

# Modeling of Transport Phenomena in A PEM Fuel Cell

Kerkoub Youcef, Kerboua Ziari Yasmina, Benzaoui Ahmed

**Abstract**— In this paper, a three dimensional non-isothermal and steady state model is presented. This model takes into account the transport of reactants, heat, charge species and fluid flow in all parts of the cell in conjunction with the electrochemical reaction. The solid collectors are also included in this model in view to approach a realistic system representation. These processes have a significant impact on water management. Water management ensures that the membrane remains fully hydrated to maintain good ionic conductivity and performance. This work focuses on the effect of gradients of pressure between the anode and cathode, on the performance of the cell and also investigates the effect of these parameters on water management within the cell. Different cases of these gradients have been investigated and compared to the experimental results reported by Wang [2000].

**Index Terms**— PEMFC— fuel cell—energy—hydrogen—electrical performance.

## I. INTRODUCTION

The PEMFC (Proton Exchange Membrane Fuel Cell) using very thin polymer membrane has been considered as a promising candidate for future power sources for transportation and residential applications Pinar [2011] and Lobato [2010]. The difficulties related to the fuel cell systems experimental environment have stimulated efforts to develop models that could enable simulation and prediction of multi-dimensionally coupled transport of reactants, heat and charge species. The model based on Ohm's law and Butler-Volmer (or Tafel) equation is the first kind of model which describes the performance of the PEM fuel cell. Ticianelli [1988] and Srinivasan [1988] were among the first

to use the empirical equation in order to analyze their experimental polarization results. However, they do not provide insight into the underlying transport and electrochemical phenomena that occur inside the fuel cells. More detailed analysis of the multiple transport and electrochemical mechanisms requires the use of numerical models (CFD). The first applications of CFD methods to fuel cells focused on two-dimensional models Gurau [1998] and

Singh [1999]. More recently, CFD and improved transport models have allowed the development of increasingly more realistic computational models Ozmen [2011], accounting for fluid, thermal and electrochemical transport, complex three-dimensional geometries including flow and cooling channels and two-phase transport Berning [2002] and Hao [2009].

## II. HYPOTHESIS MODEL

Equations of transport in the PEMFC are highly nonlinear interdependent. Solving these equations in a part of the cell requires the resolution in all elements. Therefore, simplifying assumptions are needed to solve the system. These assumptions are:

- Reactive gases are ideal
- The speed of the reactive gas is small, so the flow is considered laminar and incompressible.
- The water produced by the electrochemical reaction is considered to the vapor phase and the phase change is not considered.
- The porous layers are considered homogeneous isotropic is
- The membrane is impermeable to gas

## III. MODEL EQUATIONS

The main equations dealing with transport phenomena are: continuity, momentum, conservation of species, conservation of energy and conservation of electric charge. These equations can be written in the same way throughout the computational domain of the cell PEMFC.

However, diffusive and convective terms and sources change from one element to another depending on local properties of the region. For example the term source of the consumption of hydrogen is enabled only to the catalyst layer of the anode and for the same oxygen consumption and the production of the water where they are activated only in the catalyst layer of the cathode.

The equations of this model are below. Terms of diffusion and sources are described below for each layer  
Continuity equation is given as follows:

$$\nabla \epsilon \rho \vec{u} = S_{H_2} + S_{O_2} + S_{H_2O} \quad (1)$$

Where  $\epsilon$  is the porosity,  $\rho$  is the density.

The motion amount in three directions is given by:

$$\nabla (\epsilon \rho \vec{u} \vec{u}) = -\epsilon \Delta P + \nabla (\epsilon \mu \nabla \vec{u}) + S_{mom} \quad (2)$$

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Where  $\mu$  : is the dynamic viscosity;  $P$  is the pressure and  $S_{mom}$  is the source terms representing the viscous pressure drop (as Darcy).

The energy equation is given by:

$$\rho C p_{eff} \nabla(\vec{u}T) = \nabla(k^{eff} \nabla T) + S_{rev} + S_{ohm} + S_{ac} \quad (3)$$

The source terms  $S_{rev}$ ,  $S_{ohm}$  et  $S_{ac}$  represent the heat release through an electrochemical reaction, Joule effect and overvoltage activation respectively.

