FINITE VOLUMES MODELLING OF THE HEAT AND MASS FLUXES IN A CELL OF PEMFC. MODELLING OF THE REAL GEOMETRIES OF THE ANODE AND CATHODE CHANNELS.

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ABSTRACT
The Proton Exchange Membrane Fuel Cell is an electrochemical device generating heat and electrical power. Such a system is complex to define and to be modeled. Indeed, numerous phenomena drive these systems involving electronic, chemical, physical, thermal and fluid mechanics sciences. One of the key points is the distribution of internal temperatures, the hygrometry of the feeding gas, particularly at the cathode. The aim of this paper is to describe a complete 3D finite volumes modelling of the behavior of the cell involving the heat and mass transfers in the cell considering the real geometries of both gas channels. Heat power of the electrochemical reactions are considered in the model together with the friction losses and the gas partial pressures. The coupling system between the channels allows evaluating the cell temperature for calculating the water content and the efficiency of the transfer of protons. The final main advantage is to forecast and to locate the phenomena of local condensation phases at the origin of the lower efficiency of the stack.

1. INTRODUCTION

Nowadays, the PEMFC (Proton Exchange Membrane fuel Cell) are clearly the most studied and developed. Application fields are most of them concerned by the car development so that for stationary and mobile applications. Some main advantages compared to other types of stacks are the relatively low working temperature permitting also a quicker start and a higher dynamic. Moreover, this relatively low temperature doesn't simplify the heat management. Indeed, it can be at the origin of local problems of condensation in the both gas channels. Main consequence is the flooding of the chemical reaction areas inducing a lower efficiency. One of the key points for simplifying the whole management of the system and particularly the thermal management is to carry out a faithful modelling and the heat and mass transfers through the cell allowing to determine the accurate internal temperature field at the interfaces fluid-solid of the channels where the condensation phenomena could appear.
BEDET and al [1] have developed an experimental setup based on the magnetic resonance device for studying the storage area where the water appears. Despite heavy difficulties, they succeeded to show local heterogeneities of hygrometry in the membrane coming from the channel geometries and also due to swelling effects.
For forecasting the condensation phenomena in the feeding gas channels, the knowledge of the boundary conditions at the interfaces is very fundamental. In this way, NGUYEN and al [2] have developed a 2D model of the heat and mass transfers between the two channels. It permits to define the model parameters needed for channels modelling and to repeat it until convergence between the anode and the cathode modelling. BERNARDI and VERBRUGGE [5] have described the influence of the vapour pressure in the air and the hydrogen on the efficiency of the stack. More recently, an isothermal model developed by SPRINGER and al [6] shows the strong relationship between the water content of the membrane and the efficiency of the proton transfer in the cell. All these models should permit to validate and to determine the boundary conditions of heat and mass transfers between the gas channels and the solid structure of the cell. DUTTA and al [7] have carried out a 3D numerical computation based on the Navier-Stockes equations for a linear channel and they have directly shown that the transfers of different chemical species are absolutely dependent on the consumed feeding gas. Same authors have carried out this work on a real geometry of a PEMFC cell [8]. Very few works

considers such geometries and most of them simplified geometries [9]. This presented work describes a whole computation of the cell, taking into account the real geometries of the anode and cathode channels, whereas the relationship between these two channel models uses the theoretical equations developed by DUTTA [7],[8]. This paper gives the chosen model and presents computed results of friction losses in the channels and local temperatures in the stack. Finally, authors present results with condensation phenomena along the air ducts. The initial conditions of the computations are relative to an experimental works of DUMERCY [9], for different current densities and hygrometries. The influence of the water channel for the cooling of the stack at the nominal operation is considered through Dirichlet boundary conditions. The latent heat of the chemical species is not at the moment taken into account. The only considered heat power generations are the chemical reaction enthalpies and the Joule effect.

