)
$F$	Faraday's constant ( $\text{C kmol}^{-1}$ )
$\bar{h}_{ai}^{\text{in}}, \bar{h}_{ci}^{\text{in}}$	anode (cathode) inlet partial molar enthalpies ( $\text{J mol}^{-1}$ )
$\bar{h}_i^s$	partial molar enthalpies at stack temperature ( $\text{J mol}^{-1}$ )
$i$	stack current density ( $\text{A m}^{-2}$ )
$i_L$	limiting current density ( $\text{A m}^{-2}$ )
$i_0$	exchange current density ( $\text{A m}^{-2}$ )
$I$	stack current (A)
$K_i$	valve molar constants
$K_r$	constant dependent on Faraday's constant and number of electrons in the reaction ( $\text{kmol (s A)}^{-1}$ )
$M^s$	mass of the cell unit (kg)
$n$	number of electrons participating in the reaction
$N_{\text{H}_2}$	hydrogen flow that reacts ( $\text{kmol s}^{-1}$ )
$N_i^{\text{in}}, N_i^{\text{o}}$	molar flow rates ( $\text{mol s}^{-1}$ ) of the $i$ th reactant at the cell input and output, respectively
$N_i^r$	reaction rate ( $\text{mol s}^{-1}$ ) of the $i$ th reactant
$N_o$	number of cells in stack
$N_{\text{ta}}^{\text{in}}, N_{\text{tc}}^{\text{in}}$	anode (cathode) total inlet molar flow ( $\text{mol s}^{-1}$ )
$p$	cell pressure (atm)
$P_{\text{dc}}$	stack dc power (W)
$r$	ohmic resistance ( $\Omega \text{ m}^2$ )
$R$	gas constant ( $8.31 \text{ J (mol K)}^{-1}$ )
$R_{ai}, R_{ci}$	anode (cathode) total rate of production of species ( $\text{mol s}^{-1}$ )
$T^s$	stack solid average temperature (K)
$T^0$	temperature constant (K)
$V$	compartment volume ( $\text{m}^3$ )
$V_{\text{dc}}$	cell voltage (V)
$V_e$	volume of the cell unit ( $\text{m}^3$ )
$V_o$	open-circuit reversible potential (V)
$x_{ai}^{\text{in}}, x_{ci}^{\text{in}}$	anode (cathode) inlet mole fractions
$x_i$	mole fractions of species

### Greek letters

$\alpha$	electron transfer coefficient of the reaction at the electrode
$\alpha_r, \beta_r$	ohmic resistance constants
$\eta_{\text{act}}$	activation losses (V)
$\eta_{\text{con}}$	concentration losses (V)
$\tau_{\text{H}_2}$	time constant associated with the hydrogen flow and is a function of temperature (s)
$\xi$	total gas components in anode or cathode

contrast to [8], applies also to multivariable systems, allows a more general representation (using base functions) for the static nonlinearity, and where the consistency of the estimates is guaranteed even in the presence of colored output noise. As in Ref. [8], the main computational tools employed by the algorithm are least-squares estimation (LSE) and singular value decomposition (SVD), which results in numerical robustness under weak assumptions on the persistency of excitation of the inputs. Key on the derivations of the results in Ref. [17] is the use of base functions for the representation of the linear and the nonlinear blocks in the Hammerstein model.

The paper is organized as follows. In Section 2, general principles of SOFC are explained. The multivariable Hammerstein model is introduced and the identification problem is formulated in Section 3. Simulation examples illustrating the performance of the algorithms on SOFCs are presented in Section 4, and finally, conclusions are provided in Section 5.

## 2. Solid oxide fuel cell dynamic model

The proposed stack model is based on the following assumptions:

- (1) Stack is fed with hydrogen and air, therefore, the fuel processor dynamics is not included.
- (2) A uniform gas distribution among cells is assumed, since there is a small deviation of the gas distribution among the cells.
- (3) There is no heat transfer among cells. Each cell has the same temperature and current density [1].
- (4) The channels that transport gases along the electrodes have a fixed volume, but their lengths are small, so that it is only necessary to define one single pressure value in their interior. The ratio of pressures between the interior and exterior of the channel is large enough to consider that orifice is choked [1,18].

Fig. 1 shows the dynamic model of SOFC, along with its major chemical reactions.

