

PEM automotive stack model with experimental validation

J.C. Gómez^{1*}, J.K. Dombrovskis², M. Serra¹, A. Husar¹

¹Institut de Robòtica i Informàtica Industrial (CISC-UPC), C. Llorens i Artigas 4-6, 08028 Barcelona, Spain

²PowerCell, Ruskvädersgatan 12, 418 34 Göteborg, Sweden

(*) Corresponding author: jgomez@iri.upc.edu

Keywords: PEM stack, dynamic modeling, automotive power system, experimental validation, galvanostatic operation

1. Introduction

Dynamic models of PEM stacks are the basis to design controllers for optimizing performance, efficiency and minimizing degradation. Fluid dynamic models of different dimensions can be found in the literature; however, these models are rarely used to improve the control laws and strategies. This work presents a 1+1D control oriented model, distributed in the direction of the stack flow channels. The model, which is based on first principles as described by Mangold [1], is implemented in MATLAB Simulink. Moreover, in this work we introduce the conversion from potentiostatic to galvanostatic mode of operation, because this is the operating mode in automotive applications. The model presented by Luna et al. [2] has similar objectives; however, we propose an improved solution to the distribution of current along the channels in galvanostatic, what gives an improved calculation of the distributed consumption of species in both the anodic and cathodic semi-reactions. The model is validated using experimental data of a Powercell stack.

2. Model description

2.1 System description

The stack modelled has 335 cells and 300 cm² of active area. The flow of reactants in the channels are in a counterflow configuration. Since the model is aimed at automotive applications, excluding the start up, which is potentiostatic, it uses a load control device to set the current that circulates through the stack, that forces a galvanostatic mode of operation.

2.2 Model description

The model presented in this work is based on a first principles model with partial derivatives to describe the variation of the relevant fuel cell variables along the channel's direction (z-direction) [1]. In order to take into account concentration gradients in the direction perpendicular to the MEA (y-direction) in the catalyst and diffusion layers, our model adds to the z-direction distribution axis a second distribution axis in y-direction.

On the other hand, the model in [1] has voltage as an input and calculates the dynamics of the current as an output (potentiostatic mode), but our automotive application requires a galvanostatic operation, therefore, the model needs to be reversed. In [2], this change was done by including the Nernst equation to calculate the voltage for a specific current and partial pressure of gases. However, the condition that the voltage at the terminals is the same along the z-direction was disregarded. In section 2.3, we present a methodology to solve the system of equations for galvanostatic operation, at the same time that the current distribution is computed.

In the rest of this section, the most relevant model equation of a single cell are given. To obtain the stack model, we simply extrapolate linearly to the the number of cells in the stack.

The cathodic and anodic catalyst layers have no mass storage capacity. Then, the semi-reaction at the discretization points read as:

Equation 1: $\mathbf{0} = \dot{n}_{O_2} - \frac{1}{2}r^C$; $\mathbf{0} = \dot{n}_{H_2} - r^A$

The rate of reaction in the anode and the cathode catalyst layers are given,



$$\text{Equation 2: } r^A = f^v \frac{i_{A0}}{2F} \left\{ \exp \left(\frac{2F}{RT^S} (\Delta\Phi^A - \Delta\Phi_{ref}^A) \right) \frac{\xi_{H_2}^{CA} p^A}{p_{H_2,ref}} - 1 \right\}$$

$$\text{Equation 3: } r^C = f^v \frac{i_{C0}}{2F} \exp \left(-\frac{\Delta G_0}{R} \left(\frac{1}{T^S} - \frac{1}{T_{ref}} \right) \right) \frac{\xi_{H_2}^{CC} p^C}{p_{O_2,ref}} \exp \left(\frac{\alpha 2F}{RT^S} (\Delta\Phi^C - \Delta\Phi_{ref}^C) \right)$$

The voltage drop on the catalyst layers depend on the difference between the reaction rates and the flow of protons across the membrane,

$$\text{Equation 4: } C^A \delta^{AC} \frac{\partial \Delta\Phi^A}{\partial t} = i^M - 2F r^A; C^C \delta^{CC} \frac{\partial \Delta\Phi^C}{\partial t} = 2F r^C - i^M$$

From simple algebraic substitution of equations in [1], it can be shown that the voltage drop on the membrane, $\Delta\Phi^M$, depends on the water content, gradients of concentration water and protons on the membrane, and the current density,

$$\text{Equation 5: } \Delta\Phi^M = \frac{\delta^M}{K(\Lambda)} i^M + \frac{\delta^M t_w(\Lambda)}{F} \nabla \mu_{H_2O} + \frac{\delta^M}{F} \frac{RT^S}{\xi_{H^+}(\Lambda)} \nabla \xi_{H^+}$$

2.3 Solving the system of equations for galvanostatic operation

The mean current density through the stack, $i_{st} = \frac{I_{st}}{A_{cell}}$, its known because the current through the stack, I_{st} , is an input variable. The unknown variables are the cell voltage, U , and the distribution of the current densities, $i_{M,i}$. The cell voltage is composed of three voltage drops the cathodic, anodic and the membrane (Equation 6). Since the total current is imposed, the current at any point of discretization is not independent of the rest, and the system has to be solved as a whole.

