Pore network simulation of water condensation in Gas Diffusion Layers of PEM Fuel Cells

B. Straubhaar[1], J. Pauchet[2] & M. Prat[1]

[1] Institut de Mécanique des Fluides de Toulouse, France
[2] CEA (LCPEM, LITEN), France

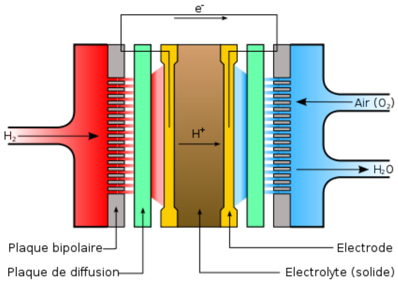
Outline

1. Introduction
2. Pore Network Model
3. Water transfer $(\Delta T \neq 0)$
4. Conclusion

Outline

Introduction : Proton Exchange Membrane Fuel Cells (PEMFC)

- = Stack
- Creates electricity/heat with hydrogen and oxygen
- Operating between 60 and 80°C

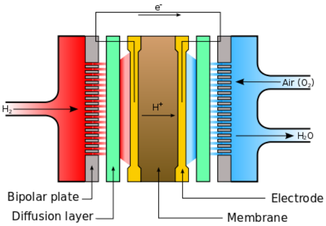


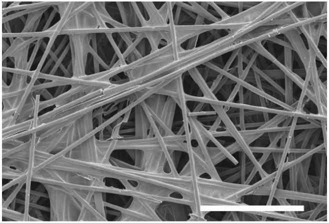
Introduction : Gas diffusion layer (GDL)

The GDL is a carbon fiber-based medium :

- hydrophobic
- 170 to 400 μm of thickness
- 0,21 to 0,73 g/cm^2 of density
- 70 and 80 % of porosity ; resulting pores between 20 and 50 μm

$\Rightarrow$ **GDL = Thin porous medium**

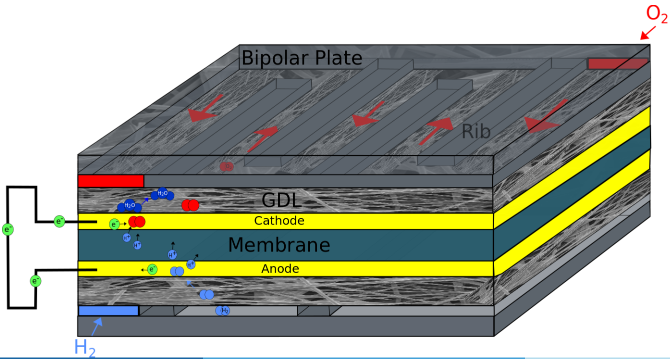




Introduction : Gas diffusion layer (GDL)

The main challenges in a GDL are :

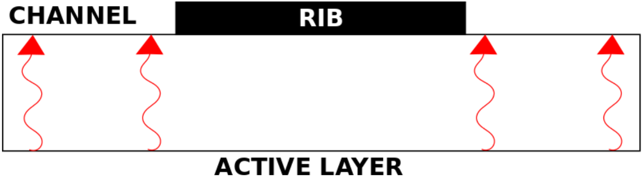
- ✔ To diffuse reactant gas uniformally from the channel to the active layer
- ✔ To keep the membrane hydrated for proton transfer
- ✔ To evacuate excess water to avoid cell flooding and let oxygen reach the active layer = Water management issue



What kind of water transfer in the GDL ?

First option

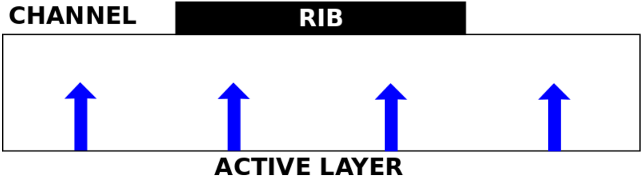
☞ Only vapor transfer ?



What kind of water transfer in the GDL ?

Other options

- Only vapor transfer ?
- ☞ Only liquid transfer ? e.g. Pasaogullari et al., J. Elec. Soc. 151 (3), A399-A406 (2004)

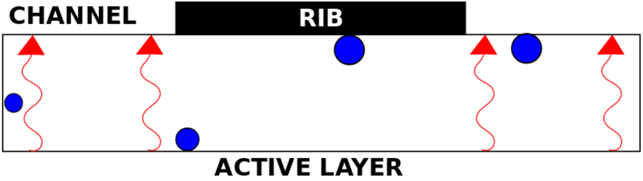


What kind of water transfer in the GDL ?