### 2.1. Electrochemical model

The change in concentration of each specie that appears in the chemical reactions can be written in terms of input and output flow rates and exit molarity due to the following chemical reaction [19,20]:

$$\frac{V}{RT} \frac{d}{dt} p_i = N_i^{\text{in}} - N_i^{\text{o}} - N_i^r \quad (1)$$

In agreement with the basic electrochemical relationships, the molar flow that reacts can be calculated as:

$$N_i^r = \frac{N_o I}{2F} = 2K_r I \quad (2)$$

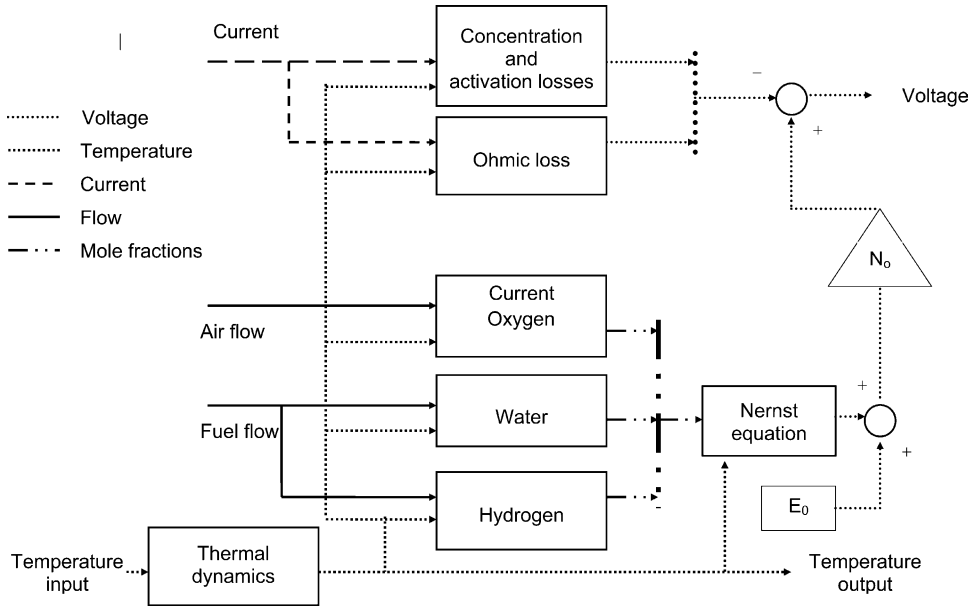


Fig. 1. Dynamic model of SOFC.

The cell utilization is defined through the input and output hydrogen flow rates as follows:

$$u = \frac{N_{H_2}^{in} - N_{H_2}^o}{N_{H_2}^{in}} \quad (3)$$

For orifice that is choked [18], molar flow of any gas through the valve is proportional to its partial pressure inside the channel according to the following expressions [1]:

$$\frac{N_{H_2}}{p_{H_2}} = K_{H_2}, \quad \frac{N_{H_2O}}{p_{H_2O}} = K_{H_2O} \quad (4)$$

Considering the hydrogen partial pressure,

$$\frac{V}{RT} \frac{d}{dt} p_{H_2} = N_{H_2}^{in} - N_{H_2}^o - 2K_r I \quad (5)$$

Applying the Laplace transformation to the above equations and isolating the hydrogen partial pressure, yields the following expressions:

$$p_{H_2} = \frac{\frac{1}{K_{H_2}}}{1 + \tau_{H_2} s} (N_{H_2}^{in} - 2K_r I) \quad (6)$$

$$\tau_{H_2} = \frac{V}{K_{H_2} RT} \quad (7)$$

### 2.2. Thermal model

The fuel cell power output is closely related to the temperature of the cell unit. The heat storage in the thin fuel unit gas or oxidant gas layer is neglected. The thin fuel unit or oxidant gas layers are lumped to the cell unit and gas layers are assumed to have the same temperature as the cell unit [2–4].