An auxiliary distributed variable Q (Equation 7) is used. Q_i represents the voltage on the discretization if the ohmic resistance was null, and is a function of the states and the terms independent of i_M .

$$\text{Equation 6: } U = \Delta\Phi_i^C - \Delta\Phi_i^A - \Delta\Phi_i^M$$

$$\text{Equation 7: } Q_i = U + \delta^M \frac{i_{M,i}}{K(\Lambda_i)}$$

In Figure 1, an equivalent electrical system is presented. The electrical power of the single fuel cell $P = I_{st} \cdot U$. The electrical branches represent the voltages of the discretizations. At any time, the current is distributed following the system of equations. Both the resistivity of the membrane, $\frac{\delta^M}{K(\Lambda_i)}$, and Q_i are known.

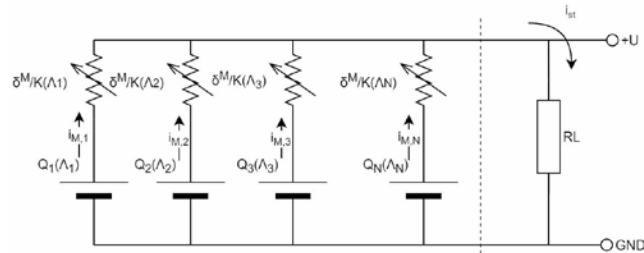


Figure 1: Distributed current equivalent circuit

$$A i_M = B \rightarrow \begin{bmatrix} \frac{\delta^M}{K(\Lambda_1)} & -\frac{\delta^M}{K(\Lambda_2)} & 0 & \dots & 0 \\ \delta^M & 0 & -\frac{\delta^M}{K(\Lambda_3)} & \ddots & 0 \\ \frac{\delta^M}{K(\Lambda_1)} & \vdots & \ddots & \ddots & \vdots \\ \frac{\delta^M}{K(\Lambda_1)} & 0 & 0 & 0 & -\frac{\delta^M}{K(\Lambda_N)} \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix} \begin{bmatrix} i_{M,1} \\ i_{M,2} \\ i_{M,3} \\ \vdots \\ i_{M,N} \end{bmatrix} = \begin{bmatrix} Q_1 - Q_2 \\ Q_1 - Q_3 \\ \vdots \\ Q_1 - Q_N \\ N * i_{st} \end{bmatrix}$$

Figure 2: Linear system of distributed currents

Knowing that the potential at the terminals is the same, we use the following constraint.

$$\text{Equation 8: } Q_i - \delta^M \frac{i_{M,i}}{K(\Lambda_i)} = Q_j - \delta^M \frac{i_{M,j}}{K(\Lambda_j)}, \quad \forall i, j$$

The total current of the stack is the sum of currents from each discretization. Due to the fact that the discretizations are of the same size, the mean of the current densities of the discretizations equal the total current density.

$$\text{Equation 9: } \frac{1}{N} \sum_{i=1}^N i_{M,i} = i_{st}$$

Taking into account Equation 8, Equation 6 and Equation 9 there are N equations and only the current densities as unknown. Then, the linear system, $A i_M = B$, is solved in Figure 2.

The value of the coefficients of the matrix A represent the electrical resistivity of each discretization along the membrane. Analyzing the structure of matrix, A , we can demonstrate that it is always solvable as long as the conductivities are strictly positive, $K(\Lambda_i) > 0$. Hence, the linear system is solved by $i_M = A^{-1}B$.

Proof: The determinant of A is $(\prod_{i=1}^N \frac{\delta^M}{K(\Lambda_i)}) (\sum_{j=1}^N \frac{K(\Lambda_j)}{\delta^M})$. The value of both $\delta^M, K(\Lambda_j)$ are strictly positive which leads to a strictly positive determinant.

Then, in order to calculate the total potential of the cell, U , we can use any discretization and add up the terms of membrane, cathodic and anodic voltage drops using Equation 6.

3. Experimental validation

We test our model against the experimental data provided by PowerCell. Figure 3 shows the variables measured and the simulated results. The experiment consists of changes in stoichiometry (a), relative humidity (b), current (d) with constant outlet pressure (c) in both channels.

