State Observers Design for PEMFC Systems

Julio Luna, Attila Husar, Maria Serra

Institut de Robòtica i Informàtica Industrial (CSIC-UPC), C/ Llorens i Artigas 4-6, 08028 Barcelona, Spain

RESUMEN: *Este trabajo presenta el desarrollo de un observador de estados no lineal para la estimación de los perfiles de concentraciones en un sistema de energía basado en una Pila de Combustible de Membrana de Intercambio Protónico (PEMFC). La selección de los estados a estimar está basada en la funcionalidad y desempeño del observador. Las ecuaciones en derivadas parciales son discretizadas en dos sentidos a partir de un modelo 1+1D para aprovechar las condiciones de contorno del problema. Una acción de corrección basada en métodos deslizantes de segundo orden es implementada para reducir el error de estimación a cero en un periodo finito de tiempo. Se presentan resultados de simulación para mostrar el rendimiento del observador en la reconstrucción de los valores de los estados y para extraer conclusiones para futuro trabajo de investigación.*

ABSTRACT: *This work presents the development of a nonlinear state observer to estimate the values of the different gas species concentration profiles in a Proton Exchange Membrane Fuel Cell (PEMFC) energy system. The selection of the estimated states is based on the functionality and performance of the observer. The implementation is based on the discretization of a PEMFC distributed 1+1D model. Forward and backwards discretization of the partial derivative equations is performed to take advantage of the boundary conditions of the problem. A second-order sliding-mode control super-twisting corrective input action is implemented to reduce the estimation error to zero in a finite amount of time. Simulation results are presented to show the performance of the observer to estimate the values of the states and to extract conclusions for future research work.*

Palabras clave: *PEMFC, modelo distribuido, observadores no-lineales, super-twisting, estimación.*
Keywords: *PEMFC, distributed model, nonlinear observers, super-twisting, estimation.*

1. INTRODUCTION

To operate properly, different physical variables have to be measured from the PEMFC, which make possible to implement output-feedback control laws. While a certain number of these measurements are feasible to perform with the current existing sensor technology, due to the enclosed construction of the system, there are parts that are inaccessible and therefore, state estimation techniques are needed to obtain the internal state values.

A limited number of works have been published regarding the nonlinear observation in PEMFC systems aimed to design appropriate controllers and perform diagnosis. The membrane water content estimation [1] is a critical aspect of the water management problem, which is crucial when operating a PEMFC. The inlet oxygen flows [2] and fuel cell hydrogen estimation [3] through the measurement of the output manifold pressures are necessaryto maintain a proper reactant amount in the system and to decrease the hydrogen consumption respectively.

The model-based nonlinear state observation approach has an extensive amount of advantages due to the consideration of the nonlinear dynamics of the system. It allows the implementation of output-feedback nonlinear control techniques that allow the system to operate far away from its nominal working point, which is a common situation in PEMFC energy systems. The main contribution of this paper relies on the implementation of a nonlinear observer topology [4] based on a distributed parameters model [5] of a PEMFC.

The rest of the document is organized as follows. In section 2 the mathematical model of the PEMFC is developed. The analysis of the observed variables is presented in Section 3. Section 4includes the design of the nonlinear observer. Simulation results are shown in Section 5. Finally, in Section 6, the conclusions of this research work are presented.

2. MATHEMATICAL MODEL

A schematic representation of the single-channel PEMFC modeled for the present work is shown in Fig. 1. The dynamic modeling of the system considers discretized partial derivative equations (PDE) along the z-axis (backwards and forwards discretization techniques are applied to the original equations [5] to take advantage of the boundary conditions of the problem). The reacted hydrogen, oxygen and water transport flows through the membrane are perpendicular to the supply channels (y-axis direction) and are depicted as lump parameters. The PEMFC model [5] includes the mathematical representation of the anode and

cathode gas channels, gas diffusion layers (GDL), catalyst layers (CL) and the electrolyte membrane.

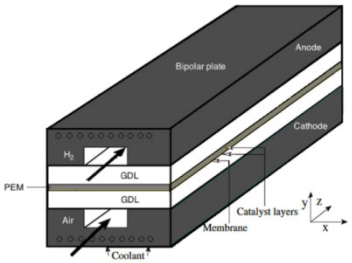

Fig. 1. Single-channel PEMFC representation.

