

Bond Graph model of a PEM fuel cell stack

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Abstract: The fuel cell is a complex system, in which several disciplinary fields are concerned: hydraulics, chemical, thermal and electric. In this paper, we present the hydraulic part of the model of a PEM fuel cell stack via the Bond Graph formalism. The developed model enables to simulate the pressure losses inside the fuel cell. Firstly the basis of Bond Graph modelling is recalled. Then, the structure of the model and its elements are described. Secondly, the model is exploited to study the effects of operating conditions on the pressure losses attached to the distribution of gases in the electrodes.

1. Introduction

Fuel cells are electrochemical reactors generating electricity and heat directly from reactions of fuels, typically hydrogen and oxygen, pure or from the air. The fuel cell is a complex energetic system, in which several interactions have to be considered in order to establish a multi-physical model. Different disciplinary fields are concerned: hydraulics, chemical, thermal and electric. Thence, the bond Graph formalism is particularly well adapted to modelling this multidisciplinary system [1] as shown in [2, 3] in which the Bond Graph models of the electrochemical, electric and thermal phenomena are explained. In these former works, the hydraulic part of the system where represented by perfect sources of pressure, neglecting the pressure losses inside the fuel cell. Indeed, there are hydraulic pressure losses in the gaz feeders and inside the fuel cell depending on the

configuration of the channels in the bipolar plates and their geometrical parameters (diameter, length and width). They impact the working point and, reciprocally, they depend on the operation point as well. Then the pressure losses are an important term in the fuel cell efficiency and design. It has to be modelled.

2. Constitution of a PEM fuel cell

A PEMFC (Proton Exchange Membrane Fuel Cell) uses an electrolyte with polymeric membrane which allows operation at low temperature less than 90°C. At such low temperatures, the chemical reactions need a catalyst: platinum is often used. The figure (1) shows the schematic diagram of cell configuration and its constitution, and basic operation principles.

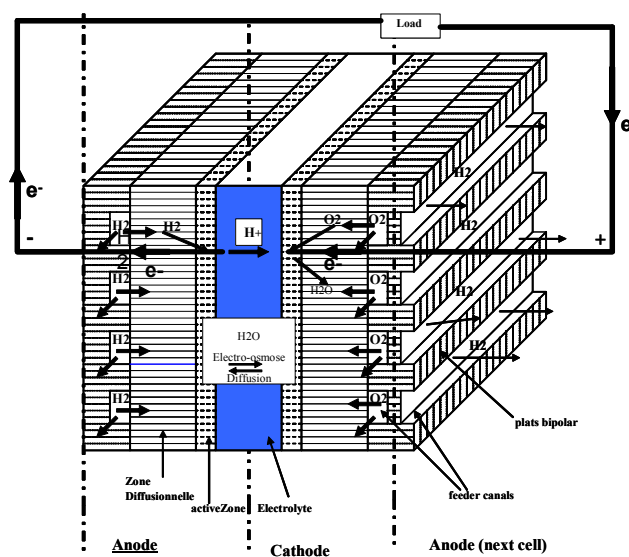
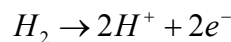


Figure 1: constitution of a PEM fuel cell

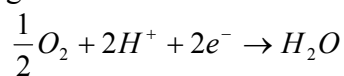
On the figure 1, we can distinguish:

- The two electrodes (anode and cathode), generally made of carbon cloth or carbon fibre paper ;
- the membrane which acts as the electrolyte for ensuring the transfer of the protons from the anode to the cathode;
- the bipolar plates, generally made of graphite or metal. They involve the channels to bring the reactive gases until the site's reactions at the active layer situated at the interface of the electrode and the electrolyte.
- An external electric circuit with an electric load as a motor or light... etc.

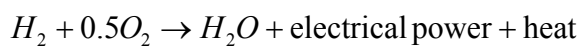
The hydrogen side is negative and is called the anode where the following reaction:



The oxygen side of the fuel cell is positive and is called the cathode, where the following reaction:



The electrochemical reaction exploited by this fuel cell is given by the following reaction:



The water is created on the cathode and must be evacuated out of the fuel cell.