The energy balance equation for each cell unit is as follows:

$$M^s C_p^s \frac{dT^s}{dt} = N_{ta}^{in} \left[ \sum_{i=1}^{\xi} x_{ai}^{in} (\bar{h}_{ai}^{in} - \bar{h}_i^s) \right] - \sum_{i=1}^{\xi} \bar{h}_i^s R_{ai} + N_{tc}^{in} \left[ \sum_{i=1}^{\xi} x_{ci}^{in} (\bar{h}_{ci}^{in} - \bar{h}_i^s) \right] - \sum_{i=1}^{\xi} \bar{h}_i^s R_{ci} - P_{dc} \quad (8)$$

Under the ideal gas supposition, the partial molar enthalpies are calculated using

$$\bar{h}_i = \bar{h}_i^{ref} + \int_{T_{ref}}^T c_{p,i}(u) du \quad (9)$$

and coefficients of the specific heats  $c_{p,i}$ ,

$$c_{p,i} = a_i + b_i T + c_i T^2 + d_i T^3 \quad (10)$$

are encountered in standard reference tables. The reference enthalpy stands for energy at standard reference temperature and considers the heat of formation for each gas species to account for energy change on chemical reaction.

### 2.3. Nernst's equation

Applying Nernst's equation and Ohm's law (taking into account ohmic, concentration, and activation losses), the stack is connected in series and the stack output voltage is represented as follows [19–21]:

$$V_{dc} = V_o - rI - \eta_{act} - \eta_{con} \quad (11)$$

$$V_o = N_o \left( E_o + \frac{RT}{2F} \left[ \ln \frac{x_{H_2} x_{O_2}^{0.5}}{x_{H_2O}} \right] \right) \quad (12)$$

For the reason that the reactant is consumed at the electrode by electrochemical reaction, there is a loss of potential due to the inability of the surrounding material to maintain the initial concentration of the bulk fluid. Concentration loss equation is given by [2,19–21]:

$$\eta_{\text{con}} = \frac{RT}{nF} \ln \left( 1 - \frac{i}{i_L} \right) \quad (13)$$

Activation polarization is existent when the rate of an electrochemical reaction at an electrode surface is controlled by sluggish electrode kinetics [20,21]. Activation loss equation is as follows:

$$\eta_{\text{act}} = \frac{RT}{\alpha nF} \ln \left( \frac{i}{i_0} \right) \quad (14)$$

$\alpha$  is the transfer coefficient, which is considered to be the fraction of the change in polarization that leads to a change in the reaction rate constant and its value is usually 0.5 for the fuel cell application.

Tafel plots provide a visual understanding of the activation polarization of a fuel cell. They are used to measure the exchange current density, given by the extrapolated intercept at  $\eta_{\text{act}} = 0$  which is a measure of the maximum current that can be extracted at negligible polarization, and the transfer coefficient (from the slope).

The usual form of the Tafel equation that can be easily expressed by a Tafel plot is

$$\eta_{\text{act}} = a + b \ln i \quad (15)$$

where  $a = (-RT/\alpha nF) \ln i_0$  and  $b = RT/\alpha nF$ .

The term  $b$  is called the Tafel slope and is obtained from the slope of a plot of  $\eta_{\text{act}}$  as a function of  $\ln i$ . The Tafel slope for an electrochemical reaction is about 110 mV/decade at room temperature.

Ohmic losses occur because of resistance to the flow of ions in the electrolyte and resistance to the flow of electrons through the electrode materials. This resistance is dependent on the cell temperature and is obtained by Ref. [21]

$$r = \alpha_r \exp \left[ \beta_r \left( \frac{1}{T^0} - \frac{1}{T} \right) \right]. \quad (16)$$

### 3. Hammerstein model identification

#### 3.1. Problem formulation

A multivariable Hammerstein model is symbolized in Fig. 2. The model consists of a zero-memory nonlinear element  $\mathcal{N}(\cdot)$  in cascade with a linear time invariant (LTI) system with transfer function matrix  $G(q) \in H_2^{m \times n}(\mathbb{T})$ . It is accepted that the measured output  $y_k$  contains an unknown additive noise component  $v_k$ .

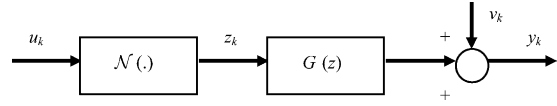


Fig. 2. Multivariable Hammerstein model.