The equation of species conservation is expressed as:

$$(\varepsilon \vec{u} C_i) = \nabla(D_{i,m}^{eff} \nabla C_i) + S_i \quad (4)$$

$\sigma_s$  et  $\sigma_m$  are polymer solid phase electrical conductivity and  $\phi$  is the potential

#### A. Inside the membrane

The equation of species conservation is only applied to water. The reason is that the membrane is supposed to be impermeable to reactive gas. This equation will take into account a source term which describes water transportation by electro-osmosis (water molecules accompanying each  $H^+$  proton crossing the membrane). This term is expressed by:

$$S_{H2O} = -\nabla\left(\xi \frac{i}{F}\right) \quad (5)$$

$\xi$ : Transportation by electro-osmosis coefficient

The mean density current produced by the cell is:

$$i_{moy} = \frac{1}{L} \int_0^L \sigma_m \frac{\partial \phi_m}{\partial x} \quad (6)$$

Where  $L$  is the membrane thickness

#### IV. SIMULATION

The flow diagram for this numerical algorithm is represented in Figure (1)

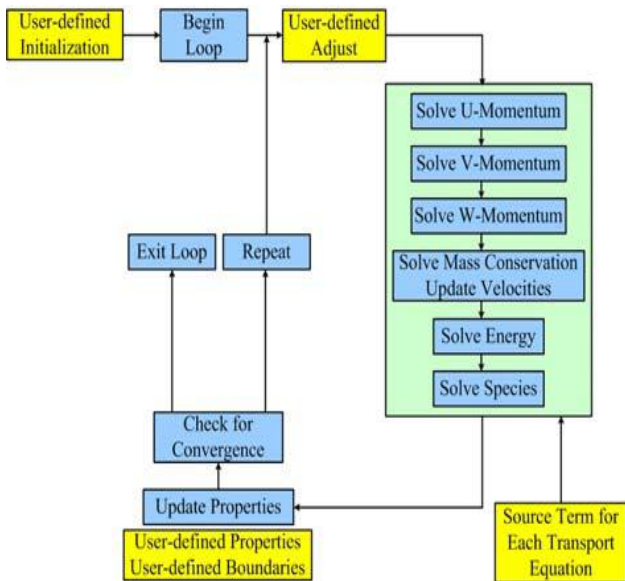


Figure 1. A flow diagram for the solution procedure

#### V. VALIDATION

The current model is validated against experimental data measured with an in-house developed PEM fuel cell Wang [2003]. Figure (2), compares the computed and measured polarization curves. In the activation and the ohmic regions (low and mid-range current densities) of the polarization curve, the results derived by using the proposed model are in a good agreement with the experimental ones, with deviations less than 5.0%. As expected, the model is unable to reproduce the experimental data at high current densities. The discrepancy in this region is attributed in part to the assumption of single phase transport. In practice, however, the formation of liquid is expected to limit mass transport at higher current densities Sivertsena [2005]. Another effect that may lead to a drop in the cell voltage at higher current densities is the shift of the reaction zone in the catalyst layer away from the membrane interface at higher currents Sivertsena [2005]. The protons need to be transported further out in the catalyst layer due to the depletion of oxygen in the catalyst, and this leads to an increased ohmic losses.

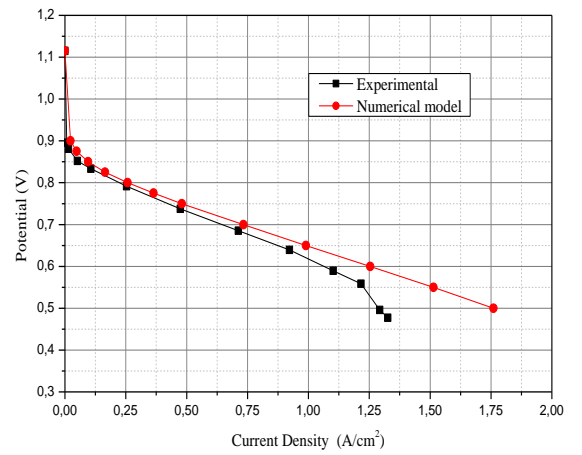


Figure 2. Polarization curve: comparison of simulations and experiments Wang [2003]

#### VI. HUMIDIFICATION OF THE MEMBRANE

Wetting well the membrane is essential to reduce the resistance to proton transport in order to obtain good electrical performance. It is interesting to observe the distribution of the water content in the thickness of the membrane as a function of operating conditions (relative humidity of inlet gas, current densities). For this, we study two cases. In the first case, hydrogen is perfectly hydrated  $RH = 100\%$  and the air  $RH = 30\%$ . Otherwise, in the second case, the air is perfectly hydrated  $RH = 100\%$  and humidity  $RH = 30\%$  hydrogen.

