Nonlinear Predictive Control for the Concentrations Profile Regulation in a PEM Fuel Cell Anode Gas Channel

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***Abstract*— In this work, a nonlinear model predictive control (NMPC) strategy is proposed to regulate the concentrations of the different gas species inside a Proton Exchange Membrane Fuel Cell (PEMFC) anode gas channel. The purpose of the regulation relies on the rejection of the perturbations that affect the system. The model of the anode channel is derived from the discretization of the Partial Differential Equations (PDE) that define the dynamics of the system, taking into account spatial variations along the channel. Forward and backward discretizations of the distributed model are employed to take advantage of the boundary conditions of the problem. Simulation results are presented to show the performance of the proposed control method over a given case study. Different cost functions are compared and the one with minimum error is identified. Suitable dynamic responses are obtained facing the different considered disturbances.**

I. INTRODUCTION

Fuel cells are an interesting alternative for clean energy production. Particularly, Proton Exchange Membrane Fuel Cells (PEMFC), with a high power density, are very promising for mass market applications such as automotive and stationary combined heat and power systems. Currently, researchers from all over the world are dedicating a great effort to improve efficiency, reduce degradation and decrease production costs of this technology. In the automatic control field, new estimation, diagnosis and control systems are being developed.

Therefore, there is already an important number of works focusing on the dynamic control of PEMFC. Different control objectives and different control techniques can be found in the literature: stoichiometry, flow rates, temperature and water management are among the most frequent control objectives [12], [13]; linear controllers, model-based controllers, predictive controllers, variable structure controllers are some of the used control techniques [3], [15]. In order to continue exploiting the control engineering potential to improve PEMFC performance, distributed parameter models have acquired increasing importance [11], [10]. This is due to the increasing concern about the effects of the variation of certain variables along the system. This work is based on a distributed model of the anode channel of a PEMFC, proposing as a control objective to regulate the gas concentration profiles along the channel towards constant setpoint profiles.

As any real system, PEMFC is plenty of behaviors and variables bounded by physical limits which should be considered when a control law is designed, e.g., ranges of voltages, currents, flows. Moreover, the interaction of the diverse compositional sub-systems determines the definition of several operational constraints that, in the same way as the variable bounds, should be taken into account when formulating a closed-loop control scheme. In this sense, model predictive control (MPC) has been recognized as a powerful methodology since it has the intrinsic ability to deal with system constraints in a systematic and straightforward manner [9]. Added to this fact, there exists other strong reasons for utilizing this control technique such as the capability of considering several variables (multi-variable systems) and control objectives (multi-objective control) as well as the inclusion of system disturbances handling in on-line mode.

Although MPC is sensitive to the model accuracy since the control computation is precisely based on a mathematical model of the plant (in this case, the fuel cell), this dependence opens several ways on how to design the MPC controller from the point of view of the nature of the PEMFC model: from the purely nonlinear MPC (NMPC) [16], to linear approaches [4], [1], piece-wise affine (PWA) models [7], [5] and hybrid systems forms [6].

The NMPC approach has several advantages due to the consideration of the nonlinear dynamics of the system, key aspect when driving the system far away from its nominal working point (a common situation in PEMFC energy systems). On the other hand, one of the main problems that can be encountered when using this control strategy is the high computational burden. The main contribution of this paper relies on the implementation of a NMPC strategy based on a nonlinear distributed parameters model of a PEMFC anode channel in such a way that the proposed regulation of the anode gas concentration can be reached by considering simpler but accurate model and physical/operational system constraints. To this end, a prestablished disturbance profile (PEMFC load) is considered.

The remainder of the paper is organized as follows. In Section II, the general system description and statement of the control problem are presented. In Section III, the mathematical model of the plant, based on distributed parameters is presented and explained. In Section IV, the NMPC problem is stated and implemented considering the model of the anode gas channel. In Section V, the results extracted from the simulation are presented and analyzed in detail. Finally, in Section VI, the conclusions of this work are presented and some research lines for future work are proposed.

