Macroscopic modeling and representation of a PEM fuel cell gas supply taking into account the water phenomena

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The objective of this paper is to propose a model to develop control laws and energy management of a fuel cell system and of a fuel cell vehicle. Water phenomena into the device have a great influence on the stack efficiency and on faulty conditions. Henceforth the gas supply model must be able to work with a multi-species gas mix and to describe biphasic effects. To tackle the control objective, a formalism called Energetic Macroscopic Representation is presented and used. This paper presents an experimental validation of the proposed model.

Keywords-* *Fuel cell; Water phenomena; Energetic Macroscopic Representation; EMR; modeling; flooding; gas supply

I. INTRODUCTION

In order to improve the global efficiency of a Fuel Cell Vehicle (FCV), the local management of the Fuel Cell System (FCS) has to be optimized.

The water phenomena have an impact at two efficiency levels. Firstly, the water content of the membrane modifies the membrane equivalent resistor and consequently, the stack efficiency [1]. Secondly, the water management of the FC is strongly dependant of the air supply management: at low temperature, a good water management requires a high air stoichiometry [2,3]. For vehicular applications, the air supply subsystem is often based on a compressor. Such a device uses 25% of the power produced by the stack [4]. As a consequence, the FCS efficiency is water management dependant.

The water management is directly linked with flooding and drying fault occurrence [5-7]. They can lead to performance drop or device degradation. This study is focused on the flooding conditions but the proposed model allows considering drying as well. From a stack point of view, flooding (i.e. water accumulation in channels) leads to the gas channels blocking. The reactants cannot reach the catalytic sites and a starvation phenomenon appears (i.e. FC degradation). From a FCS point of view, flooding can be fixed using a purge. Nevertheless, such a technique has an important energetic cost. From a vehicle point of view, a purge leads to an interruption in the FC power production during which the requested power has to be supplied by auxiliary sources.

The global objective of the project is to work on FCV control and energy management. A specific work on FCS and water issues is a mandatory step. Water phenomena are impacted by the thermal control of the FCS, the gas supply (compressor) and the humidification subsystem. The current which drives the electrical behavior is supposed to be imposed to the device. Consequently, controlling the water phenomena leads to act on different parts of a whole multi-physics system.

In this paper, a model of a PEMFC gas supply that takes into account the water issues is presented. Its representation and degree details allow the development of control and of energy management laws [8].

Energetic Macroscopic Representation (EMR) is identified as a relevant methodology for this specific work. It allows a structured study of such a system with a highlighted control objective [9-11]. The control objective leads to a dynamic modeling. The energy management modeling imposes to take into account the different losses. Moreover, information can be obtained to know when a purge is requested.

II. THEORETICAL FUNDAMENTALS OF THE STUDY

A. Energetic Macroscopic Representation

EMR is a graphical formalism (see Appendix) able to describe power exchanges within dynamic multi-physics systems such as FCS and FCV. It has been presented in several publications [9-11]. Its main feature is to propose a systematic control structure design methodology. However, this paper is focused on the modeling and simulation part.

EMR is organized around three core principles:

- The arrows represent the causality and not the sign of the exchanged power. The action of an element to an other element yields a reaction of the second one to the first one.

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- The product of the two exchange variables between two elements is consistent with a power (Watts).
- The internal relations of an element are governed by the physical causality principle. The accumulation elements represent an energy accumulation, the relationship between their input and their output is integral (i.e. physical). The derivate causality is avoided.

The internal relationships of the converters and the couplings are not time dependant. The coupling elements represent the power flow repartition.

B. *Water phenomena into a fuel cell*

Figure 1 summarizes the water phenomena in a PEMFC.

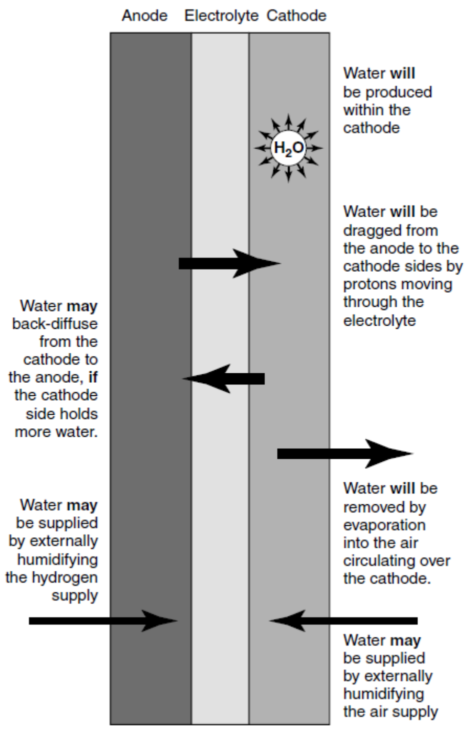

Figure 1. Summary of the water phenomena in a PEMFC (without exhaust on the anodic side) [2]