The input–output relationship is then given by

$$y_k = G(q)\mathcal{N}(u_k) + v_k \quad (17)$$

where  $y_k \in \mathbb{R}^m$ ,  $u_k \in \mathbb{R}^n$ , and  $v_k \in \mathbb{R}^m$  are the system output, input, and measurement noise vectors at time  $k$ , respectively. It will be assumed that the nonlinear block can be specified as

$$\mathcal{N}(u_k) = \sum_{i=1}^r a_i g_i(u_k) \quad (18)$$

where  $g_i(\cdot) = \mathbb{R}^n \rightarrow \mathbb{R}^n$  ( $i = 1, \dots, r$ ) are known nonlinear base functions and  $a_i \in \mathbb{R}^{n \times n}$  ( $i = 1, \dots, r$ ) are unknown matrix parameters. Typically, the nonlinear functions  $g_i(\cdot)$  are polynomials that allow the representation of smooth nonlinearities, but they can also be radial base functions (RBF) or base functions generated by translations and dilations of a mother function (e.g., wavelets). Any smooth function in an interval can be represented with arbitrary accuracy by a polynomial of sufficiently high order.

From another point of view, the LTI system will be represented using rational orthonormal bases as follows:

$$G(q) = \sum_{l=0}^{p-1} b_l \mathcal{B}_l(q) \quad (19)$$

where  $b_l \in \mathbb{R}^{m \times n}$  are unknown matrix parameters and  $\{\mathcal{B}_l(q)\}_{l=0}^{\infty}$  are rational orthonormal bases.

The identification problem is to estimate the unknown parameter matrices  $a_i \in \mathbb{R}^{n \times n}$  ( $i = 1, \dots, r$ ) and  $b_l \in \mathbb{R}^{m \times n}$  ( $l = 0, \dots, p-1$ ) characterizing the nonlinear and the linear parts, respectively, from an  $N$ -point data set  $\{u_k, y_k\}_{k=1}^N$  of observed input–output measurements.

#### 3.2. Identification algorithm

Substituting Eqs. (18) and (19) in (17), the input–output relationship can be written as

$$y_k = \sum_{l=0}^{p-1} \sum_{i=1}^r b_l a_i \mathcal{B}_l(q) g_i(u_k) + v_k \quad (20)$$

From Eq. (20), the parametrization (18) and (19) is not unique. A technique that can be used to obtain uniqueness is to normalize the parameter matrices  $a_i$  or  $b_l$ , for example, assuming that  $\|a_i\|_2 = 1$  or  $\|b_l\|_2 = 1$ . Under this assumption, the parametrization is unique.

Specifying now

$$\theta \triangleq [b_0 a_1, \dots, b_0 a_r, \dots, b_{p-1} a_1, \dots, b_{p-1} a_r]^T \quad (21)$$

$$\phi_k \triangleq \begin{bmatrix} \mathcal{B}_0(q) g_1^T(u_k), \dots, \mathcal{B}_{p-1}(q) g_r^T(u_k), \dots \\ \vdots \\ \mathcal{B}_{p-1}(q) g_1^T(u_k), \dots, \mathcal{B}_{p-1}(q) g_r^T(u_k), \dots \end{bmatrix}^T \quad (22)$$

Eq. (20) can be written as

$$y_k = \theta^T \phi_k + v_k \quad (23)$$

which is in linear regression form. Regarding the  $N$ -point data set, the last equation, and defining

$$Y_N \triangleq [y_1, y_2, \dots, y_N]^T \quad (24)$$

$$V_N \triangleq [v_1, v_2, \dots, v_N]^T \quad (25)$$

$$\Phi_N \triangleq [\phi_1, \phi_2, \dots, \phi_N]^T \quad (26)$$

the next equation can be written

$$Y_N = \Phi_N^T \theta + V_N \quad (27)$$

The estimate  $\hat{\theta}$  that minimizes a quadratic criterion on the prediction errors  $\varepsilon_N = Y_N - \Phi_N^T \theta$  is determined by

$$\hat{\theta} = \Phi_N^T Y_N \quad (28)$$

The problem is how to calculate the parameter matrices  $a_i$  ( $i = 1, \dots, r$ ) and  $b_l$  ( $l = 0, \dots, p - 1$ ) from the estimate  $\hat{\theta}$  in (28). From