2. METHODOLOGY

The used methodology consists in the computation of the flows in the air and hydrogen channels with the CFD code Fluent, for a given current density and for a chosen the air input hygrometry. The cooling water temperature is about 323 K and is given as a Dirichlet inhomogeneous condition. All the temperatures and pressures at the input and output gas (air and H2) channels are well known and taken as input parameters of the computed model. These conditions correspond to experimental measurements on a low power stack of 500W. Results of these two computations give the interfaces temperatures conditions used for the calculus of the NGUYEN equations e.g; figure 1.

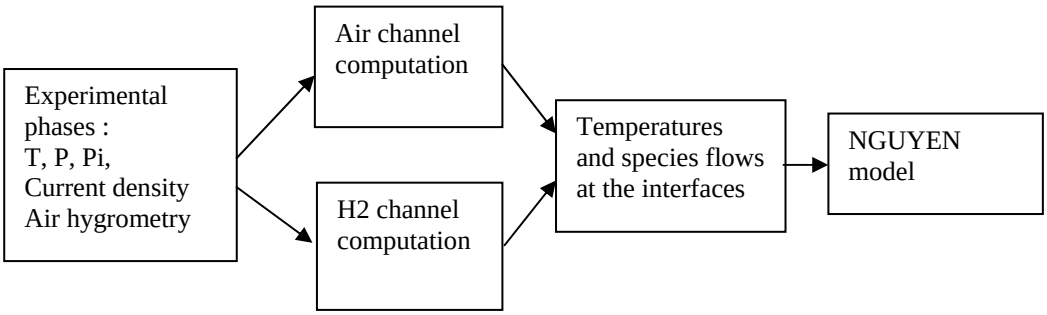

Fig.1: Following methodology

The results of the computation are compared to those given by the Dumercy's model [9]. This comparison is the validation criterion. Moreover, as it will be shown in the results paragraph, the taking into account of the real internal geometries seems to give better results on MEA temperature profiles.

3. MODEL EQUATIONS

Equations for the conservation of mass, momentum, energy and species are solved in the gas channels, the diffusion layers and the membrane. The general form of these equations for a steady state, 3D model can be written as:

$$\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial w}{\partial z}=S_m \quad (1)$$

$$u\frac{\partial(\rho\phi)}{\partial x}+v\frac{\partial(\rho\phi)}{\partial y}+w\frac{\partial(\rho\phi)}{\partial z}=\frac{\partial J_\phi}{\partial x}+\frac{\partial J_\phi}{\partial x}+\frac{\partial J_\phi}{\partial x}+S_\phi \quad (2)$$

where u,v,w are the velocity components of the gas mixture flow. ϕ stands for each transported variable (momentum, energy, mass fraction of hydrogen, oxygen and water) while J_ϕ represents the diffusion flux density of ϕ. The source terms S_ϕ depend on the considered location. Their values are zero expected for the different active zones where:

$$S_{H2} = -\frac{I}{2F}.M_{H_2}.A_{CV} \quad (3)$$

for hydrogen in the anode catalyst layer

$$S_{O2} = -\frac{I}{4F}.M_{0_2}.A_{CV} \quad (4)$$

for oxygen in the cathode catalytic layer

$$S_{aw} = -\frac{\alpha}{4F}.I.M_{H_20}.A_{CV} \quad (5)$$

for water in the anode catalyst layer

$$S_{cw} = -\frac{1+2\alpha}{2F}.I.M_{H_20}.A_{CV} \quad (6)$$

for water in the cathode catalyst layer

M_ϕ is the molecular weight of ϕ; I the current density; A_{CV} the specific area of the considered control volume (this volume corresponds to the meshing of each part of the stack) and α is the water transfer coefficient computed from the Nguyen model [2]. According to these definitions, the source term S_m can be written as:

$$S_m = S_{H_2} + S_{aw} \quad (7)$$

in the anode catalytic layer

$$S_m = S_{O_2} + S_{cw} \quad (8)$$

in the cathode catalytic layer

Concerning the equation of energy, the volume source term S_Q takes into account both the heat production given out by the electrochemical reaction and the Joule effect:

$$S_Q = 48{,}7.10^3 \frac{I}{2F}.M_{H_20}.A_{CV} + \frac{R_{me}I^2}{L_{me}} \quad (9)$$

$$\text{with } R_{me} = \frac{L_{me}}{15.\exp\left(\frac{-15048}{RT}\right)} \quad (10)$$

as given by Neubrand (2003)