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II. SYSTEM DESCRIPTION

PEMFC systems produce electrical energy from the consumption of hydrogen and air through an oxidation-reduction chemical reaction at both sides of an electrolyte membrane that separates the anode from the cathode. At the anode side, the hydrogen is catalytically split into protons and electrons. Protons travel through the electrolyte membrane to react with the air and the returning electrons in the cathode side of the cell, generating water. Electrons travel to the load of the system, generating electrical current through the electrical connection between anode and cathode sides of the cell.

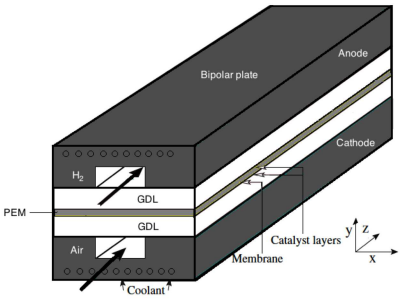

Fig. 1. Single-channel PEM Fuel Cell representation

The reaction rate at which the hydrogen is consumed depends on the power demanded by the load. Therefore, the hydrogen inflow has to be controlled in order to maintain its desired concentration along the cell channel when there are load changes. On the other side, a key aspect to the efficiency of the PEMFC is the hydration of the catalyst layer and the polymeric membrane that separates the anode from the cathode. Due to this fact, a second control objective should be considered: the regulation of the water vapor concentration along the channel.

As said, this work is focused on the anode supply gas channel of a single-channel PEMFC. The concentration profiles through the anode channel are controlled. The spatial derivatives are defined along the z-axis, while the hydrogen and water transport terms, considered as disturbances, are perpendicular to the supply channel (in the y-axis direction), see Figure 1. The nature and computation of these disturbances come from recent research work developed in [14]. In the present work, these profiles have been used as nominal inputs to design the NMPC strategy.

The anode gas channel model employed to simulate the control solutions has a z-axis length (L) of 0.4 m and a y-axis channel thickness (δ) of 0.7 mm.

III. MATHEMATICAL MODELING

In order to implement the NMPC approach (or any MPC method for that matter) to control the plant, a model that represents the dynamics of the system is needed beforehand. In this section, a mathematical model of the PEMFC anode gas channel will be derived from the partial differential equations that represent the behavior the overall mass balances, the flow velocities and the pressure drops along the channel, as developed in [10], i.e.,

$$\frac{\partial c_i}{\partial t} = -\frac{\partial v}{\partial z}\, c_i - \frac{\dot{n}_i}{\delta}, \tag{1a}$$

$$v = -K\frac{\partial p}{\partial z}, \tag{1b}$$

$$p = RT\left(c_{H_2} + c_{H_2O}\right), \tag{1c}$$

where Table I collects and describes the variables in (1). Hydrogen (H_2) and water vapour (H_2O) concentrations along the different discretized volumes of the channel are denoted as c_i, where subscript i denotes the reactant, being $i = 1$ the H_2 index and $i = 2$ the water index.

TABLE I

NOMENCLATURE AND UNITS OF VARIABLES IN (1)

Coefficient	Description, Units
c_i	Concentration of i-th gas, [mol][m^{-3}]
δ	Thickness of the channel, [m]
K	Pressure drop coefficient, [m^2][s^{-1}][Pa^{-1}]
$\dot{n}$	Molar flux density of i-th gas, [mol][m^{-2}][s^{-1}]
p	Pressure, [Pa]
R	Gas constant, [J][mol^{-1}][K^{-1}]
T	Temperature, K
v	Flow velocity, [m][s^{-1}]
Δz	Discretization length, [m]

The system has a certain set of known boundary conditions (input molar fluxes and external ambient pressure). A forward and backward discretization will be applied to the spatial partial differential equations that define the dynamics of the system in (1). As explained before, hydrogen reaction and water transport take place in the y-axis of the PEMFC. These terms are not constant along the channel. These variations explain the necessity of a spatial discretization in order to obtain a model with more information of the dynamics that govern the system than other concentrated parameter models proposed in the literature. Making use of this improved model, more advanced controllers can be designed and implemented.

The study can be generalized to the case of n discretized volumes along the gas channel (n_{Vol}). In Figure 2 the main structure of the system for this generalization is presented. Particularly, in this work 11 volumes of discretization along the z axis have been considered to implement the NMPC strategy to regulate the concentration profiles.