Other options

- Only vapor transfer ?
- Only liquid transfer ?

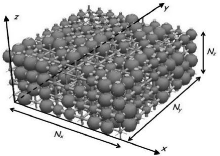
☞ Transfer with condensation and evaporation ?



Method : simulation of water transport using PNM

What numerical model ?

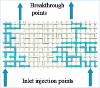
Classical 2-phase flow model based on generalized Darcy's law and macroscopic capillary pressure ?
But GDL is very thin (No length-scale separation)
$\Rightarrow$ Use of 3D **Pore Network Model (PNM)**



Outline

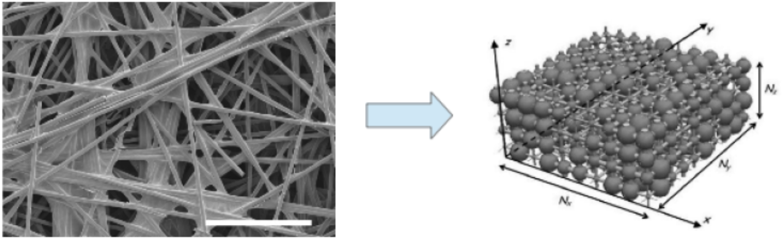
Pore Network Model (PNM)

- Allow invasion percolation process (pore with largest connected bond is invaded) or invasion with viscous effects
- Allow multiple injection points :

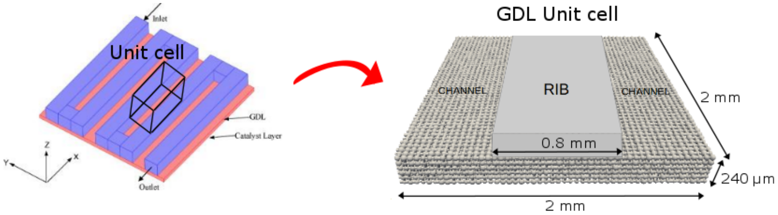


Ceballos et al., Phys. Rev. E 84, 056311 (2011)

- Less time-consuming than direct simulation (e.g. Lattice Boltzmann methods)



Properties



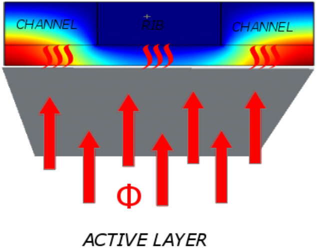
- $6 \times 50 \times 50$ pores with a $40\mu m$ step $\Rightarrow 240\mu m \times 2mm \times 2mm$ network
- Cubic pores and bonds
- Random distribution : $[d_{p_{min}} \,; d_{p_{max}}] = [24\mu m \,; 36\mu m]$ and $[d_{t_{min}} ; d_{t_{max}}] = [10\mu m \,; 24\mu m]$
- Fully hydrophobic : contact angle between water and carbon fibers : $\Theta = 110°$

Outline

Introduction

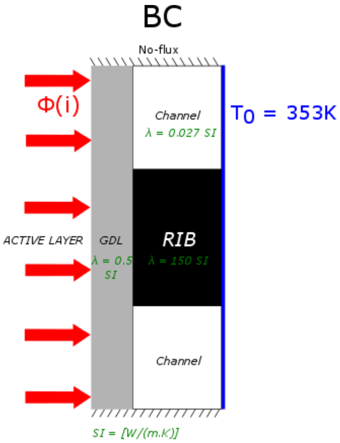
Introduction

Electrolysis $\Rightarrow$ Heat flux Φ at the GDL/active layer interface
Non uniform temperature in the GDL $\Rightarrow$ Colder zone $\Rightarrow$ Possibility of condensation



Calculation of temperature field with Finite-volume method

→ Two cases : a) Isotropic and b) Anisotropic thermal conductivity



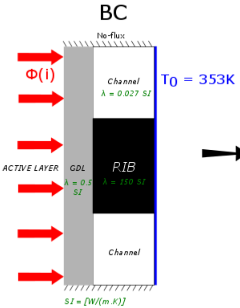
λ (W/(m.K))