III. MODELING AND REPRESENTATION OF A GAS PIPE

For this first step of the work, the objective is to model a simple gas pipe. The gas consumption and the water production in a fuel-cell channel are not considered.

A. *Mono-species gas mixture*

The gas pipe modeling is based on a thermal-electric analogy [12,13]. Pressures are represented by voltages and gas flows by currents. To take into account the gas dynamics, [14] shows that a gas pipe can be represented with a "T" circuit (Fig. 2). The resistors model charge losses and the capacitor models the gas accumulation into the pipe.

Such an analogy implies flow dependant resistors. In many cases, the effect is neglected [10]. Nevertheless, the water management objective may need a wide range of flow variation [3]. For instance, the model presented in this paper is experimentally validated for an up to 5 air stoichiometry factor. The varying ratio of the upstream resistor of the model is 7. This flow dependence is generally modeled with a linear function [14].

The model representation with EMR is straight and easy (Fig. 2). The resistors are represented with mono-physical converters and the capacitor with and accumulation element.

A work on the exchange variables has to be performed. EMR imposes an exchange variable product consistent with Watts. As a consequence the variables are pressure P and volume flow qv (1). In a gas pipe, the molar flow $\dot{n}$ is constant in steady state. Given to the perfect gas law (2), the volume flow is thus variable (actually, temperature (T) and pressure are modified into the equivalent resistors). In this paper, a low pressure drop is assumed and the gases are supposed to come into the device at a temperature near of fuel cell temperature. Consequently, the volume flow is considered as constant.

$$[Pa].[m^3 s^{-1}] = [W] \quad (1)$$

$$qv = \dot{n}\frac{RT}{P} \text{ with R the perfect gas constant} \quad (2)$$

The study of the inputs and the outputs is interesting. The gas supply is represented with the upstream source (on the left). It represents a compressor [10] or a flow regulator and consequently, the flow qv_{in} is imposed to the pipe. To respect the integral causality, the accumulation element imposes the pressure to the resistors. Finally, the downstream source represents the atmosphere and thus, imposes the atmospheric pressure P_{atm}.

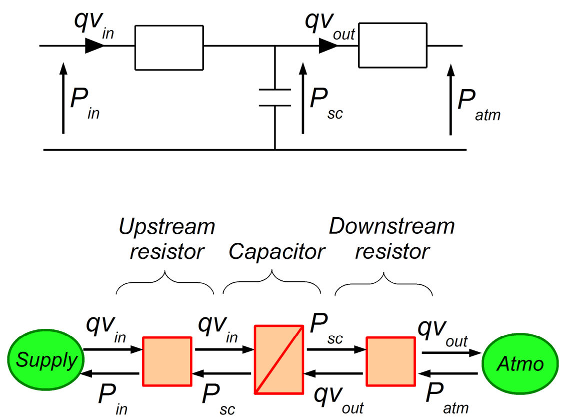

Figure 2. Electric scheme and EMR of a simple gas pipe

B. *Multi-species gas mixture*

Into a FCV, the most common configuration is based on an ambient air compressor. The air is composed by oxygen (O_2), nitrogen (N_2), and water vapor (H_2O). On the anodic side, oxygen is switched with hydrogen (H_2). Consequently, pressures and flows are vectors (3x1) of partial pressures and of partial flows (3).

Nevertheless, the behavior of the three species is not independent. For example, the three partial flows have a same sign. Basically, the absolute pressure difference imposes the absolute flow. The composition (%) of the gas mix through the element is imposed by the high pressure side (4).