With regard to the momentum equation, the diffusion and catalystic zones are considered as an isotropic porous medium with low permeability and the Darcy law can be applied to express the sink term of momentum for each direction:

$$S_{PX}=\frac{\mu u}{\beta}\ ;\ S_{PY}=\frac{\mu v}{\beta}\ ;\ S_{PZ}=\frac{\mu w}{\beta} \qquad (11)$$

μ is the dynamic viscosity of fluid depending on its composition and $\beta=10^{-12}\ m^{-2}$ is the permeability of the porous medium.

3. THE COMPUTATIONAL DOMAIN AND THE BOUNDARY CONDITIONS

The domain of interest for the simulation of flows consists of the whole cell which is partially shown in Fig.2. Each gas channel corresponds to a serpentine made up of 20 straight channels and bends. Velocity profiles and temperatures are defined for the gas flows in the inlet sections and water mass ratio is also determined in the cathode inlet section. Considering a high efficiency of the heat release device (water circulation), temperature on the gas channels boundaries has been set to a constant value (323K).

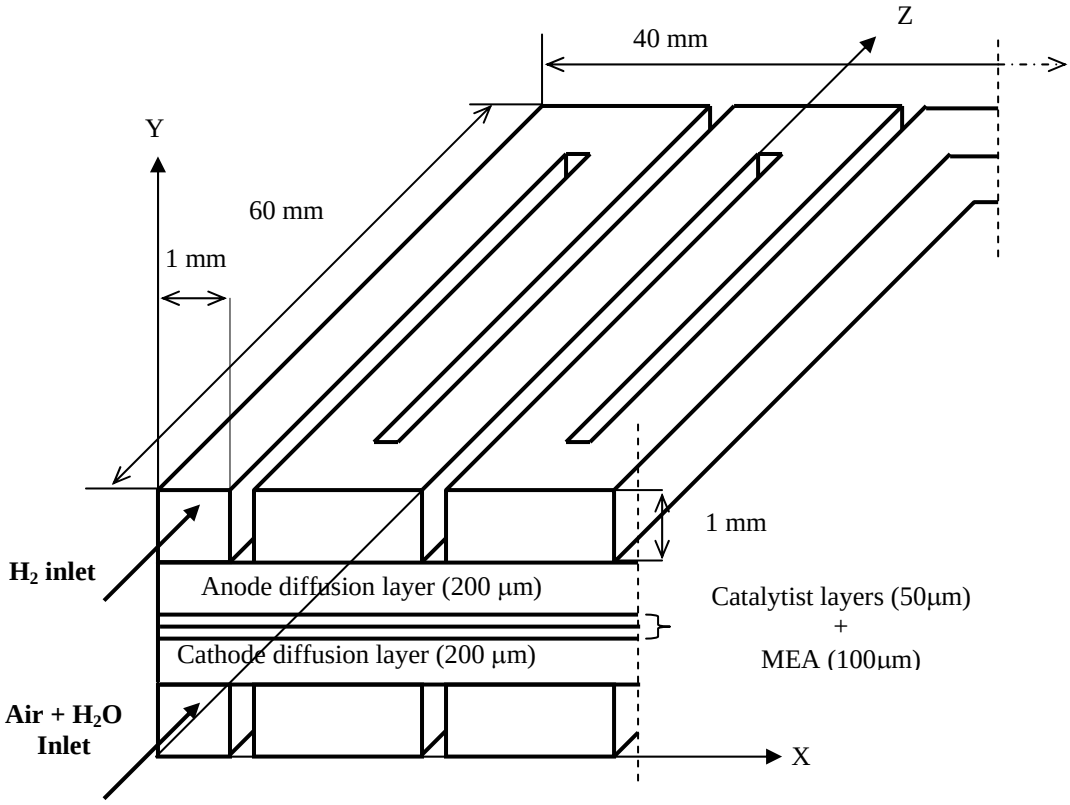

Fig.2: The computational domain (inexact scale)