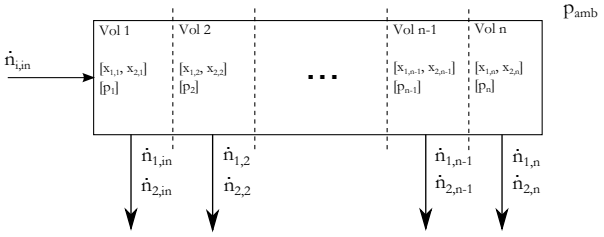

Fig. 2. Generalized model of the discretized anode gas channel

The discretization of the differential equations in (1) yields

the following system:

$$\dot{c}_{i,j} = \frac{v_{j-1}c_{i,j-1}}{\Delta z} - \frac{v_j c_{i,j}}{\Delta z} - \frac{\dot{n}_{i,j}}{\delta}, \tag{2a}$$

$$v_j = \frac{K}{\Delta z}\left(p_j - p_{j+1}\right), \tag{2b}$$

$$p_j = RT\left(c_{1,j} + c_{2,j}\right), \tag{2c}$$

where subscript j is refered to the discretized volume (e.g., $c_{2,3}$ is the H_2O concentration value at the third volume of the spatial discretization).

The boundary conditions are given by $v_{j-1}c_{i,j-1} = \dot{n}_{i,in}$ for the first volume of discretization and $p_{j+1} = p^{\text{amb}}$ for the last one [10]. From this development, three kind of state equations using (2) are developed for the first, middle and last volumes. These spatial-discretized equations will be used for the implementation of the NMPC algorithm.

The manipulated variables are the inflow molar densities for both H_2 and H_2O (named $\dot{n}_{i,in}$). The molar flux densities for the hydrogen reaction rate and the water transport through the channel (named $\dot{n}_{i,j}$) are included in the model as measured disturbances, the future profiles of which are assumed to be known. The temperature will be considered as constant along the channel, as well as the ambient pressure value. Moreover, full-state feedback to the controller is also assumed, as seen in Figure 3.

IV. NMPC CONTROLLER DESIGN

A. Control-oriented model

From (2), the following discrete-time dynamic model is obtained:

$$x_{i,j}(k+1) = x_{i,j}(k) + \left[\frac{\alpha_{j-1}(k) - \alpha_j(k)}{\Delta z} - d(k)\right], \tag{3a}$$

$$v_j(k) = \frac{K}{\Delta z}\left(p_j(k) - p_{j+1}(k)\right), \tag{3b}$$

$$p_j(k) = RT\left(x_{1,j}(k) + x_{2,j}(k)\right), \tag{3c}$$

with $\alpha_j(k) = v_j(k)x_{i,j}(k)\Delta t$ and $d(k) = \frac{\dot{n}_{i,j}(k)}{\delta}\Delta t$, where the state variables are $x_{1,j}$ (H_2 concentration) and $x_{2,j}$ (H_2O concentration), both along the j volumes of the channel. Moreover, the control inputs are $u_1 \triangleq \dot{n}_{1,in}$, corresponding to the hydrogen molar inflow, and $u_2 \triangleq \dot{n}_{2,in}$, which denotes the humidification molar inflow. Here, Δt is the sampling time that, for this case study, is 10 ms and k is the discrete-time variable.

B. Control objectives

The control objectives for this system are straightforward: it is needed to maintain a certain value of H_2 and H_2O concentrations (x_1^{ref} and x_2^{ref}) along all the channel no matter what PEMFC reaction consumption profile is given. The reaction terms are considered measured disturbances and the global control problem can be also defined as a disturbance rejection problem.

The hydrogen concentration is directly related to the PEMFC output voltage and thus, the generated power of the system. Besides, it is important to properly hydrate the membrane (but not too much) to guarantee the suitable performance of the overall system. Concentrations x_1^{ref} and x_2^{ref} are the reference point for which the designed NMPC controller should steer the system to its stationary point in finite time, in spite of the disturbance profile $\dot{n}_{i,j}$ given by the electrical consumption of the load, which is known beforehand.