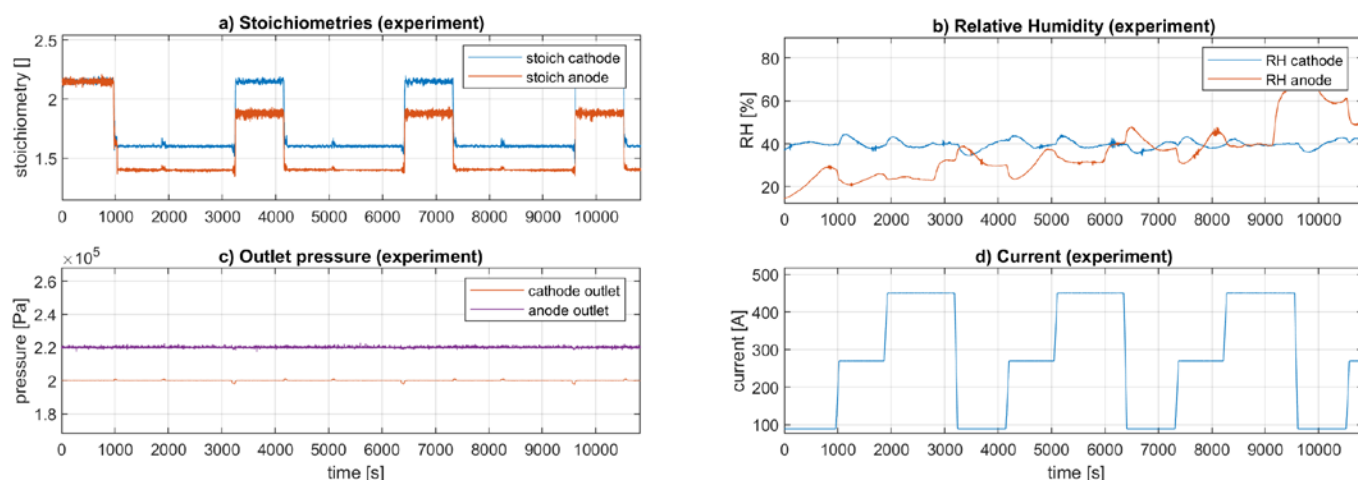


Figure 3 Experimental results and input condition for the simulation

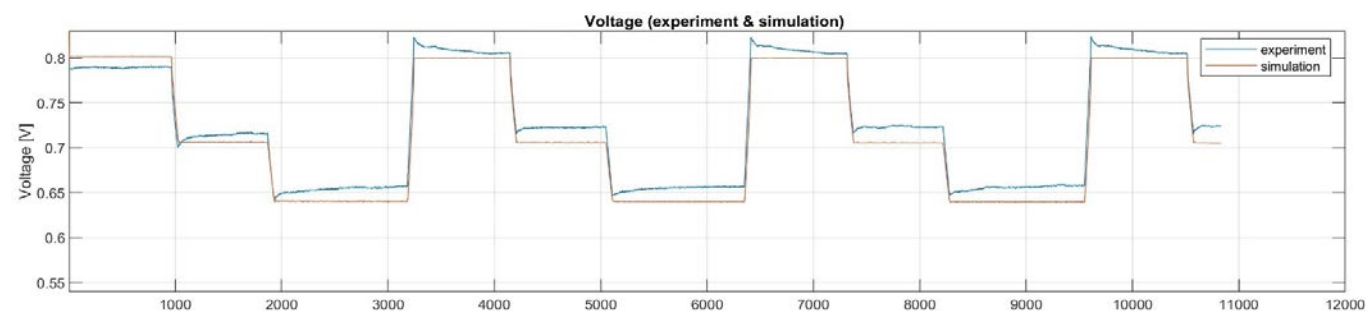


Figure 4 Single cell voltage, experimental and simulated

The results of the simulation shown in Figure 4, confirm that the model reproduces the trends of the real system in a multivariate scenario. The simulated voltage curve of our model estimates the experimental voltage taking into account the behaviour of the operating conditions: relative humidity, pressure or stoichiometry. It represents correctly both the steady-states and the transients with an error that is within the order of tens of millivolts.

4. Conclusions

A dynamic control-oriented model of an automotive PEM stack has been modelled and experimentally validated. The distribution of current along the z direction has been calculated solving the mathematical problem through the inversion of a matrix.

5. Acknowledgements

This work was done with the support of European Union's Horizon 2020 research and innovation programme through the INN-BALANCE project (ref. H2020-JTI-FCH-2016-1-735969), the Spanish national project MICAPEM (ref. DPI2015- 69286-C3-2-R, MINECO/FEDER) and the Spanish State



Research Agency through the María de Maeztu Seal of Excellence to the Institut de Robòtica i Informàtica Industrial (MDM-2016-0656).

6. References

- [1] X. Mangold et al., Passivity based control of a distributed PEM fuel cell model, J. Process Contr. (2009), doi:10.1016/j.jprocont.2009.11.008.
- [2] J. Luna, C. Ocampo-Martinez and M. Serra. Nonlinear predictive control for the concentrations profile regulation under unknown reaction disturbances in a fuel cell anode gas channel, Journal of Power Sources, 282: 129-139, 2015