3.1. Temperature profiles along 0,Y axis.

Figure 3 shows two computed structures. The first one is the air channel modelled with the FLUENT software and represents the real geometries of the duct whereas the second one is the simplified geometry with deployed linear channels. In that last representation [9], the friction losses are not taken into account, inducing finally dubiousness on final results and particularly on species pressure. According to the chosen axis imposed by Dumercy's, the simplified geometry could bring us to very different temperature profiles. Indeed, the nodal network used by [9] only considers three principal ducts of gas inducing also variable temperature profiles according to the location of the chosen axis. Moreover, the friction losses are not taken into account. At the opposite, in our case, the homogeneity of the channel disposition leads to a priori faithfully results. Moreover, whatever could be the chosen axis, the temperature profiles are similar.

3.2. Experimental conditions

As previously explained, the experimental results feeding the computed model are issued from tests performed on a low power PEMFC stack. The computed results are given for dry hydrogen. The hygrometry of the air is given first dry and then at 50%. Input temperatures of the feeding gas has been set to 333K corresponding to the previous heating before being consumed by the stack. Results are given for two current densities of 0,3 and 0,5 A.cm^2. For all the studies, the output pressures of the gas are assumed to the atmospheric pressure (10^5 Pa).
The cooling channel is considered in our case thanks to a symmetrical applying of Dirichlet conditions on temperature on external face of the bipolar plate. The cooling channel is modelled by finite differences in model [9].