C. System constraints

The overall problem constraints are mainly given by the equipment employed to inject both the hydrogen and water molar inflows into the channel. This paper focuses on the theoretical development of the NMPC controller, a necessary step prior to the implementation in a real system. Because of this, the values have been obtained from the data reported in [10], where the theoretical nonlinear model of a PEMFC stack, employed here, is proposed. Those bounding constraints are defined as

$$0 \leq u_1 \leq 40, \tag{4a}$$

$$0 \leq u_2 \leq 15. \tag{4b}$$

The values for the input steady state values are the nominal for the given disturbance vector at a given initial operation condition employed during the case study

$$u_1^{\text{ss}} = 35\ \frac{\text{mol}}{\text{m}^2\,\text{s}}, \quad u_2^{\text{ss}} = 10\ \frac{\text{mol}}{\text{m}^2\,\text{s}}.$$

Apart from the input constraints, there is another set of hard constraints related to the admissible concentration values throughout the channel, not only in the controlled volumes. These constraints are

$$0 < x_{1,j} \leq 20, \quad \forall\, j, \tag{5a}$$

$$0 < x_{2,j} \leq 4, \quad \forall\, j, \tag{5b}$$

where (5a) is related to the hydrogen concentrations. Since all the volumes are constrained to have concentration values higher than zero, there will always be enough H_2 in the anode to satisfy the power demanded by the load variations within normal operation conditions. However, it is possible that if the power demand is enough to saturate the H_2 molar inflow, the system enters in starvation, a situation that would result in a failure to meet constraint (5a) in one or more of the discretized volumes. Constraint (5b) is related to the water concentration of the channel, affecting the humidification of the membrane, which has to be adequate to operate the system within suitable conditions of conductivity and degradation.

D. Cost function

Given the control objectives stated for this problem, the resultant cost function can be written as

$$J(k) = \sum_{j=0}^{n_{\text{Vol}}} ||x_j - x_j^{\text{ref}}||^2_{W_x} + ||\Delta u||^2_{W_u}, \tag{6}$$

where $x_j = [x_{1,j}, x_{2,j}]^T$ and $\Delta u = [\Delta u_1, \Delta u_2]^T$ with $\Delta u_i(k) \triangleq u_i(k) - u_i(k-1)$. Similarly, $x_j^{\text{ref}} = [x_{1,j}^{\text{ref}}, x_{2,j}^{\text{ref}}]^T$. Moreover, notation $||\cdot||^2_W$ indicates the quadratic norm and

W_x and W_y are weighting matrices defined as $W = \gamma_p \mathbf{I}$, with $\gamma_p \in \mathbb{R}$ prioritizing each objective and $\mathbf{I}$ an identity matrix of suitable dimensions. The cost function is applied to each one of the discretized volumes of the channel as denoted by n_{Vol}.

Notice that, apart from the error, minimization terms for the slew-rate of the two manipulable inputs have been included. This is in order to avoid severe changes in the inputs that could damage the considered devices. The optimal tuning of the weighting matrices and other MPC configurable aspects are out of the scope of this paper.

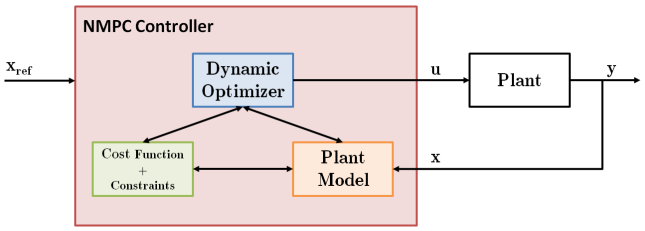

Fig. 3. Closed-loop control scheme of the case study

E. NMPC Algorithm

The algorithm employed for the disturbance rejection approach has been taken from the works presented in [8] and it has been adopted for the proposed case study. The parameters of the algorithm and their units can be found in Table II. Therefore, the design of the NMPC controller for the proposed case study in this paper is based on Problem 1.