Assuming that the Gibbs free energy can be converted into electrical energy, the theoretical potential E of the fuel cell corresponds to Gibbs free energy, ΔG , of the above reaction:

$$E = -\frac{\Delta G}{nF}$$

Where n is 2, the number of electrons involved in the above reaction, and F is the Faraday's constant (96,485 Coulombs / electron-mol).

At 25°C and atmospheric pressure, the theoretical potential of fuel cell is:

$$E^0 = 1.23 \text{ Volts.}$$

Several elementary cells are connected together through their bipolar plates so as to constitute a fuel cell stack. The bipolar plates enable a direct electric serie connecting while the gas feeding is done in parallel in the channels.

3. Bond graph modelling of the hydraulic part of the fuel cell

3.1 Hydraulic part of the fuel cell

The channels have to bring in and out flows of gases and water. The geometry of the channels and their dimensions are determining on the water and gas flow in the stack and on the pressure drop between the inlet and outlet, i.e,

$$\Delta P = P_{Tank} - P_{Stack}$$

Three types of parallel-channel configurations can be encountered in classical PEM fuel cells: Z form, U form and serpentine form. The figure (2) shows that in each configuration of the types Z and U, there are two heads for the entry and the other for the exit of flows. For each channel, we specify dimensions (the length, the thickness, and the width) [4]. In a Z-type configuration, the inlet to the assembly is near the first channel and the outlet is near the last channel. In a U-type configuration, both the inlet and the outlet of the assembly are connected near the first channel.

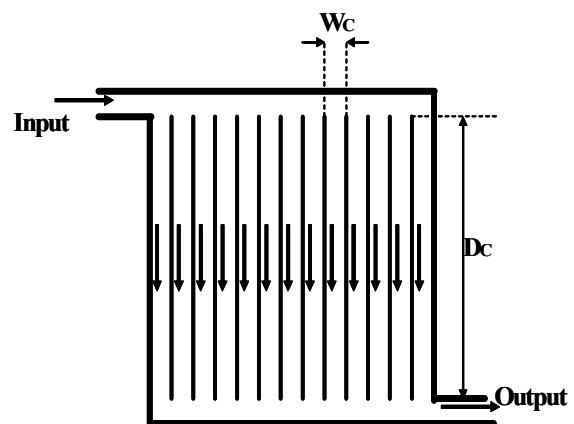


Figure 2: Z-type configuration

The geometric parameters of one channel are determined in the following table:

Length Dc(m)	0.066
Width Wc (m)	0.002
Depth (m)	0.002
Diameter inlet (m)	0.003
Depth inlet (m)	0.025

Table 1: geometric parameters of a channel

3.2 Recalls on Bond Graph

In Bond Graphs [5, 6], the energy exchanges within a system are described by bonds which represent the power exchanges. Two variables, effort and flow, are associated with each bond (Fig. 3). These factors have different interpretations in the different fields of physics (Table 2). The product of these two variables is the transferred power. The bond is arbitrarily oriented by a half arrow which indicates the positive power flow orientation. Furthermore, causality is a fundamental concept in Bond Graphs: it defines the cause-effect relations. The causal bar indicates the effort direction (Fig. 3).

Only a limited number of elements are necessary to describe the majority of systems. Table 2 gives these main elements: dissipative element R , inertial element I and storage element C . The connections between these elements are implemented through junctions. There are two types of junctions (Table 3): 1-junctions and 0-junctions which respectively correspond to series connections and parallel connections in electricity. They express in fact the generalized Kirchoff's laws. The transformers and the gyrators are used to pass from a field of physics to another. Causal rules impose that only one port can fix the flow through a 1-junction or only one port can fix the effort at a 0-junction. For instance, an effort source connected to a 0-junction fixes the effort at the junction; the rest of the system fixes the flows through this junction.

