

Distributed Parameter Nonlinear State Observer with Unmatched Disturbance Estimation for PEMFC Systems

Julio Luna¹, Elio Usai², Attila Husar¹ and Maria Serra¹

¹Universitat Politècnica de Catalunya. Institut de Robòtica i Informàtica Industrial (CSIC-UPC). C/Llorens i Artigas 4-6. 08028 Barcelona, Spain

²Università di Cagliari. Dipartimento di Ingegneria Elettrica ed Elettronica (DIEE), Piazza d'Armi, Cagliari, Italy

{jluna,ahusar,maserra}@iri.upc.edu, eusai@diee.unica.it

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ABSTRACT

In this paper a nonlinear state observer based on a distributed parameter model is proposed for a proton exchange membrane fuel cell (PEMFC). The estimation technique is implemented using a model-based nonlinear observer with a nonlinear disturbance observer in parallel. To implement the model, a finite element discretisation is performed to take advantage of the boundary conditions of the problem and also to apply lumped systems theory in the observer synthesis procedure. By means of this double observation technique it is possible to reconstruct the gases concentrations internal states in the gas channels of the PEMFC in the presence of disturbances. The reaction rates and water transport terms that cross the membrane are considered as unknown unmatched disturbances of the model, henceforth the implementation of a disturbance observer to estimate them. Simulation results of the proposed solution are provided and discussed.

1 INTRODUCTION

Measuring the internal states in a PEMFC is virtually impossible due to the enclosed construction of the overall system. However, in order to implement advanced control techniques that improve the efficiency and life expectancy of the plant, these internal states are required to be known. Moreover, the knowledge of the internal variables can be used for the diagnosis of the state of health of the PEMFC. The concentrations of the different gas species along both gas channels (anode and cathode) are critical variables for the efficient and lasting operation of the PEMFC. To reconstruct their values from the measured outputs, a nonlinear state observer with unmatched disturbance estimation is proposed in this paper.

Some authors have proposed nonlinear observers [1] based on concentrated parameter models of the PEMFC [2] for the estimation of unmeasurable variables in dynamical systems. In this paper, the observer is model-based on a distributed parameter model [3,4].

This approach allows to describe in detail the internal dynamics of the PEMFC and to represent the full profile behaviour of the states in the direction of the gas channels. Forward and backward discretisation of the model is performed to take advantage of the boundary conditions of the problem, which are the input molar flows and the external ambient pressure. The measurements used to reconstruct the internal states are the input and output flow rates and pressures.

The hydrogen and oxygen reaction terms and the water transport flows across membrane are considered as unmeasured disturbances. The effect of the disturbances in a dynamical system define the robustness of the control and estimation solutions applied to it. Two different kinds of disturbances can affect the system: matched and unmatched. Matched disturbances affect the input signals of the plant (i.e. actuator faults) while unmatched disturbances are model and parameter uncertainties. Recent research works [5, 6] only focus on the treatment of matched and unmatched disturbances from the control point of view. In this paper a nonlinear disturbance observer (NDOB) [7] is implemented in parallel with the main state observer to estimate the values of the unmatched disturbances and inject them into the main observer to recover the values of the states.

As introduced before, the main state estimator is model-based. From the modelling domain point of view, the PEMFCs can be represented by 1D models through the membrane, by 2D models or by more complex and precise 3D models. Combinations between models can be made: i.e. it is possible to combine models to obtain 1+1D and 2D+1D variations. The trade-off between the complexity of the model and the level of detail is the main argument when selecting a mathematical representation of a PEMFC. In the 1D modelling approach, some researchers have studied the distributed dynamical behaviour of the membrane and channels variables along one direction [8] with isothermal assumptions. More advanced studies include non-isothermal models [9]. Other authors have developed 1D control-oriented models for PEMFC systems [2]. More complex 2D models can be found in the literature. In particular, in [10] a 2D model that focuses on the behaviour of the fluid hydrodynamics and electrochemical kinetics of a PEMFC is developed. A quasi-two-dimensional (1+1D) distributed parameter model is developed in [4]. Further complexity and detail can be found in 3D models. From computational PEMFC dynamical research [11] that studies the interactions between mass transport and electrochemical kinetics, to models [12, 13] focused in parameter sensitivity analysis and experimentation.