Problem 1 (NMPC Design): Let[1]

$$\mathbf{u}(k) \triangleq (u(0|k), \ldots, u(H_p - 1|k)) \tag{7}$$

be the sequence of control inputs over a fixed-time prediction horizon H_p, depending also on the initial condition $x(0|k) \triangleq x_0$. Hence, the NMPC design is based on the solution of the open-loop optimization problem (OOP)

$$\min_{(\mathbf{u}(k) \in \mathbb{R}^{m H_p})} J(x_0, \mathbf{u}(k)), \tag{8}$$

subject to

- system model in (3) over H_p,
- input constraints in (4) over H_p,
- state constraints in (5) over H_p,

where $J(\cdot) : \mathbb{U}^{m H_p} \times \mathbb{R}^{H_p} \mapsto \mathbb{R}$ in (8) is the cost function, with $m = 2$ and $H_p = H_u$. Assuming that the OOP (8) is feasible, there will be an optimal solution for the sequence of control inputs

$$\mathbf{u}^*(k) \triangleq (u^*(0|k), u^*(1|k), \ldots, u^*(H_p - 1|k)) \tag{9}$$

and then, according to the receding horizon philosophy, $u_i^*(0|k)$ is applied to the system, while the process is repeated for the next time instant k.

[1]Here, $z(k+i|k)$ denotes the prediction of the variable z at time $k+i$ performed at k. For instance, $x(k+i|k)$ denotes the prediction of the system state, starting from its initial condition $x(0|k) = x(k)$.

V. SIMULATION RESULTS

The initial state for all simulations is x_0 = ($x_{1,1}$, $x_{1,2}$, $x_{2,1}$, $x_{2,2}$, ...) = (24.75, 7.15, 23.34, 6.83, 21.87, 6.49, 20.33, 6.13, 18.70, 5.74, 16.97, 5.31, 15.11, 4.84, 13.09, 4.30, 10.84, 3.66, 8.25, 2.88, 5.02, 1.82) in [mol][m^{-3}]. The simulations have been carried out using `fmincon` function in MATLAB® R2011a (32 bits), running in a PC Intel® Core™ i7-3770 at 3.40GHz with 8GB of RAM.

A. Simulation scenario

The simulation scenario starts with the system working in an equilibrium point under known hydrogen and water transport reaction terms. From this initial stationary point a known load profile is applied to the PEMFC.

There exists a direct relation between the electrical current of the load and the hydrogen reaction rates of the cell [17]. An hydrogen consumption spatial profile (for each volume of the channel) has been considered in every time instant of the simulation. The water transport terms are computed proportionally from the hydrogen curve since the hydration is also a function of the hydrogen consumption of the system. The profile of the hydrogen consumption multiplier for all of the discretization volumes versus time is shown in Figure 4.

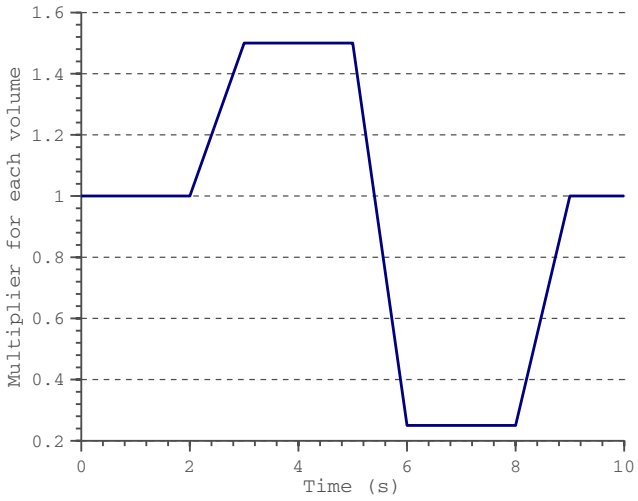

Fig. 4. Hydrogen rate multiplier applied to each volume of the discretized anode channel

Different combinations of controlled volumes will be simulated and analyzed in subsequent sections in order to determine which one is the most appropriate control strategy for the dynamical behaviour of the energy system studied in this work.