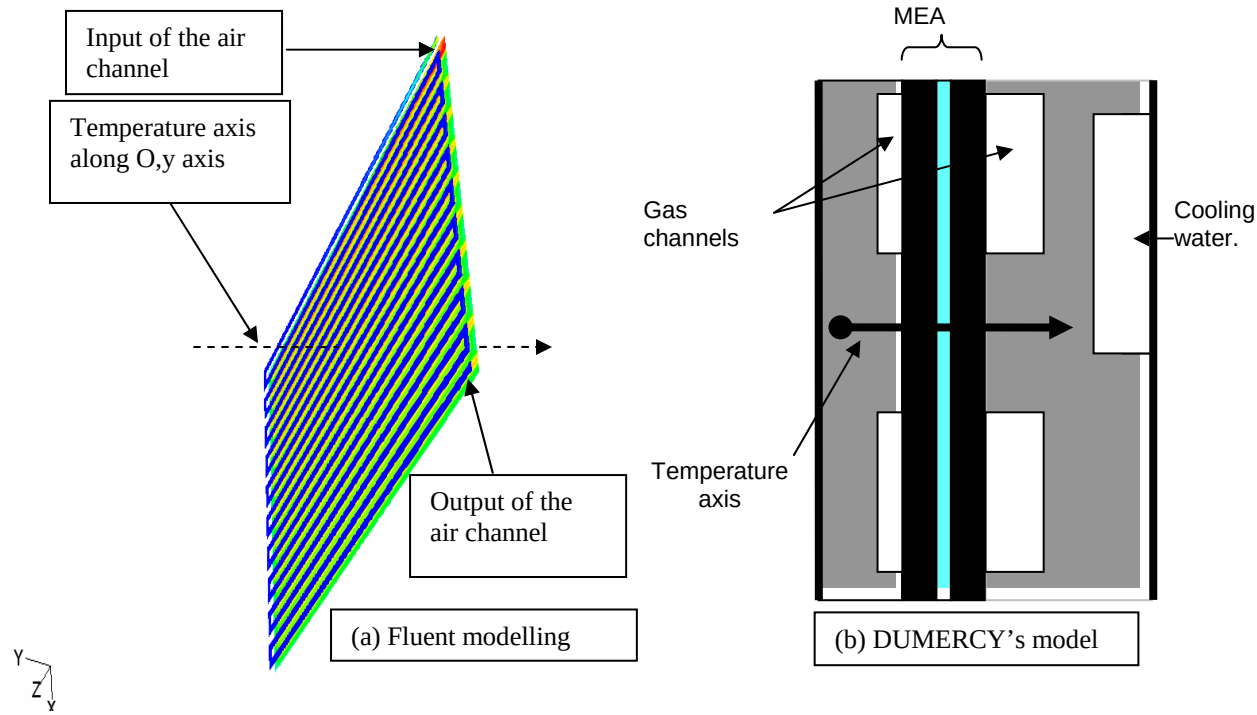

Fig.3: Chosen temperature profiles locations for the two modelling

4. RESULTS AND DISCUSSION

4.1 Modelled temperature profiles through the MEA.

Figure 4 describes and compares the results of modelled temperature profiles through the MEA along the 0,Y axis as defined in figure 2 for different current densities and for the two models. It can be observed that the temperature gradients in the stack modelled with FLUENT are higher than for the Dumercy's studies. In the FLUENT modelling, the distribution of the species on the chemical reaction areas is more homogeneous. For the Dumercy's profile, it avoids the feeding gas channel inducing also lower temperatures. The choice of an other axis would have led to an other temperature profile and particularly if this axis is close to the H_2 and air channels.

4.2. Friction losses in the air duct.

Friction losses results are only detailed for the air channel as shown in figure 5. Moreover, it could be observed that the influence of the hygrometry is absolutely insignificant on the friction losses of the air duct, and finally, whatever could be the air temperature.

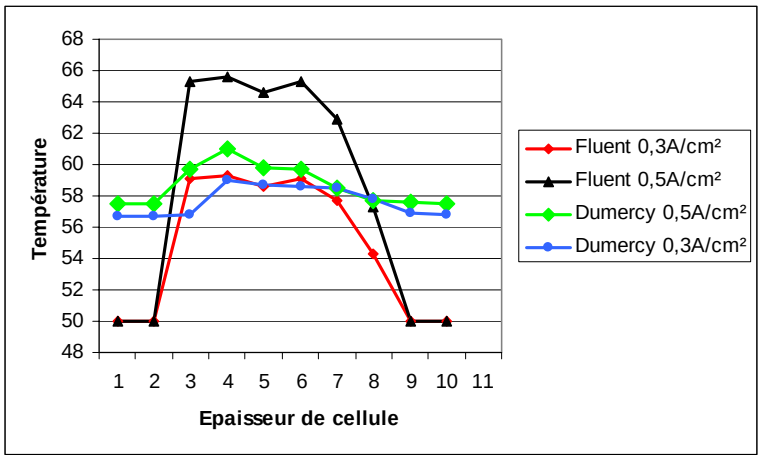

Fig 4 : Temperature profiles through the MEA

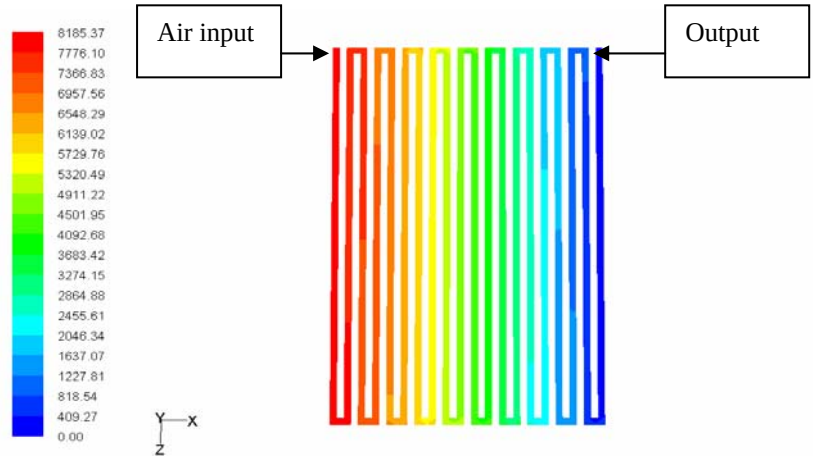

Fig 5 : Friction losses in the air duct for a standard output pressure.