The main contribution of this paper relies on the implementation of a nonlinear distributed parameter observer (NDPO) with unmatched disturbance estimation of the reaction and water transport terms for a distributed parameter 1+1D PEMFC model. From the results of the study, conclusions about the internal dynamics of the system and the effect of the reaction disturbances can be extracted.

This paper is organised as follows. In Section 2 the model for the PEMFC is introduced, following first physical principles. In section 3 the observation-oriented model is developed and the main observer described. The NDOB for the unmatched disturbances is described in Section 4. Simulation results for the observer with disturbance estimation are presented and analysed in Section 5. Finally some conclusions are extracted and discussed in Section 6.

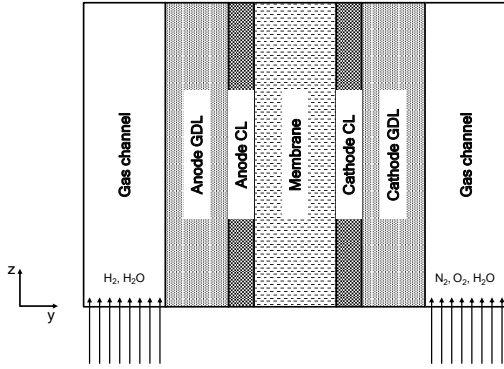


Figure 1: PEMFC modelling domain.

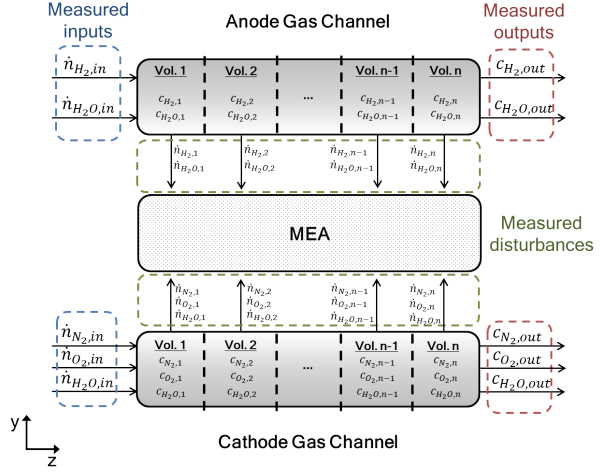


Figure 2: Discretised PEMFC.

2 MATHEMATICAL MODELLING

In this section the distributed parameter model for the PEMFC is presented. Certain assumptions have been considered [4] in order to simplify the understanding of the dynamics. First of all, the fluid in the gas channels and in the GDLs behaves like an ideal gas. Moreover, the liquid water formation is not considered neither in the gas channels nor in the GDLs. The electrical energy that the PEMFC produces is injected into a load. It is assumed that the gas channels possess a storage capacity for mass. Finally, the temperature of the model follows an isothermal behaviour.

2.1 Modelling domain

The modelling domain for the PEMFC system studied in this paper is portrayed in Figure 1. The layers, according to their physical distribution and functionality in the PEMFC are the gas channels (anode and cathode), gas diffusion layers (GDLs), catalyst layers (CLs), and the membrane.

Nevertheless, since the observer considers the internal layers variables as unknown unmatched disturbances (that will be estimated through the NDOB), only the differential equations for the gas channels are given in this paper, though the rest of the layer domains are included in the simulation model. The justification for the use of the gas concentrations as the main modelling domain variables to synthesise the observer and the whole PEMFC model were given in [14].

2.2 PEMFC gas channel model

The gas channels (anode and cathode) are modelled following a nonlinear mass balance equation for the gas transport in the z-direction of the PEMFC

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

$$v(t) = -K \frac{\partial p(t)}{\partial z}, \quad (1b)$$

$$p(t) = RT \sum_i c_i(t), \quad (1c)$$

where subscript i stands for the reactant, being $i = \text{H}_2$ the hydrogen index, and $i = \text{H}_2\text{O}$ the water index in the anode side. At the cathode side, $i = \text{N}_2$ denotes the nitrogen, $i = \text{O}_2$ the oxygen and $i = \text{H}_2\text{O}$ the water. Molar flux densities \dot{n}_i are the reaction and water transport terms for the five gas species of the model in the y-direction. It is assumed that they are unmeasured uncertainties of the model.