$$\theta = \text{blockvec}(\Theta_{ab}) \quad (29)$$

where  $\text{blockvec}(\Theta_{ab})$  is the block column matrix obtained by stacking the block columns of  $\Theta_{ab}$  on top of each other, and

where  $\Theta_{ab}$  has been defined as

$$\Theta_{ab} \triangleq \begin{bmatrix} a_1^T b_0^T & a_1^T b_1^T & \dots & a_1^T b_{p-1}^T \\ a_2^T b_0^T & a_2^T b_1^T & \dots & a_2^T b_{p-1}^T \\ \vdots & \vdots & \dots & \vdots \\ a_r^T b_0^T & a_r^T b_1^T & \dots & a_r^T b_{p-1}^T \end{bmatrix} \quad (30)$$

where  $\Theta_{ab} = ab^T$  and the following definitions for the matrices  $a$  and  $b$ ,

$$a \triangleq [a_1, a_2, \dots, a_r]^T \quad (31)$$

$$b \triangleq [b_0^T, b_1^T, \dots, b_{p-1}^T]^T \quad (32)$$

An estimate  $\hat{\Theta}_{ab}$  of the matrix  $\Theta_{ab}$  can then be obtained from the estimate  $\hat{\theta}$  in (28). The question now is how to estimate the parameter matrices  $a$  and  $b$  from the estimate  $\hat{\Theta}_{ab}$ . It is clear that the closest estimates  $\hat{a}$  and  $\hat{b}$  are those that solve the following optimization problem

$$(\hat{a}, \hat{b}) = \arg \min_{a,b} \left\{ \|\hat{\Theta}_{a,b} - ab^T\|_2^2 \right\} \quad (33)$$

The solution to this optimization problem is supplied by the SVD of the matrix  $\hat{\Theta}_{ab}$ .

The structure (17)–(19) of the identified Hammerstein model can be interpreted as an equivalent LTI model whose inputs are the actual inputs  $u_k$  filtered by the nonlinear base functions  $g_i(\cdot)$  used to represent the static nonlinearity in the Hammerstein model. This interpretation of the Hammerstein model is represented in the block-diagram of Fig. 3.

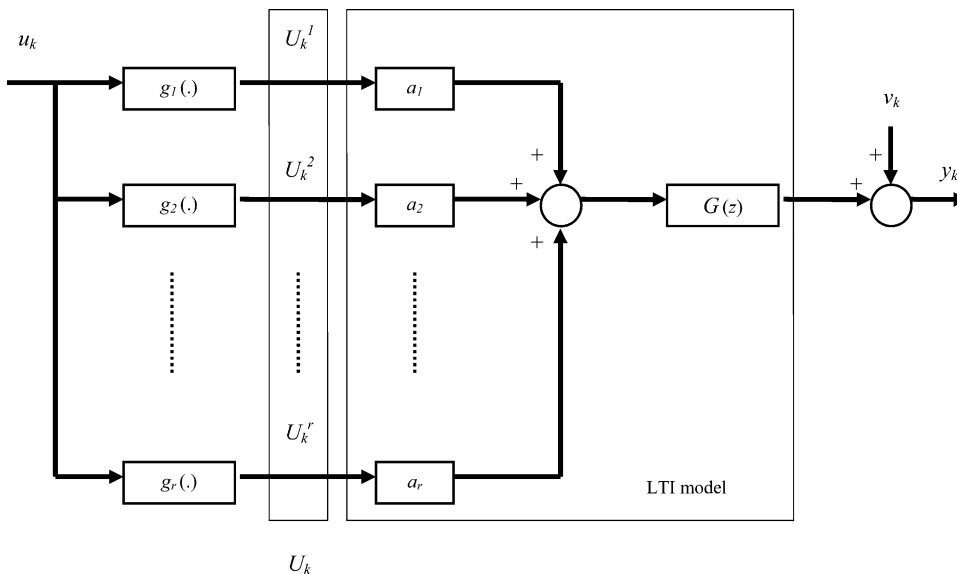


Fig. 3. Equivalent LTI model.