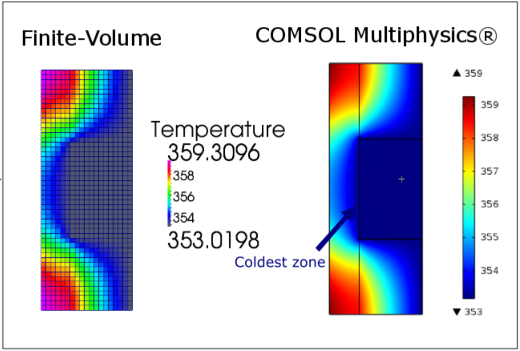
	in-plane	through-plane
x1	0,5	0,5
x10	0,5	5
x100	0,5	50

Anisotropy

$$\Phi(i) = (\Delta H_{liq}/2F - U)\, i$$

a) **Isotropic thermal conductivity** in the GDL $\rightarrow \lambda = 0.5 W/(m.K)$

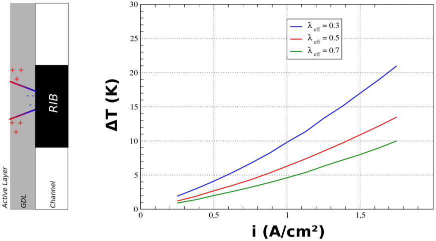


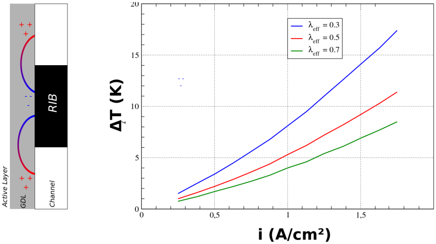


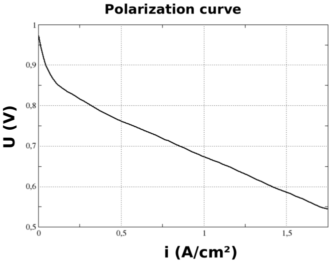
$$\Phi(i) = (\Delta H_{liq}/2F - U)\, i$$

Temperature field

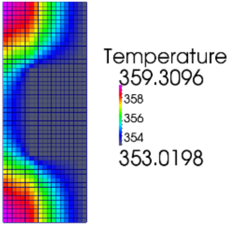
At 80°C, $\frac{\Delta H_{liq}}{2F} = 1,48$. U and i are taken from the polarisation curve below.

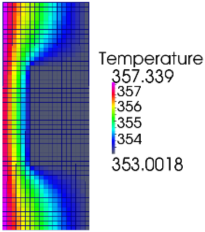


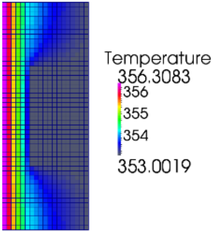




b) **Thermal anisotropy** in the GDL $\rightarrow \lambda = 0.5 W/(m.K)$ in through-plane direction and $\lambda = 5$ or $50 W/(m.K)$ in in-plane direction (for i = 1 A/cm²)







in-plane λ [SI]	0.5 (isotropic)	5	50

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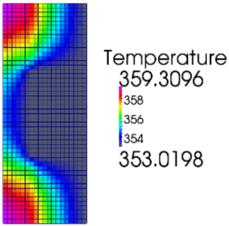
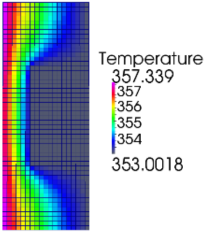
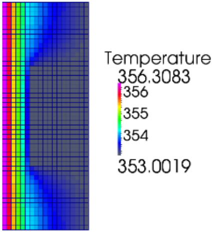
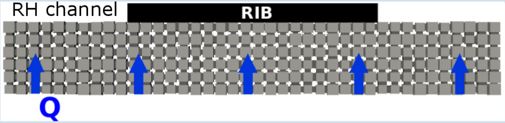
			
in-plane λ [SI]	0.5 (isotropic)	5	50

☞ Anisotropy tends to make the in-plane temperature uniform

Water production rate



$$Q = \frac{iA}{2F}$$

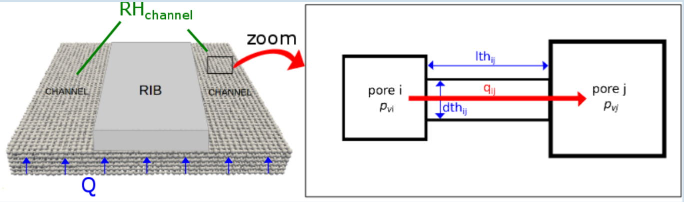
- i : current density
- A : cross-sectional area
- F : Faraday constant

Is it possible to transfer this flux in vapor phase accross the GDL ?