System	e : Effort (unit)	f : Flow (unit)
Electrical	v : Voltage (V)	i : Current (A)
Mechanical	F : Force (N)	V : Velocity (m s ⁻¹)
Chemical	μ : Chemical potential (J mol ⁻¹)	dn/dt : Molar flow (mol s ⁻¹)
Hydraulic	P : Pressure (N)	dq/dt : Volume flow (m ³ s ⁻¹)
Thermal	T : Temperature (K)	ds/dt : Entropy flow (JK ⁻¹ s ⁻¹)

Table 2: examples of effort and flow

Element	Represents	Equation without causality
$R:r$	Resistance	$e - rf = 0$
$I:i$	Inertia	$e - i \frac{df}{dt} = 0$
$C:c$	Capacitance	$f - c \frac{de}{dt} = 0$
Se	Effort source	$e = cst$
MSe	Modulated effort source	$e = e(input)$
Sf	Flow source	$f = cst$
MSf	Modulated flow source	$f = f(input)$

Table 3 bond Graph elements

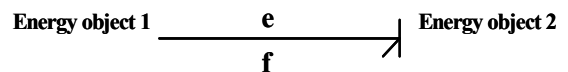


Figure 3: bond graph with causality bar

3.3 Bond graph model of the hydraulic part and assumptions

In the hydraulic field, the efforts are the gas pressures P_{gas} in bars, and the flows are the gas volumic flows D_{gas} ($m^3 s^{-1}$). The gas pressures are input parameters of the model. We can model a channel as a combination of a C element of storage and a R dissipative element which models the

pressure losses in the channel. Indeed, in Bond Graph, the volumes occupied by gas can be represented by C elements corresponding to a fluidic capacity (storages of gas under pressure). The pressure losses are modelled by R dissipative elements. The constitutive equations of these elements depend on the geometry of the channels and on the nature of the losses. The pipe which connects the fuel cell to the tank is also represented by a (R, C) association.

In our model we only consider Z type rectangular channels as in the figure (2).

The main assumptions for the hydraulic model are:

1. one-dimensional modelling
2. rectangular shaped channels
3. the number of channel in the bipolar plate is 23
4. the input gases are pure O₂ and pure H₂
5. laminar gases flows in the channels
Re < 2000 (Re : Reynolds number).
6. the temperature is known and constant inside the cell.
7. the pressure losses between the channels are negligible

The main tank is modelled by a C element, considered either under constant volume and variable pressure, or under variable volume and constant pressure. Figure 4 shows the Bond Graph model of the hydraulic part elaborate with regard to these assumptions.

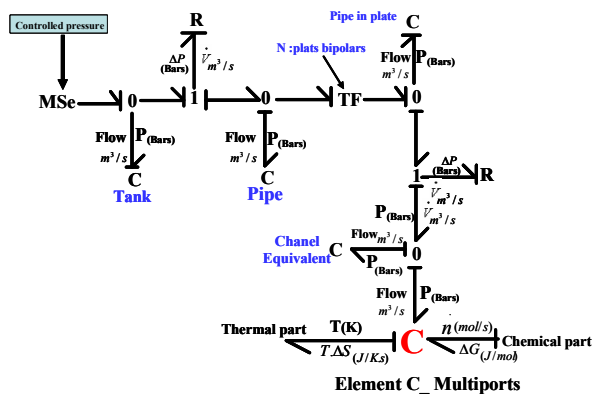


Figure 4: Bond Graph Model of the hydraulic part

The modulated source of effort models either the imposed pressure or the constant volume. In this part, the pressure is imposed by an effort source Se.

3.4 Calculation of the pressure losses in a channel

The pressure losses in a channel result of a fluid flow through the channel. Because of viscosity a part of the energy of the fluid, liquid or gas is transformed into heat by friction. We can define the pressure losses referring to this irreversible transformation and write:

$$Pressure\ losses = R_{hydra} * flow$$

The R_{hydra} hydraulic resistance is calculated with respect to the geometrical parameters of the channel and the gas viscosity in this channel. For a rectangular channel, hydraulic resistance is given by:

$$R_{Hydra} = 8 * \eta * L / (\pi * D^4) \quad (1)$$

Where

L: length of the channel in (m)

η : Gas viscosity in (Pa)

D: hydraulic diameter (m) of the channel given by:

$$D = \frac{2 * (Dc * Wc)}{Dc + Wc} \quad (2)$$

We can write the formula to calculate the pressure losses in the hydraulic part according to (1) and (2):

$$pressure_losses = \frac{8 * \eta * L}{\pi * D^4} * Q_{gas} \quad (3)$$

4. Exploitation of the model

In order to exploit this model of the hydraulic part, it is inserted in the global model of a fuel cell stack [5, 7]. Then the operation pressure, the temperature, molar flow and the current output of the stack are varied. The conditions of simulations are a

fixed pressure at 2 bars, and a variable temperature lower than 90°C.