Both anode and cathode gas channels follow Darcy's mass balance equations that relate the concentrations $\dot{c}$, pressure p and velocity v along the channel to model the gas transport in the z-direction

$$\dot{c}_{i,j}^{k} = \frac{v_{j-1}^{k} c_{i,j-1}^{k}}{\Delta z} - \frac{v_{j}^{k} c_{i,j}^{k}}{\Delta z} - \frac{\dot{n}_{i,j}^{k}}{\delta^{k}}, \quad (1a)$$

$$v_{j}^{k} = \frac{K^{k}}{\Delta z}\left(p_{j}^{k} - p_{j+1}^{k}\right), \quad (1b)$$

$$p_{j}^{k} = RT^{k} \sum_{i} c_{i,j}^{k}, \quad (1c)$$

where subscript i refers to the component mass index (i = H_2, H_2O on the anode side and i = O_2, N_2, H_2O on the cathode side) and subscript j indicates the discretized volume. Molar flux densities $\dot{n}_{i,j}^{k}$ are assumed to be perpendicular to the channels in the y-direction. Superscript k indicates that the equations are valid for both gas channels. The discretization step is represented by Δz.

Fick's second law of diffusion

$$\dot{c}_{i} = D_{i} \frac{\partial^{2} c_{i}}{\partial y^{2}}, \quad (2)$$

describes the transport gradient from the anode and cathode gas channels through the GDLs to the CLs of the PEMFC.

The electrochemical reaction takes place in the CLs. The molar fluxes are function of the anodic and cathodic reaction rates r_{j}^{k} and are assumed to be unidimensional. Moreover, these values are obtained from the diffused concentration values after applying Equation (2) to the gas channels concentrations. For the anode side, the molar fluxes include H_2 and H_2O transports along the y-axis

$$\dot{n}_{H_2,j}^{A} = r_{j}^{A}, \quad (3)$$

$$\dot{n}_{H_2O,j}^{A} = \dot{n}_{H_2O,j}^{AM}. \quad (4)$$

Three molar fluxes are modeled in the cathode

$$\dot{n}_{O_2,j}^{C} = \frac{1}{2} r_{j}^{C}, \quad (5)$$

$$\dot{n}_{H_2O,j}^{C} = \dot{n}_{H_2O,j}^{CM} - r_{j}^{C}, \quad (6)$$

$$\dot{n}_{N_2,j}^{C} = 0. \quad (7)$$

A complete water transport model [6] is implemented in the membrane layer of the PEMFC. Water plays a key role in the dynamics of the proton transport and the water content which is defined as the relation between the number of water molecules and the moles of polymer in the membrane and it is included in the model.

3. STATES TO OBSERVE

The implemented model for this work includes several states. Nonetheless, the observation of the gas species concentrations $\dot{c}_{i,j}^{k}$ is going to be the focus of the study. The predominant reason behind this decision is that the knowledge of the gas species concentrations values allows for designing controllers and diagnosis tools based on output-feedback techniques that consider the internal variables of the PEMFC.

Furthermore, the degree of complexity when designing the observer for the gas concentrations is lower than with other states, since the mass balance model presented in Equation (1) does not depend on the water content (which introduces a great level of mathematical complexity) as much as other state variables in the PEMFC model do.

4. NONLINEAR STATE OBSERVER DESIGN

4.1. Structure of the observer

The main structure of the observer follows a model-based approach of the literature [4] for an n-order system

$$\dot{\hat{\boldsymbol{x}}} = \boldsymbol{f}(\hat{\boldsymbol{x}}, \boldsymbol{u}) + \boldsymbol{g}(\hat{\boldsymbol{x}})\boldsymbol{u_0}, \quad (8a)$$

$$\hat{\boldsymbol{y}} = \boldsymbol{h}(\hat{\boldsymbol{x}}), \quad (8b)$$

where the generalized observed state vector $\dot{\hat{\boldsymbol{x}}} \in \mathbb{R}^{n}$ and observed output variable $\hat{\boldsymbol{y}} \in \mathbb{R}^{p}$. The function $\boldsymbol{f}(\hat{\boldsymbol{x}}, \boldsymbol{u})$ contains the nonlinear part of the model. The vector function $\boldsymbol{g}(\hat{\boldsymbol{x}})$ provides the observer with full relative degree n with respect to the input vector $\boldsymbol{u}$. The correction input $\boldsymbol{u_0}$ is designed to achieve null estimation error in a finite amount of time using super-twisting algorithms based in SMC control techniques [7].