Estimation of Critical Relative Humidity

Critical RH = RH within the GDL marking the onset of condensation

Calculation of vapor partial pressure field by PN approach



In each pore i, mass conservation : $\sum_{j=1}^{nb_{neighbours}} q_{ij} = 0$

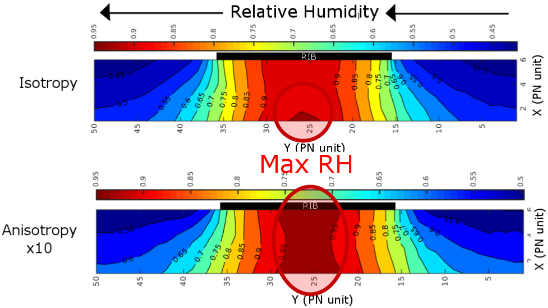
$q_{ij} = g_{ij}(x_{vi} - x_{vj})$ is the local vapor flux from pore i to pore j

$g_{ij} = cD_{w/a} dth_{ij}^2 / a$

- c : mole concentration $(= p/RT)$
- dth_{ij} : width of the throat between i and j
- a : lattice distance
- $D_{w/a}$: molar diffusion coefficient between air and water

Example for i = 1 A/cm^2 - RH channel = 50 %

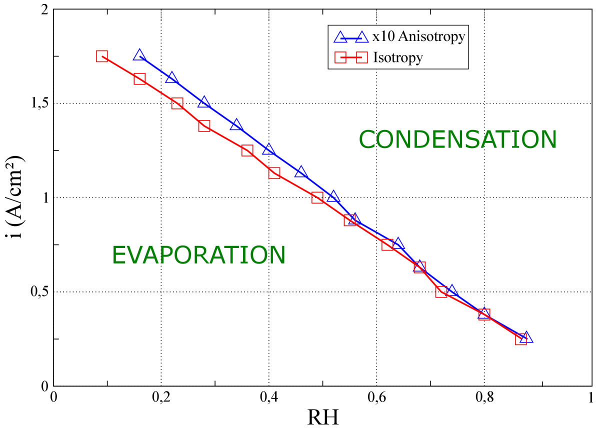
$$RH_{local} = \frac{p_v(x,y,z)}{p_{vs}(T(x,y,z))}$$



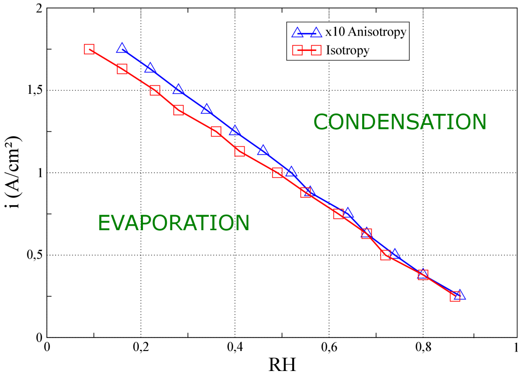
⇒ Isotropy : Maximum of local Relative Humidity at the GDL/AL interface
⇒ Anisotropy : Maximum of local Relative Humidity under the rib and at the GDL/AL interface
⇒ No condensation as long as local RH < 1 in the GDL

Phase diagram

From many simulations varying i and RH channel



Pore Network Model with condensation and evaporation

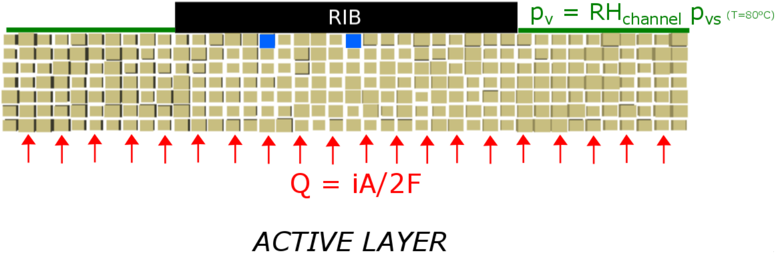


If condensation is possible $\Rightarrow$ 2 steps : nucleation and growth of liquid clusters