4.1 - Influence of current on the pressure losses

The figure 5 shows the results of simulations with the global model. It can be noticed that the variation is linear. This linearity relies on constant stoichiometry. We can also observe that the pressure losses are much higher at cathode side where the oxygen gas, which is well-known.

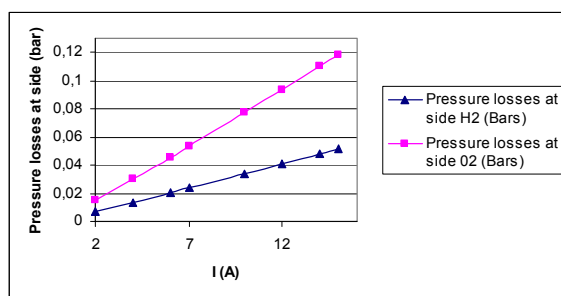


Figure 5: T=65°C, P=2 bars

4.2 - Influence temperature on the pressure losses

Figure 6 shows the influence of the temperature on the pressure losses under a given current density. We note that the pressure losses increase with the increase of the operating temperature in the fuel cells, because the viscosity and the density of gas change according to the temperature. The relationship between the viscosity and the temperature is given by the law of Sutherland [8]:

$$\text{For the gas: } \frac{\eta}{\eta_0} = \sqrt{\frac{T}{T_0}} \frac{1 + C/T_0}{1 + C/T}$$

Where:

- T: The temperature inside the fuel cell.
- T_0 : The initial temperature.
- C: a constant for a given gas:
 $C_{H_2} = 504K^{-1}$, $C_{O_2} = 945K^{-1}$

The thermal conductivity of materials constituting the bipolar plates, the anode, cathode, and the channels vary according to the temperature.

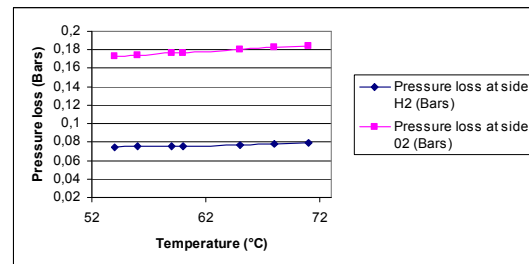


Figure 6 : I=15A

Actually, we note that the maximum of pressure losses corresponds to an important temperature and a high density of current. This temperature is produced by the electrochemical reaction. Alex Hakenjos et al. [9] showed that when the temperature increases, it is distributed in the channels of gases and in the zones where there is no water flow.

4.3 - Influence of channel dimensions on the pressure losses

The simulation allows to study the influence of the diameter of the pipe which connects the fuel cells with the gas tank. Figure 7 shows that the losses vary non-linearly according to this diameter. In our model, we consider that there are two parts of pressure losses:

- Pressure losses inside the fuel cell; it is possible to exploit the thermo hydraulic conditions to control these losses.
- Pressure losses in the pipe, where the temperature in the pipe is considered. To decrease the pressure losses it is necessary to increase the diameter.

The more the diameter decreases, the more the pressure losses increase considerably. For this model, the normal used diameter of the pipe is 9 mm.

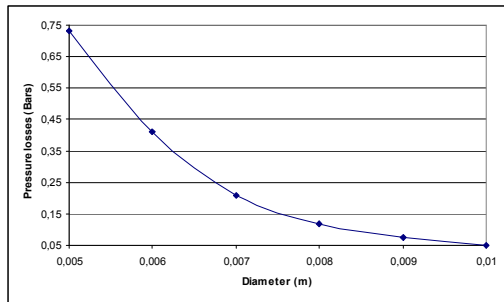


Figure 7: T=298K, I=15A

5. Conclusion

In this paper, we have presented a Bond Graph model of the hydraulic part of a fuel cell stack and some examples of exploitation in order to study the influence of the operational parameters on the pressure losses. The model elements are well described by linear or non linear constitutive laws which govern the pressure losses according to the operational conditions. The model parameters are identified and determined by using actual geometrical data. This model is integrated into the whole Bond Graph model of the fuel cell with chemical, electric and thermal parts. It will enable us to study by simulation the effects of coupling between the electric use and the hydraulic aspects on the global performances.

6. References

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