4.2. Nonlinear observability condition

For the nonlinear case, the observability condition arises from the computation of the observability matrix $\mathcal{O}$ that maps the outputs of the

system to the initial values computing all the repeated Lie derivatives of the output vector field $\boldsymbol{y}$

$$\mathcal{O}(\boldsymbol{x}) = \frac{\partial}{\partial \boldsymbol{x}} \begin{bmatrix} \boldsymbol{h}(\boldsymbol{x}) \\ L_{f(x)}\boldsymbol{h}(\boldsymbol{x}) \\ \dots \\ L_{f(x)}^{(n-1)}\boldsymbol{h}(\boldsymbol{x}) \end{bmatrix}, \qquad (9)$$

where the Lie derivative can be written as the tensor field defined by

$$L_{f(x)}\boldsymbol{h}(\boldsymbol{x}) = \frac{\partial \boldsymbol{h}(\boldsymbol{x})}{\partial \boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x}). \qquad (10)$$

The full state vector is observable if $rank\big(\mathcal{O}(\boldsymbol{x})\big) = n$.

4.3. Implementation of the observer for the PEMFC model

The design of the gas species concentrations observer is developed from the main observer structure shown in Equation (8), having studied the observability condition beforehand. Assuming that the $\dot{n}_{i,j}^{k}$ reaction terms are measured disturbances, it is possible to obtain two separated nonlinear state space models for the anode and cathode gas channels concentrations. Therefore, their estimation is solved as two separated estimation problems. Function $\boldsymbol{f}(\hat{\boldsymbol{x}}, \boldsymbol{u})$ includes the nonlinear dynamic descriptionpresented in Equation (1). The vector $\boldsymbol{g}(\hat{\boldsymbol{x}})$ is obtained from the observability matrix $\mathcal{O}$ presented in Equation (9)

$$\boldsymbol{g}(\hat{\boldsymbol{x}}) = (\mathcal{O})^{-1}(\hat{\boldsymbol{x}})[0,0,\dots,1]^{T}. \qquad (11)$$

To remove the observation error a corrective input $\boldsymbol{u_0}$ is included in the main observer structure [7]

$$u_{i,j}^{k} = -K_1 \left|e_y\right|^{\frac{1}{2}} sign\big(e_y\big) + v, \qquad (12a)$$
$$\dot{v} = -K_2 \frac{1}{2}\, sign\big(e_y\big), \qquad (12b)$$

being $e_y = \hat{y} - y$ the output state vector for each of the measured gas concentrations and K_1 and K_2 tuning constants of the corrective action law.

5. SIMULATION RESULTS

The initial state for all simulations is defined by the vector $\boldsymbol{x_0} \in \mathbb{R}^{5\times n_{Vol}}$, which denotes the five gas species present in both gas channels. The observers are initialized with an initial observed state vector $\hat{\boldsymbol{x}}_{\boldsymbol{0}} = \boldsymbol{0} \in \mathbb{R}^{5\times n_{Vol}}$. Simulations have been carried out using Simulink for MATLAB® R2011a.

5.1. Simulation scenario

Table 1 shows an example of initial operation condition to start the simulation.

Table 1. Example initial operation conditions.

Parameter	Units	Value
Anode stoichiometry	-	2.2
Cathode stoichiometry	-	3
Temperature	K	353
Cell voltage	V	0.5

From the initial operation condition the input molar fluxes for the gas species are computed. Step changes are applied at simulation time $t = 125$ s, $t = 250$ s and $t = 375$ s. The goal of these step changes is to test the dynamical behavior of the observer when the concentration values fluctuate.