Step 1 : Nucleation

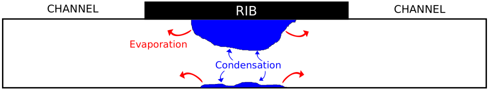
Identification of nucleation spots

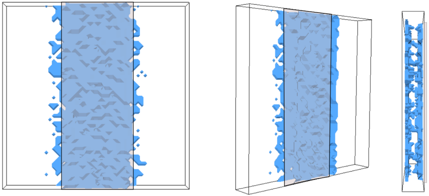
1. Compute p_v in each pore assuming no condensation
2. Identify each pore where RH is ≥ 1
3. Invade the pore where RH is ≥ 1 and is maximum
4. Back to step 1 until $RH < 1$ in each remaining pore
5. Initial state for growth step



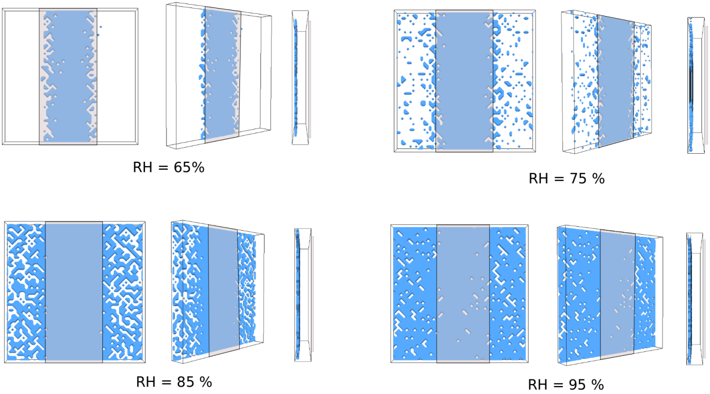
Step 2 : Pore Network Simulation of liquid cluster growth due to condensation

Growth stops when evaporation rate = condensation rate for each liquid cluster





Results (I) Isotropic Thermal Conductivity & i = 1 A/cm^2



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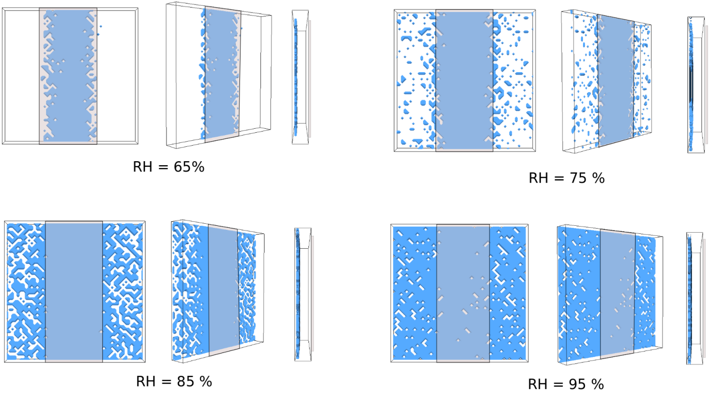
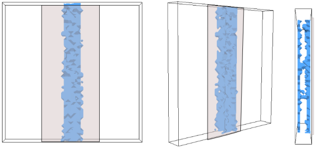
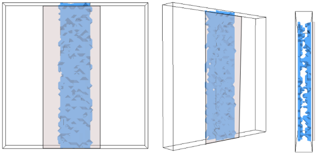


→ Condensation happens at the AL/GDL interface and water spreads over the whole AL/GDL interface

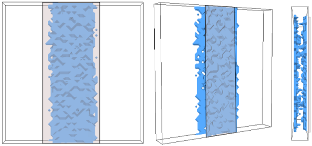
Results (II) $\times$10 Anisotropy & i = 1 A/cm^2