The whole friction losses from input to output of the air flow does not exceed 409,5 Pa. Linear friction losses are about 20,5 Pa for one length of duct at which it is necessary to add 1,1 Pa as particular friction losses issued from the bent of the duct. The theoretical calculus of the linear friction losses should have given a value of 24 Pa, inducing a relative difference of 17%. It is similar for the studies of DUTTA [7] which present differences between 15 and 25%.

4.3. Temperature profile on the chemical reaction site along the 0,X axis

It can be seen on figure 6 the temperature profile (in the plan O,X,Z parallel to O,X) of the reactive site along the 0,X axis for Z=30 mm and Y=1,050 mm (see fig.2). This interesting profile is absolutely representative of the local inhomogeneous diffusion of the chemical species from the gas channel to the active site. It could be verified that locations of lower temperatures directly face the gas channels taken at the temperature of 333 K.

4.4. Relationship current density, air hygrometry and condensation temperature

Following results presented in set of figures 7.a, 7.b, 8.a and 8.b show the profile of the hygrometry along the length of the air duct, for two current densities of respectively 0,3 and 0,5 A.cm^{-2}. Two hygrometries at the input of the air duct are presented. It can be clearly observed the appearance of the condensation along the ducts (the arrow position), inducing also an efficiency drop of the stack and

also requiring an adapted and quick control of the stack. It can be seen the quicker appearance of the condensation in the duct for an 50% air input hygrometry for the higher current density of 0,5 A.cm^{-2}.