3 PRIMARY STATE OBSERVER

The state space representation for nonlinear systems can be expressed as follows:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)), \quad (2a)$$

$$\mathbf{y}(t) = \mathbf{h}(t, \mathbf{x}(t), \mathbf{u}(t)), \quad (2b)$$

where $\mathbf{x}(t) \in \mathbb{R}^n$ is the state vector, $\mathbf{y}(t) \in \mathbb{R}^p$ the measured output vector and $\mathbf{u}(t) \in \mathbb{R}^m$ the input or control vector. For the gas channel model (1), the concentrations c_i are the state variables x_i as suggested in [14], the input and output flow rates and pressures are the measured outputs and the molar fluxes injected to the PEMFC the input vector values.

3.1 Observation-oriented model

Applying forward and backward discretisation techniques on (1) over the discretisation length Δz , and considering the constants $C_1^k = KRT/\Delta z^2$ and $C_2^k = Kp^{amb}/\Delta z^2$, it is possible to develop the generalised observation-oriented model for each one of the discretisation volumes from 1 to n_{Vol}

$$\dot{x}_{i,j}^k(t) = \begin{cases} \frac{\dot{n}_{i,in}^k(t)}{\Delta z} - C_1^k \Psi^k(j) - \frac{\dot{n}_{i,j}^k(t)}{\delta^k} & \text{if } j = 1, \\ C_1^k [\Psi^k(j-1) - \Psi^k(j)] - \frac{\dot{n}_{i,j}^k(t)}{\delta^k}, & \text{if } 2 \leq j \leq n_{Vol} - 1, \\ C_1^k \Psi^k(j-1) - C_1^k x_{i,j}^k(t) \sum_i x_{i,j}^k(t) + C_2^k x_{i,j}^k(t) - \frac{\dot{n}_{i,j}^k(t)}{\delta^k}, & \text{if } j = n_{Vol}, \end{cases} \quad (3)$$

with

$$\Psi^k(j) = x_{i,j}^k(t) \left(\sum_i x_{i,j}^k(t) - \sum_i x_{i,j+1}^k(t) \right), \quad (4a)$$

$$\Psi^k(j-1) = x_{i,j-1}^k(t) \left(\sum_i x_{i,j-1}^k(t) - \sum_i x_{i,j}^k(t) \right), \quad (4b)$$

where the state variables $x_{i,j}^k$ refer to the i -th gas concentrations at the j discretisation volume. Superscript k stands for a generalisation to specify that the variable is valid for both the anode ($k = A$) and the cathode ($k = C$) sides of the PEMFC.

The model-based NDPO developed in the consecutive sections is synthesised based on the observation-oriented model in (3).

3.2 Nonlinear Distributed Parameter Observer

Developing the model-based nonlinear observer structure proposed in [3] with the discretised observation-oriented model presented in (3) for a n -order nonlinear system, the observer structure [3] is such that

$$\dot{\hat{\mathbf{x}}} = \mathbf{f}(\hat{\mathbf{x}}, \mathbf{u}) + \mathbf{g}(\hat{\mathbf{x}})\mathbf{u}_0, \quad (5a)$$

$$\hat{\mathbf{y}} = \mathbf{h}(\hat{\mathbf{x}}), \quad (5b)$$

where the generalised observed state vector $\hat{\mathbf{x}} \in \mathbb{R}^n$ and the observed output variable $\hat{\mathbf{y}} \in \mathbb{R}^p$. The function $\mathbf{f}(\hat{\mathbf{x}}, \mathbf{u})$ contains the nonlinear dynamics of the model. The vector function $\mathbf{g}(\hat{\mathbf{x}})$ provides the observer with full relative degree n with respect to the input vector \mathbf{u} . The correction input \mathbf{u}_0 is designed to achieve null estimation error in a finite amount of time. In the present work, a Super-Twisting Algorithm (STA) based in Sliding Mode Control (SMC) techniques [15] is implemented. The details of the observability of (3) and the synthesis of the observer and corrective action were presented in [14]. The implementation of the model presented in (3) contemplates a five volume discretisation for (5), considering the trade-off between the detail of the solution and the complexity of synthesising higher order discretised observers. Likewise, five volumes are considered in this paper for the simulations ($n_{Vol} = 5$).