Vector variable is underscored as $\underline{P}_{in}$.

$$\sum \underline{P}_{in} - \sum \underline{P}_{sc} = R \sum \underline{qv}_{in} \qquad (3)$$

$$\text{if } \sum \underline{P}_{in} > \sum \underline{P}_{sc} \text{ then } \underline{qv}_{in} = \% \underline{P}_{in} \sum \underline{qv}_{in} \qquad (4)$$

For instance, with dry air $\% \underline{P}_{in} = \begin{pmatrix} 0.2 \\ 0.8 \\ 0 \end{pmatrix}$

IV. Modeling and Representation of the Fuel Cell Gas Supply

A. *Single channel without liquid water*

The main difference between a simple gas pipe and a fuel cell channel is the gas consumption and the water production (at the cathode, in vapor phase). These molar flows ($\underline{\dot{n}}_{cair}$ and $\underline{\dot{n}}_{cH2}$) are current dependant. To calculate the volume flows from (2), the temperature has to be known (5). Figure 3 shows the evolution of the output gas temperature versus the input gas and the fuel cell temperatures. In this test the air flow is constant and the FC temperature is decreased to lead to flooding. In this work, gas temperature on catalytic sites is assumed equal to the FC temperature.

The consumed and produced volume flows are represented on the electric scheme by a current source (Fig. 4). On EMR, a multi-physics converter links the FC and the previous gas pipe.

$$\underline{qv}_{cair} = \begin{pmatrix} qv_{cO2} \\ qv_{cN2} \\ qv_{cH2O} \end{pmatrix} = \frac{RT_{air}}{\sum \underline{P}_{sccat}} \begin{pmatrix} \dfrac{ni_{FC}}{4F} \\ 0 \\ -\dfrac{ni_{FC}}{2F} \end{pmatrix}$$

$$\underline{qv}_{cH2} = \begin{pmatrix} qv_{cH2} \\ qv_{cN2} \\ qv_{cH2O} \end{pmatrix} = \frac{RT_{H2}}{\sum \underline{P}_{scan}} \begin{pmatrix} \dfrac{ni_{FC}}{2F} \\ 0 \\ 0 \end{pmatrix} \qquad (5)$$

with n and F the number of cells of the stack and the Faraday constant, respectively.

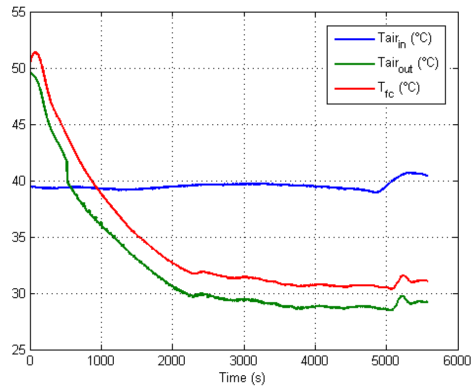

Figure 3. Evolution of the gas temperature. Experimental results

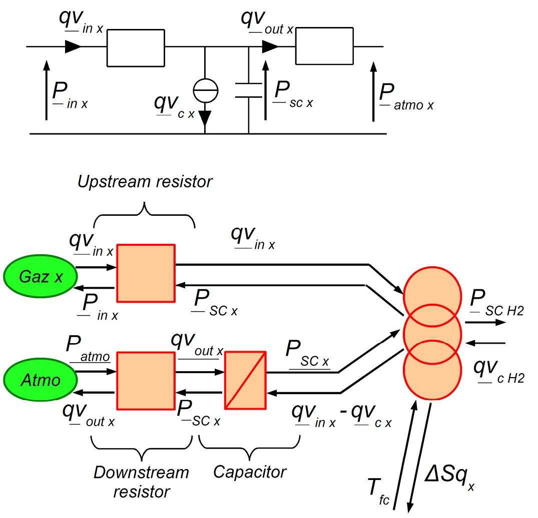

Figure 4. Electric scheme and EMR of a FC channel (x stands for H_2 or air)

B. *Single channel with liquid water*

EMR represented on figure 4 shows only the FC gas behavior. The represented flows are only gas flows. Relations presented in this part are realized in the multi-physics converter.

1) *Liquid water creation*

In a channel, liquid water is formed if the relative humidity ϕ reaches 100% (6). The relative humidity represents the water content of a gas mix. If ϕ*=100%*, the gas cannot store more vapor water. This storage ability of the water is highly temperature dependant [2] and is represented with the saturated vapor pressure P_{sat} (7).