B. Controller setup

NMPC algorithms are highly configurable via the tuning of its parameters (control and prediction horizons, penalization terms, etc.). As it was said previously, the fine tuning of this parameters is out of the scope of the present work, but it has to be stated that there exists the possibility of future improvement for the performed simulations.

Table II shows the controller setup parameters and the computational burden of each one of the simulations performed with the machine previously described.

TABLE II
NMPC SETUP PARAMETERS

Parameter	Variable	Value
H_2 reference penalization	α	10
H_2O reference penalizacion	β	0.1
Prediction horizon	H_p	5
Control horizon	H_c	5
Sampling time	Δt	10 ms
Simulation time	T_{sim}	10 s
Computing time	CPU_t	30 min

In some of the simulations there will be multiple controlled volumes, for which constant weighting terms will be assumed.

C. Results and discussion

To study and to compare the obtained simulation results, the mean absolute error

$$MAE = \frac{1}{n_{\text{Vol}}} \sum_{i=1}^{n_{\text{Vol}}} |e_i| = \frac{1}{n_{\text{Vol}}} \sum_{i=1}^{n_{\text{Vol}}} |x_i - x_i^{\text{ref}}|$$

has been used. This error is computed by comparing the state values at a given moment of the simulation with their reference values, which are constant.

In Table III the average mean absolute errors (MAE) over all the simulation time are presented for six possible combinations of controlled volumes.

TABLE III
MEAN ABSOLUTE ERROR OF THE SIMULATIONS

Control volume(s)	Acronym	Average MAE (%)
First	$(F)_V$	3.48
First-Middle	$(F\text{-}M)_V$	2.73
Middle	$(M)_V$	2.69
Middle-Last	$(M\text{-}L)_V$	2.93
Last	$(L)_V$	5.62
First-Last	$(F\text{-}L)_V$	2.68

The computing time for each of the simulations is around 30 minutes each time the algorithm runs to study 10 seconds of the behavior of the system. This may be a problem when implementing the controller in a real system, for which this time has to be drastically decreased below the real response time of the system.

The behavior of the MAE for all of the different considered cost functions is represented in Figure 5. As it can be extracted from the figure, the behavior of the disturbance rejection is similar for the majority of the cases. Some exceptions appear, like when only the last discretized volume is controlled.

From the average MAE and the results presented in Table III, it can be extracted that the best performance is

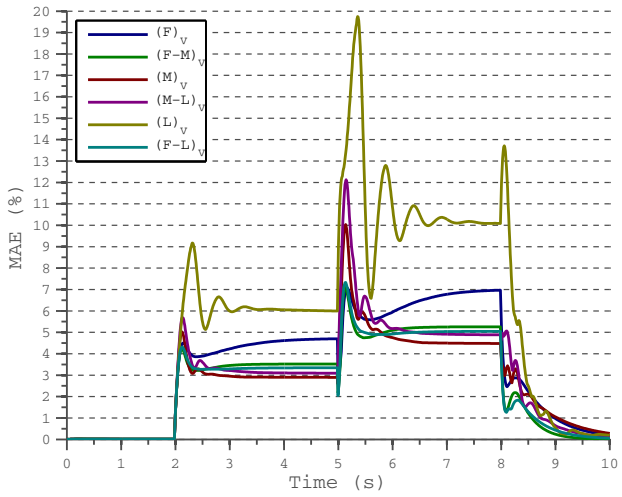

Fig. 5. Mean absolute error profile for six control volumes combinations

obtained with the configuration that has the first and last volumes as controlled volumes. This is due to the lower average mean absolute error of the disturbance rejection problem and the lower overshoots of the error for this combination. Also notice that the full regulation of two volumes in steady state is not possible because there are not enough degrees of freedom with two manipulated inputs.

The dynamical behaviour of the controlled outputs for the two controlled volumes in this case and the manipulated inputs applied to the system in order to regulate the concentrations to the reference point $\left(x_1^{\text{ref}} = 24.75, x_2^{\text{ref}} = 7.15\right)$ are shown in Figure 6.

It is possible to plot the whole range of the concentrations profile during the duration of the simulation process. This is presented in Figure 7 and shows that with the proposed control method, the concentrations remain in a narrow bounded band of values that guarantee an stable behavior of the energy system no matter the load current variation (and thus, reaction disturbances).