The study assumptions include an isothermal model, the input molar flows as measured inputs, the last volume concentration values as measured outputs and the y-direction reaction rates and water transport terms as measured disturbances.

5.2. Results and discussion

Even though the estimation is done for all the selected states, simulation results only show the estimation at the middle point of the gas channels.

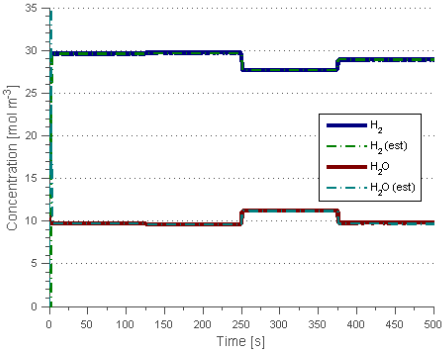

Fig. 2. State estimation anode gas channel.

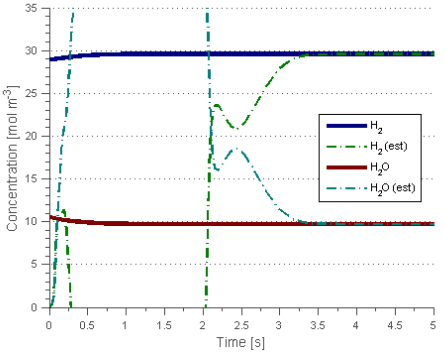

Fig. 3. State estimation anode gas channel (detailed zoom).

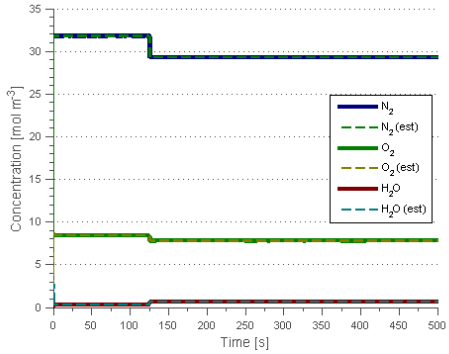

Fig. 4. State estimation cathode gas channel.

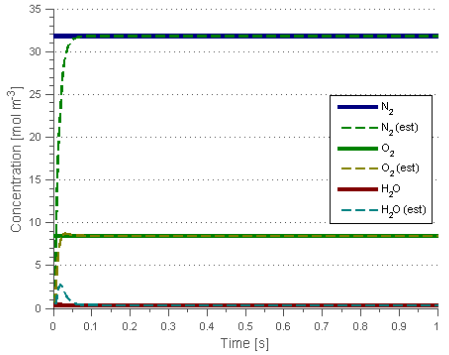

Fig. 5. State estimation cathode gas channel (detailed zoom).

As it can be extracted from Fig. 3 and Fig. 5, the observation of the gas species concentrations (dashed lines denoted by *est* in the figures) is performed properly in a simulation environment. For the reconstruction of the anode gas channel gases, the convergence occurs in less than 3.5 seconds, while in the cathode side the observer converges faster. The difference between the state reconstruction times depend on several conditions such as the K_i gains of the observers, the initial observed state vector $\hat{\boldsymbol{x}}_{\boldsymbol{0}}$ or the initial values of the real states of the system. The tuning of these parameters is out of the scope of the present work.

After the observers converge toreal values, the estimated states remain with a reconstruction error equal to zero, even after the step changes for the dynamic analysis are injected to the PEMFC plant.

6. CONCLUSIONS

The presented nonlinear state observer designed for a PEMFC energy system, described by a distributed parameter model, allows the recovering of unknown information about the internal state variables. The performance of the observer has been evaluated, obtaining satisfactory observation of the anode and cathode gas concentrations for a specific simulation scenario.

In this work, the reaction and water transport terms have been considered as measured disturbances. The continuation of the research includes the analysis of the degree of model and input uncertainties that can be included into the design of the observer.

A total of five discretization volumes have been taken into consideration to perform the simulations. It is possible to generalize the results to a higher number of volumes to obtain concentration profiles with higher level of detail. Nevertheless, the increasing of discretization volumes introduces complexity when obtaining the observer. A trade-off situation arises between the required level of detail of the recovered state information and the mathematical complexity of obtaining the observer.

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