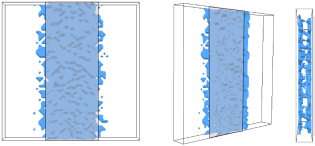
RH = 65%



RH = 75 %

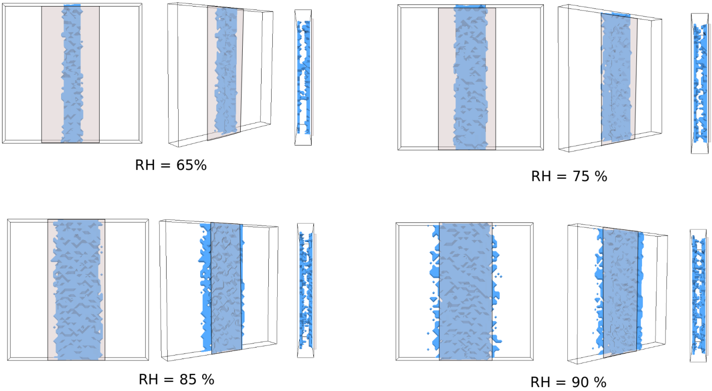


RH = 85 %



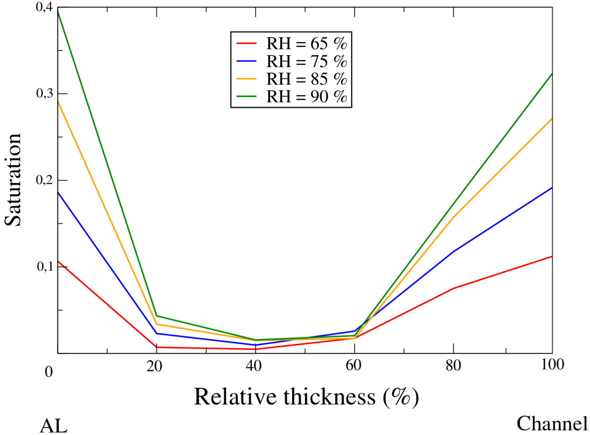
RH = 90 %

Results (II) $\times$10 Anisotropy & i = 1 A/cm^2

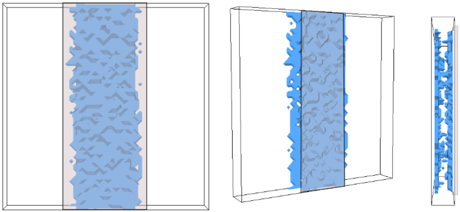


→ Condensation located under the rib and at the AL/GDL interface

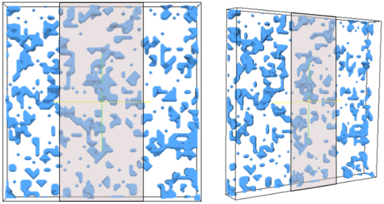
Results (III) Slice saturation (Anisotropic case)



Comparison with previous works (PNM)



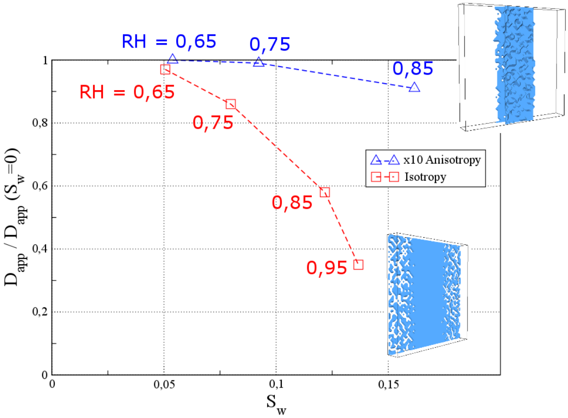
Cond. RH=85%



IP

⇒ Patterns are very different... Can affect the O_2 diffusion

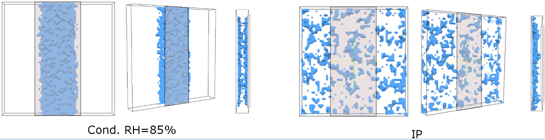
Apparent O_2 diffusion coefficient



Outline

Conclusion

- ✔ Most of previous works using PNM = Invasion Percolation in liquid phase from catalyst layer
- ✔ Temperature field is computed → Temperature variations within the GDL leading to condensation under the rib and at the GDL/AL interface
- ✔ Temperature field control is a key of water management
- ✔ Thermal anisotropy has a strong impact on temperature
- ✔ Thermal anisotropy has a beneficial impact on O_2 transfer
- ✔ Produced liquid water can be transferred through the GDL up to high RH channel
- ✔ Liquid patterns due to condensation are different from patterns using PNM(IP from active layer)



Prospects

- Coupling with non uniform current density at the GDL/AL interface
- Compare with in situ vizualisations for automotive applications ('IMPALA' project)

Acknowledgements :

Financial support from European Union's Seventh Framework Program (FP7/2007-2013) for the Fuel Cells and Hydrogen Joint Undertaking (project 'IMPALA') is gratefully acknowledged

THANK YOU FOR YOUR ATTENTION

QUESTIONS ?