Table 1  
Operating point data

Power (kW)	100
Stack voltage (V)	286.3
Stack current (A)	300
Number of cells	384
Number of stacks	1
Open circuit voltage for each cell (V)	0.935
Input fuel flow ( $\text{kmol s}^{-1}$ )	$1.2 \times 10^{-3}$
Input air flow ( $\text{kmol s}^{-1}$ )	$2.4 \times 10^{-3}$
Cell area ( $\text{cm}^2$ )	1000
Cell temperature ( $^{\circ}\text{C}$ )	1000
Transfer coefficient $\alpha$	0.5
Ohmic resistance constant $\beta_r$	-2870
Ohmic resistance constant $\alpha_r$	0.2
Temperature constant $T^0$ (K)	923
Limiting current ( $\text{A m}^{-2}$ )	0.8
$K_{\text{H}_2}$ ( $\text{kmol (atm s)}^{-1}$ )	$8.43 \times 10^{-4}$

#### 4. Results

The identification algorithm is used to estimate a Hammerstein model based on simulation data of a SOFC. The white-box model consists of a set of coupled equations, as established in Section 2.

The inputs to the system are the temperature input ( $u_1$ ), the fuel flow ( $u_2$ ), the air flow ( $u_3$ ), and the current ( $u_4$ ). The outputs of the system are the temperature output ( $y_1$ ) and the voltage ( $y_2$ ).

The linear subsystem in the Hammerstein model was represented using the rational orthonormal bases with fixed poles studied in Refs. [17,22]

$$B_l(q) = \left( \frac{\sqrt{1 - |\xi_l|^2}}{q - \xi_l} \right) \prod_{i=0}^{l-1} \left( \frac{1 - \bar{\xi}_i q}{q - \xi_i} \right), \quad l \geq 1 \quad (34)$$

$$B_0(q) = \left( \frac{\sqrt{1 - |\xi_0|^2}}{q - \xi_0} \right) \quad (35)$$

where  $(\xi_0, \xi_1, \dots, \xi_{p-1})$  are the poles of the bases.

In order to determine the model order of the linear subsystem, as well as initial guesses for the location of the poles of the bases, the same input–output data were used to identify a linear model of the process using a subspace method. System Identification Toolbox for use with Matlab [23] was used for the identification of the linear model. As a result of the identification process a fourth-order model was estimated as the linear part of the Hammerstein model.

On the other hand, a third-order polynomial was used to represent the nonlinear static block of the Hammerstein model. This choice for the order of the polynomial was a compromise between model complexity and variance error, and the decision was taken based on the values of Akaike's Information Theoretic Criterion (AIC).

The nominal operating conditions of the SOFC considered in this example are given in Table 1 [24,25]. For the

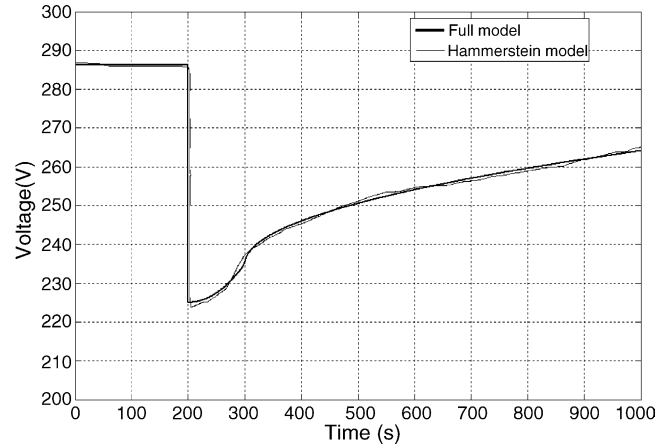


Fig. 4. Output stack voltage response due to stack current step increase.

purposes of identification, the white-box model of the SOFC was excited with band-limited white noise around the nominal value of the fuel flow ( $u_2$ ), while all the other inputs were kept constant in their nominal values. Changes in the fuel flow were produced every 40 s, with a maximum amplitude of  $\pm 100\%$  of the nominal value. A set of 10,000 data was collected from the simulation with a sampling time of 0.1 s. The first 5000 data were used for the estimation of a Hammerstein model of the fuel cell, while the remaining 5000 data were used for validation purposes.

The true (Full model) and estimated (Hammerstein model) outputs are represented in Figs. 4–6. A step change in the stack current (from 300 to 400 A) is applied. The true (solid line) and estimated (dashed line) output voltages corresponding to the identified model are represented in Fig. 4.

Fig. 5 represents the cell temperature due to this step change in the stack current.