VI. CONCLUSIONS

An NMPC controller has been designed to be applied to a PEMFC anode gas channel. This strategy allows to control the nonlinear dynamics of the concentrations profile. The performance of the controller has been evaluated, obtaining satisfactory results for a specific simulation scenario. The quantified improvement depends on the controlled volumes selected. Indeed, when stating the cost function, the selection of some combinations of controlled volumes are more convenient from the performance point of view. Specifically, the inclusion of two volumes concentrations in the cost function reduces the error and, controlling the first and last volumes, shows to be most suitable option. With the proposed control strategy, the variation of the concentrations are guaranteed to be limited to small values in all the channel.

While in the present work only 11 discretized volumes have been considered, future research will be aimed at generalizing the approach up to *n* discretized volumes. In

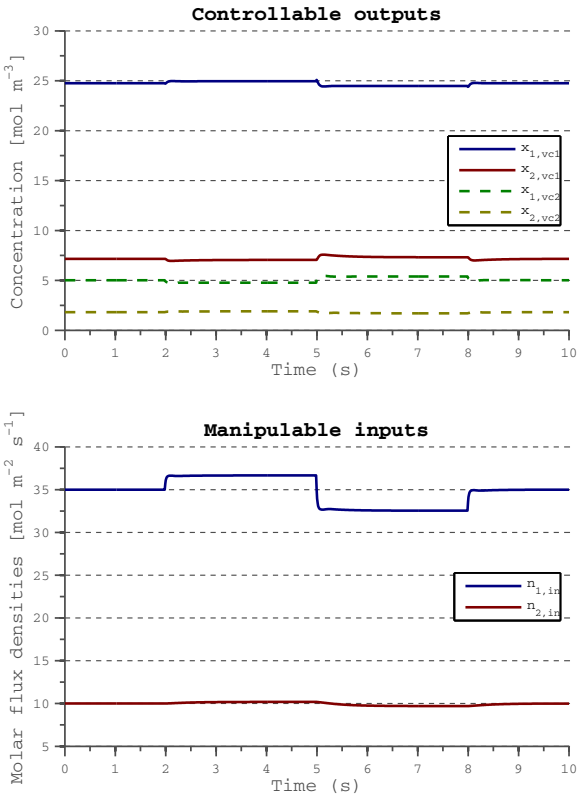

Fig. 6. Concentration profile of the NMPC case with the first and last controlled volumes (upper) and manipulated inputs

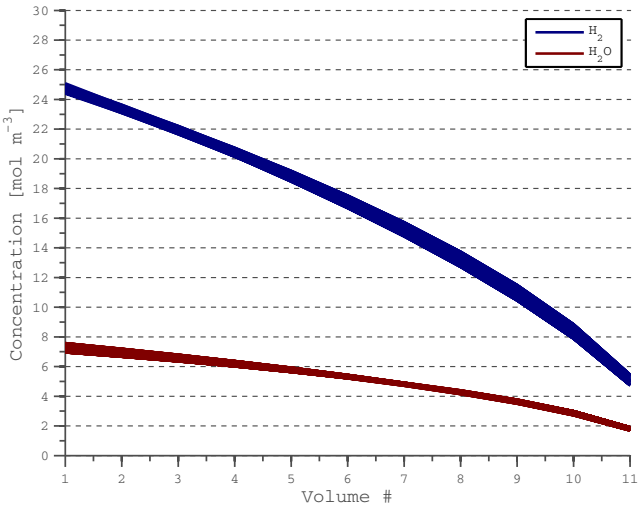

Fig. 7. Concentrations distribution through all the discretization volumes during the simulation

addition, this work presents the control approach to a single anode gas channel. However, it is forthcoming to include all PEMFC components (e.g., cathode, membrane, GDL) in order to implement the proposed controller to the entire PEMFC-based system, even over a real test-bench.

ACKNOWLEDGMENTS

This work has been partially funded by the Spanish national project MESPEM (Ref. DPI2011-25649) and the MACPERCON project (Ref. 201250E027) of the Spanish National Research Council (CSIC).

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