4 NDPO WITH DISTURBANCE OBSERVER

Rewriting the observation-oriented model (3) as a function of the dynamics of the plant (f), input gains (g_1) and unmatched disturbances (g_2):

$$\dot{x}_{i,j}^k(t) = f(x_{i,j}^k(t)) + g_1(x_{i,j}^k(t))u^k + g_2(x_{i,j}^k(t))d^k(t), \quad (6a)$$

$$y_i^k(t) = x_{i,out}^k(t). \quad (6b)$$

To estimate the nonlinear unmatched disturbances d^k in (6), a NDOB [7] is implemented in parallel with the NDPO (5)

$$\dot{p}^k = -l^k g_2(x_{i,j}^k(t))p^k - l^k [g_2(x_{i,j}^k(t))l^k x_{i,j}^k(t) + f(x_{i,j}^k(t)) + g_1(x_{i,j}^k(t))u^k], \quad (7a)$$

$$\hat{d}^k(t) = p^k + l^k x_{i,j}^k(t), \quad (7b)$$

where \hat{d}^k is the estimation of the disturbance and p^k represents the internal nonlinear dynamics of the NDOB. The gain is represented by l^k . The final topology of the estimation technique proposed in this paper is shown in Figure 3.

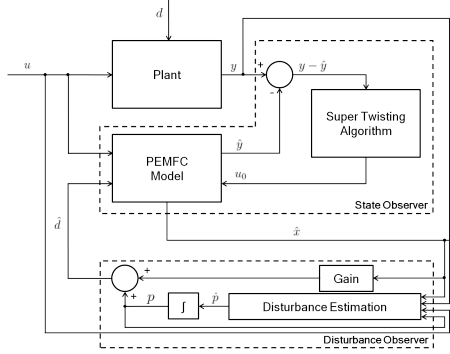


Figure 3: NDPO with NDOB topology.

5 SIMULATIONS

Consider the initial state vector $\mathbf{x}(\mathbf{0}) \in \mathbb{R}^{5 \times n_{vol}}$ for (3) and the initial observed state vector $\hat{\mathbf{x}}(\mathbf{0}) = \mathbf{0} \in \mathbb{R}^{5 \times n_{vol}}$ for (5). The initial state vector is computed from a common PEMFC operating point defined by the anode and cathode stoichiometry $\lambda_A = 2.2$ and $\lambda_C = 3$, the PEMFC temperature $T = 353$ K and voltage $U = 0.5$ V. The observer parameters are $l^A = 1e^{-9}$ and $l^C = 1e^{-12}$. The fine tuning of these parameters is out of the scope of this paper. Step variations are imposed on the system inputs at $t = 125$, $t = 250$ and $t = 375$ seconds (see Table 1) to test the dynamical behaviour of the observer when the system drives away from its initial operating point.

Table 1: Step values for the dynamical analysis

Input molar flow	Time [s]	Initial [mol m ⁻² s ⁻¹]	Final [mol m ⁻² s ⁻¹]
O ₂	125	60	30
H ₂	250	16	14
H ₂ O (anode)	375	4	3

5.1 Results and discussion

The NDPO (5) with NDOB (7) reconstructs all the internal states (gases concentrations) for each of the discretised volumes of the system (3), which are five as aforesaid. Nevertheless, for presentation purposes, only the states in the middle point of the gas channel are shown in this section. This point is of special significance due to the difficulties of sensorising it.

Figures 4 and 5 show the observation of the five gas species (dashed lines denoted by *est* in the figures) in the PEMFC. During the reconstruction of the anode gas channel states, there is an increase of the estimation error ($e_x = x - \hat{x}$) when the system drives away from its initial operating point as depicted by Figure 4 between times 250 and 375 seconds. However, these errors can be considered negligible. At the cathode side the estimation of the states remains almost perfect right after the convergence takes place. Though, a small-scale offset can be appreciated in the detail shown in Figure (5) for the H₂O estimation at the cathode.