Finally, the voltage step response of the SOFC due to the change in fuel flow input from 1.2 to 1.5  $\text{kmol s}^{-1}$  is depicted in Fig. 6.

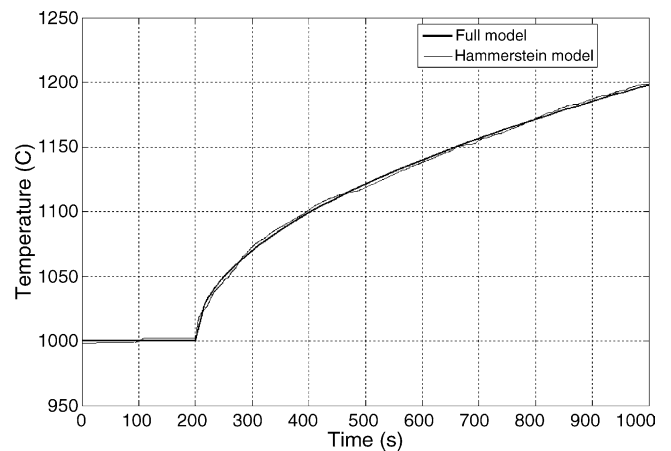


Fig. 5. Output stack temperature response due to stack current step increase.

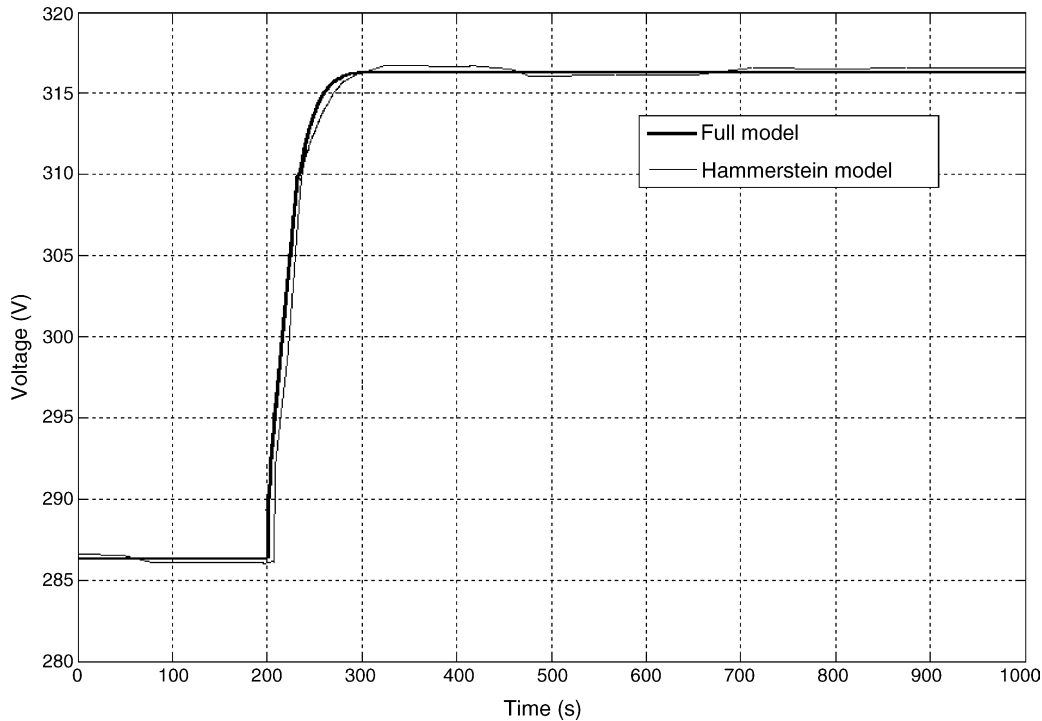


Fig. 6. Output voltage response due to fuel flow step change.

## 5. Conclusions

This paper develops a multivariable Hammerstein model of a SOFC, which can be applied for small signal and transient stability studies. The model based on electrochemical and thermal equations describes temperature dynamics and output voltage losses.

Noniterative algorithms for the identification of this multivariable Hammerstein system have been presented. The key issue in the derivation of the results is the representation of the system using base functions. The suitability of the proposed methods for their use in the identification of SOFCs has been illustrated through simulation.

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