Figure (3) shows the distribution of the water content for the first case. We can observe in this figure the influence of transport by means of electro osmosis in the internal state of the membrane. At low current densities, the water content is higher at the anode side due to the high concentration of water relative to the cathode side. The hydration of the membrane to the cathode by the water produced is low. The flow of water is required by a diffusive flux directed from the anode to the cathode. However, increasing the current density, the electro-osmosis flow is likely to carry water from the anode to the cathode. The water content decreases slightly while the

anode side and the cathode increases slightly. The production of the water is not sufficient to balance the distribution. For very high current densities, the electro osmotic flow becomes larger and the water produced by the electrochemical reactions is also important. This increases the water content of the cathode side, the distribution becomes practically uniform throughout the thickness of the membrane.

In the opposite case when air humidity  $HR_a = 100\%$  and hydrogen  $HR_c = 30\%$ , figure(3), shows the current density effect on the water content distribution. On weak current densities, the water content is at maximum on the cathode side. The water flux directed from the cathode toward the anode is forced by the main diffusive flux. By increasing the current density, the electro-osmosis flux grows and compensates the diffusive effect which leads to a water content increase on the cathode side in one hand. On other hand, on important current densities, the electro-osmosis flux takes the major place. The water is then transported from anode to cathode. Beside electro-osmosis, the water production becomes important in these densities interval, increasing the water content on the cathode side. In this case, the membrane is strongly hydrated on the cathode side, less than on the anode side. This, leads to a membrane drying risk on the anode side, which increases the protonic resistance, which lowers the fuel cell electrical performance.

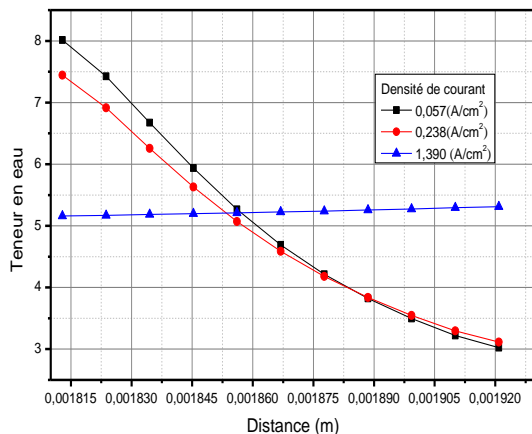


Figure3. Profile of the water content in the membrane thickness.

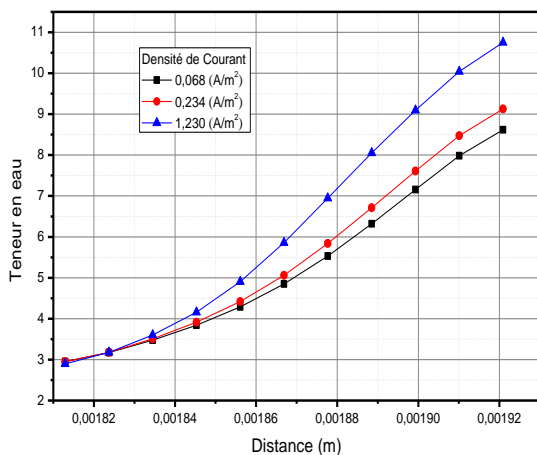


Figure4. Profile of the water content in the membrane

thickness for different values of the current density for  $HR_a = 100\%$  and  $HR_c = 30\%$ .

## VII. CONCLUSION

The stationary three-dimensional model presented includes all elements of the stack and describes the transport phenomena, the flow of reactive gases, mass transport, heat and electrical loads with the interaction of electrochemical reactions. The reactive gases perfect humidification,  $RH = 100\%$ , has a significant effect on the performance of the cell because it greatly increases the proton conductivity of the membrane. Note that the humidification of the cathode side did not have a significant effect on the performance of the cell compared to the anode side. The water production always keeps the membrane on the cathode side in a high state of hydration. It is recommended to highly humidify hydrogen and weakly the air.

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