The differences between the state reconstruction at both sides of the PEMFC depend on several conditions, such as the fine tuning of the observer for the different gas species, the

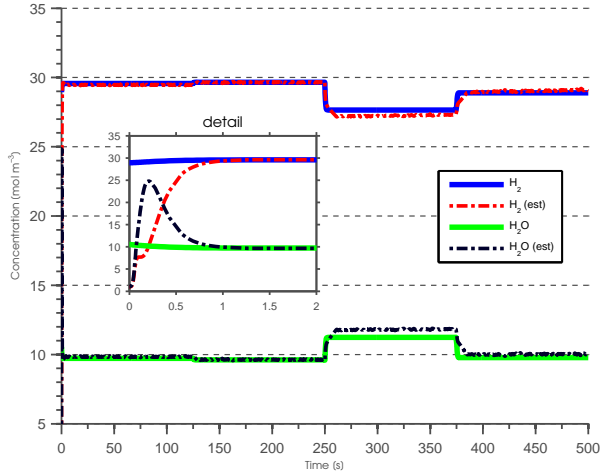


Figure 4: Estimation in the anode.

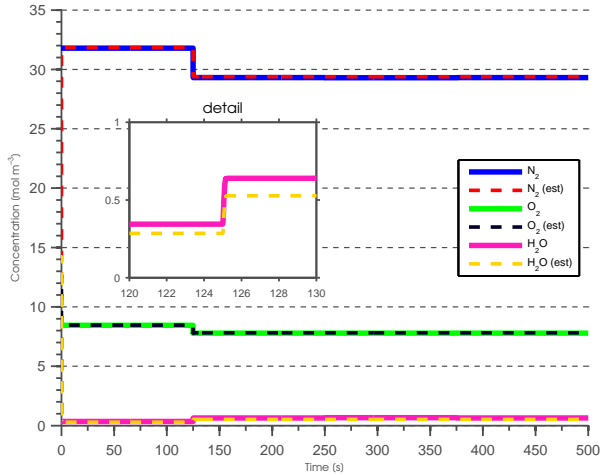


Figure 5: Estimation in the cathode.

gains of the corrective action and the difference in the dynamics that govern the internal layers of the PEMFC simulation model.

6 CONCLUSIONS

In this paper, a NDPO with nonlinear disturbance estimation is proposed to recover the full state profiles in a PEMFC system. The improved NDPO allows to estimate the reaction and water transport terms considering them as unmatched disturbances. The performance of the observer has been evaluated in a simulation scenario, obtaining satisfactory results.

The simulations presented in this paper have been carried out for a total of five discretisation points. The increase of the discretisation volumes introduces mathematical complexity when synthesising the observer. A trade-off situation arises between the required level of detail in the recovered information and the observer synthesis complexity. Nonetheless, with the configuration presented in this paper, a convenient amount of information can be extracted from the simulations.

The developed technique is suitable to design advanced controllers with output-feedback control taking into account the internal information of the PEMFC given by the observer. Furthermore, diagnosis tools to display the current PEMFC health state can be designed using the NDPO. The proposed observation technique can also be applied to other kinds of distributed parameter systems. It is forthcoming to develop new disturbance observation techniques to compare the results with the ones described in this paper.

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NOMENCLATURE

C	Volumetric capacitance	(C V ⁻¹ m ⁻³)	n_{Vol}	Discretisation volumes	-
c	Concentration	(mol m ⁻³)	p	Pressure	(Pa)
D	Diffusion coefficient	(m ² s ⁻¹)	R	Gas constant	(J mol ⁻¹ K ⁻¹)
F	Faraday constant	(C mol ⁻¹)	r	Reaction rate	(mol m ⁻² s ⁻¹)
f^V	Surface enlargement factor	-	T	Temperature	(K)
i	Current density	(A m ⁻²)	U	Fuel cell voltage	(V)
i_0	Exchange current density	(A m ⁻²)	v	Flow velocity	(m s ⁻¹)
K	Pressure drop coefficient	(m ² s ⁻¹ Pa ⁻¹)	Δz	Discretisation length	(m)
L	Fuel cell length	(m)	δ	y-axis thickness	(m)
L_x	Gas channel width	(m)	λ_A	Anode stoichiometry	-
L_z	Gas channel depth	(m)	λ_C	Cathode stoichiometry	-
\dot{n}	Molar flux density	(mol m ⁻¹ s ⁻¹)	Φ	Electrical potential	(V)

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