If ϕ*>100%* then the water flow is a liquid water flow.

$$\phi = \frac{P_{H2O}}{P_{sat}(T_{gas})} \qquad (6)$$

$$P_{sat} = 10^5 \exp\left(13.7 - \left(\frac{5120}{T_{gaz}}\right)\right) \text{ with } T_{gaz}\ [K]. \qquad (7)$$

2) Accumulation and evacuation of liquid water

The quantity of water accumulated in the FC can be calculated with a simple time integration. The evaporation phenomena are neglected. In this study, it is assumed that the liquid water is only evacuated through a purge.

C. Exchanges between the electrodes

In a fuel cell, water and nitrogen can migrate from one electrode to another one [14]. Two phenomena occur: the diffusion (H_2O and N_2) and the electro-osmosis drag (H_2O only) [15].

1) Diffusion

The diffusion equilibrates the partial pressures of vapor and nitrogen on the two sides of the membrane. A reversible flow is created between the electrodes. Nevertheless, water appears at cathode and nitrogen is brought by air. The flows are most often from the cathode to the anode.

The membrane is modeled as a resistor (8).

$$\dot{n}_{m\_y} = \frac{P_{sc\_y}}{R_{m\_y}} \quad (y \text{ stands for } N2 \text{ or } water) \qquad (8)$$

2) Electro-osmosis drag

Electro-osmosis is an electrochemical effect. It brings water from the anode to the cathode when a current is requested to the FC (9).

The coefficient K_{EO} is dependant of the water content of the membrane λ. Actually, the membrane can be seen as a sponge. λ represents the mass of water in a membrane versus the mass of the dry membrane [16,17]. The dynamics of the membrane hydration is very fast and the effect can be considered as instantaneous [14]. Several assumptions are defined to calculate the water content:

- λ is supposed between 0 and 14. The saturated conditions are neglected. Due to the post treatment of membranes, the λ value is limited to 16.8 and the assumption does not introduce important numerical errors [18].
- The water activity a is supposed equal to the relative humidity ϕ.
- λ is calculate with the sorption isotherms at 30°C [16] (10). This solution is chosen by many authors [19-23]. Nevertheless, a linear interpolation with the 80°C [24] curve is possible [25].
- K_{EO}, given by (11) is equal to 1 with a fully hydrated membrane [26].

$$\dot{n}_{EO} = nK_{EO}(\lambda)\frac{i_{FC}}{F} \qquad (9)$$

$$\lambda_z = 0.043 + 17.81a_z - 39.85a_z^2 + 36a_z^3 \text{ [7]}$$

(z stands for a (anode) or c (cathode)). Coefficient are determined for a nafion membrane. (10)

$$\lambda = \frac{\lambda_c + \lambda_a}{2}$$

$$K_{EO} = \frac{\lambda}{\lambda_{max}} \qquad (11)$$

V. Experimental validation

The experimental validation is performed on a UBZM 20cell stack (500W). The air is fully humidified and the hydrogen is dry. The proposed validation (Fig. 5) is based on the variation of the input pressure. The small signal variation is due to the current variation (gas consumption and water production) and the large signal variation is due to the input flow modification. The hydrogen flow is constant during this test (8.3*Nl.min*$^{-1}$).

The model is set with fix resistors on constant flow periods using a Newton optimization algorithm. The variation of the resistors versus the flow is obtained using a linear interpolation.

These results show the good behavior and accuracy of the model. The internal pressures are water phenomena dependant.