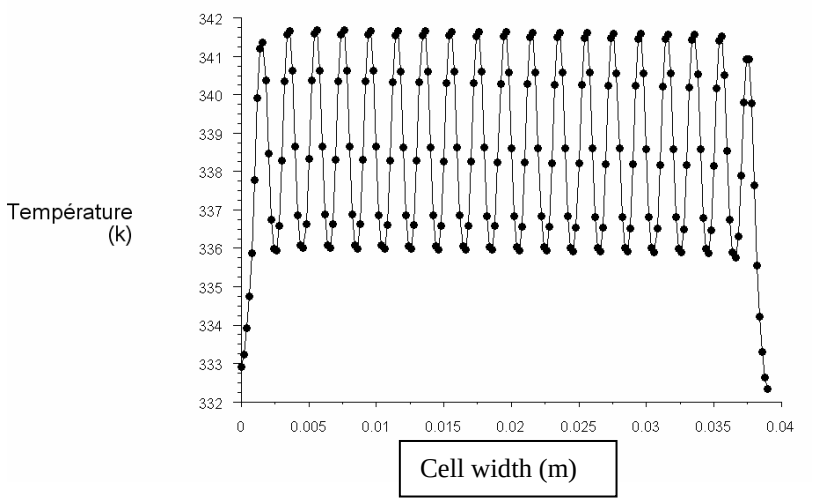

Fig. 6: Temperature profile along the active reaction site

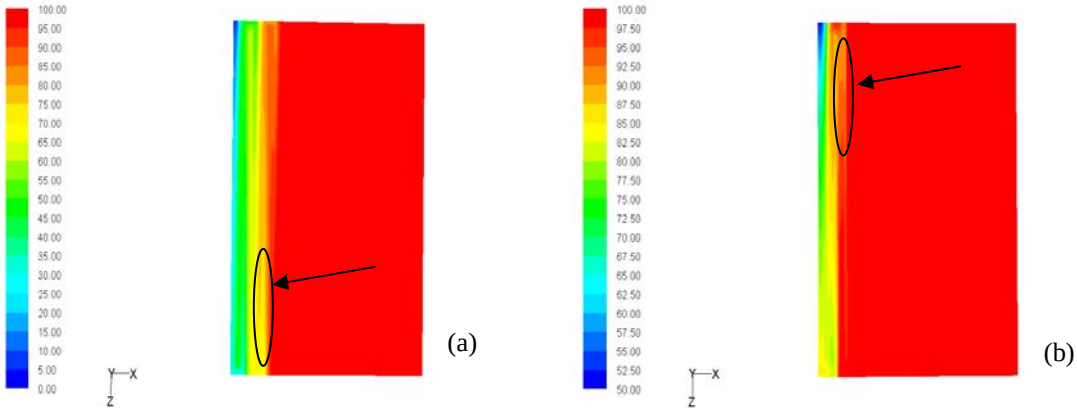

Fig 7.a and 7.b : Hygrometry profiles for 0,3A/cm² and input hygrometries of 0% (a) and 50% (b)

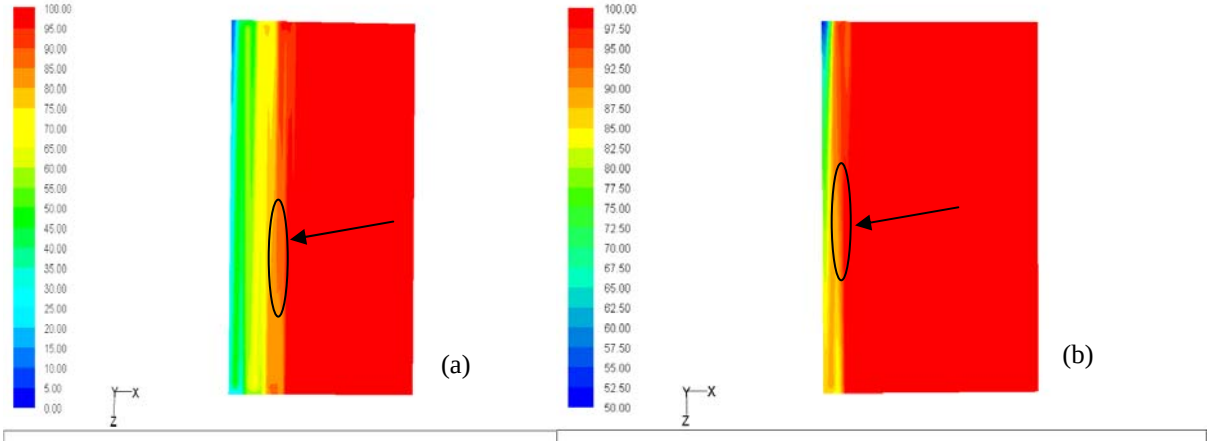

Fig 8.a and 8.b : Hygrometry profiles for 0,5A/cm² and input hygrometries of 0% (a) and 50% (b)

For a same air hygrometry, the condensation phases always appear farther from the input for lower current densities. Moreover, the more the feeding gases are humidified, the more the condensation phases soon appear. The results permit to forecast and to locate very precisely areas where this phenomenon will take place.

5. CONCLUSION

The developed model is a very complete one compared to the nowadays developed researches in this field. Indeed, it is clearly shown the influence of the simultaneous numerical resolution of the heat and mass transfers in the two feeding channels on the local temperature. The advantage of such a numerical tool is its ability to forecast the appearance of condensation phenomena which induce lower efficiencies. This behaviour forecast tool will permit to optimize in real time the control of the stack, particularly for variable load.

It should be as next step, very important to consider the internal power generation induced by the condensation phenomena. It will permit to compute more faithfully the temperatures and finally to obtain a more accurate location of the physical state changes of the water vapour for different external and internal constraints.

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