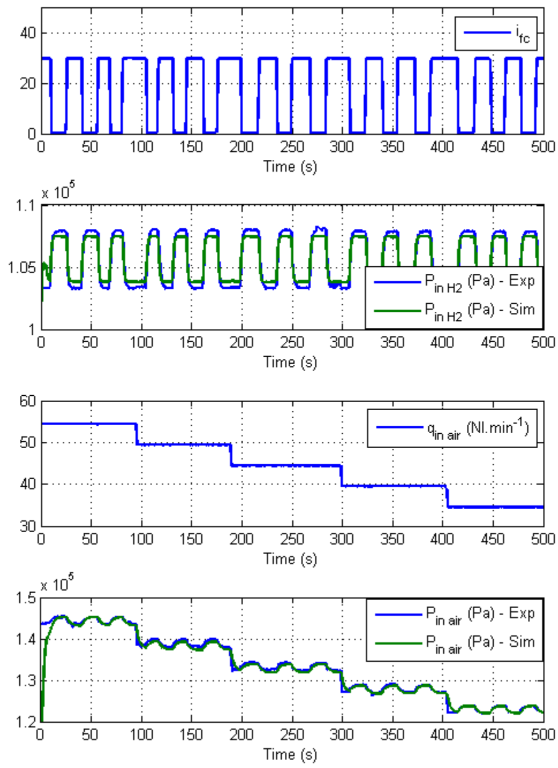

Figure 5. Experimental validation of the proposed model

VI. Representation of a PEMFC

The electrochemical model has been already presented in other publications [10,11]. It is not detailed here.

The electrochemical quasi-static model and the electrical dynamics are represented with a multiphysics converter and an accumulation element, respectively (Fig. 6). The thermal behavior of the fuel cell is represented with an accumulation element. It contains a thermal capacitor deduced from the fuel cell mass. The temperature is distributed to other parts with a mono physical coupling.

The mail differences with the previously presented PEMFC EMR (10,11) are:

- The vector exchange variables on the gas supply parts.
- The whole electrochemical model is summarized into a multiphysics coupling.
- The connection between the two gas supply parts and the FC is realized through a multiphysics coupling. Before, the gas temperature issues were neglected and the coupling was monophysical. As a consequence, the fuel cell temperature on the model behavior is increased now.
- The water phenomena are not directly represented on the scheme. They are not considered as power exchange between the different elements. Only the vapor water is taken into account in the exchange vectors.

The accumulation elements characterize the model dynamics: thermal, electrochemical, and gas supply (air and H_2).

Please notice the high coupling level between the different parts: the four central elements are interconnected. This specificity leads to many control issues [11]. Moreover, the tuning inputs (red arrows) are located on the auxiliaries.

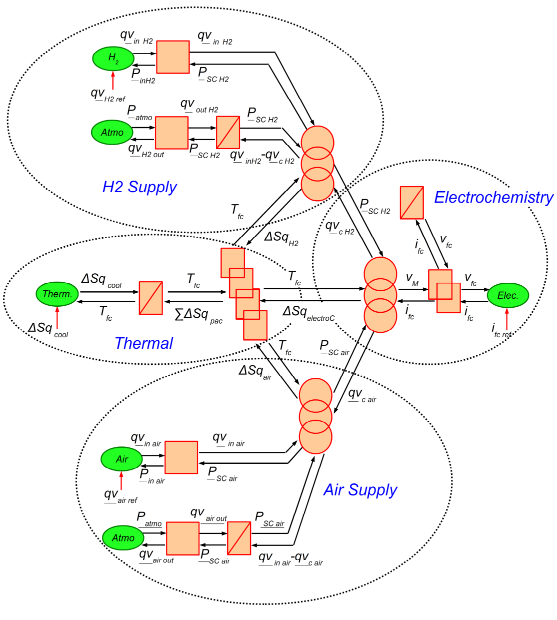

Figure 6. EMR of a fuel cell stack

VII. Conclusion

In this paper, a macroscopic model of the gas supply of a PEMFC intended for the control and the energy management design is presented. A control dedicated formalism so-called EMR is used.

The water phenomena are very important for energy management and are taken into account. The water formation on cathode is modeled as well. Moreover, the exchanges between the electrodes and biphasic effects are treated. The global behavior of the gas supply subsystem is experimentally validated.

Finally, a global EMR of a fuel cell stack is proposed.

As a consequence, this work offers several perspectives. The water accumulation into the FC will be analyzed versus flooding tests. The gas supply control and energy management will be studied. Moreover, thanks to the EMR formalism, this model will be integrated into a whole FCV model.

Acknowledgments

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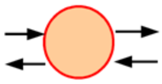
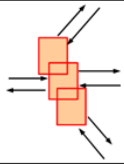
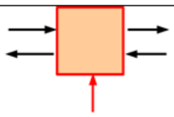
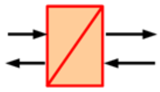
APPENDIX: SYNOPTIC OF ENERGETIC MACROSCOPIC REPRESENTATION

	Source of energy		Multi physical domain converter (without energy accumulation)		Mono physical domain coupling device (energy distribution)
	Mono physical domain converter (without energy accumulation)		Element with energy accumulation		