



HAL
open science

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

Benjamin Straubhaar, Joël Pauchet, Marc Prat

► **To cite this version:**

Benjamin Straubhaar, Joël Pauchet, Marc Prat. Pore network simulation of water condensation in Gas Diffusion Layers of PEM Fuel Cells. 7th International Conference on Porous Media - InterPore 2015, May 2015, Padova, Italie, Italy. hal-04444093

HAL Id: hal-04444093

<https://hal.science/hal-04444093v1>

Submitted on 7 Feb 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Open Archive TOULOUSE Archive Ouverte (OATAO)

OATAO is an open access repository that collects the work of Toulouse researchers and makes it freely available over the web where possible.

This is an author-deposited version published in :

<http://oatao.univ-toulouse.fr/>

Eprints ID : 14107

To cite this version : Straubhaar, Benjamin and Pauchet, Joël and Prat, Marc *Pore network simulation of water condensation in Gas Diffusion Layers of PEM Fuel Cells*. (2015) In: 7th International Conference on Porous Media - InterPore 2015, 18 May 2015 - 21 May 2015 (Padova, Italy). (Unpublished)

Any correspondance concerning this service should be sent to the repository administrator: staff-oatao@listes-diff.inp-toulouse.fr

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

B. Straubhaar¹, J. Pauchet² & M. Prat¹

¹ Institut de Mécanique des Fluides de Toulouse, France

² CEA (LCPEM, LITEN), France

Outline

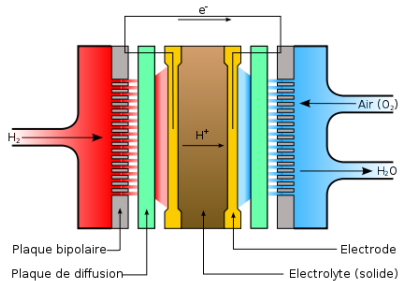
- 1 Introduction
- 2 Pore Network Model
- 3 Water transfer ($\Delta T \neq 0$)
- 4 Conclusion

Outline

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

Introduction : Proton Exchange Membrane Fuel Cells (PEMFC)

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

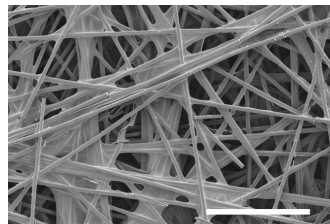
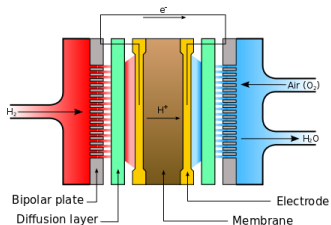


Introduction : Gas diffusion layer (GDL)

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

⇒ **GDL = Thin porous medium**

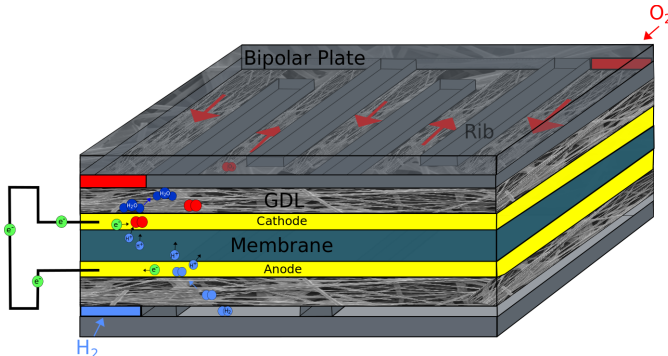


50 μm

Introduction : Gas diffusion layer (GDL)

The main challenges in a GDL are :

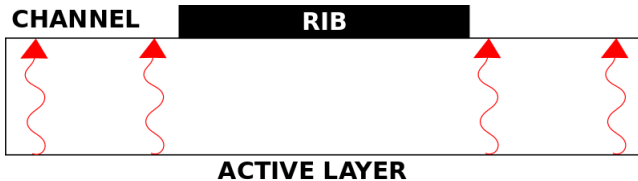
- ✓ To diffuse reactant gas uniformly from the channel to the active layer
- ✓ To keep the membrane hydrated for proton transfer
- ✓ To evacuate excess water to avoid cell flooding and let oxygen reach the active layer = Water management issue



What kind of water transfer in the GDL ?

First option

👉 Only vapor transfer ?

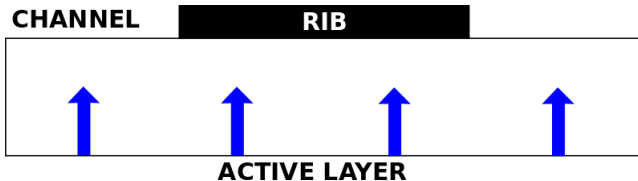


What kind of water transfer in the GDL ?

Other options

- Only vapor transfer ?

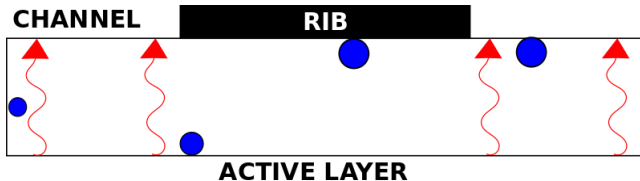
- ☞ **Only liquid transfer ?** e.g. Pasaogullari et al., J. Elec. Soc. 151 (3), A399-A406 (2004)



What kind of water transfer in the GDL ?

Other options

- Only vapor transfer ?
- Only liquid transfer ?
- 👉 Transfer with condensation and evaporation ?



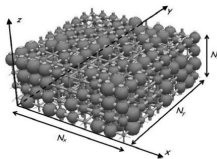
Method : simulation of water transport using PNM

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)

⇒ Use of 3D **Pore Network Model (PNM)**

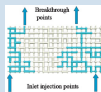


Outline

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

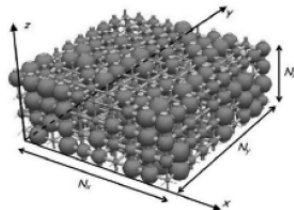
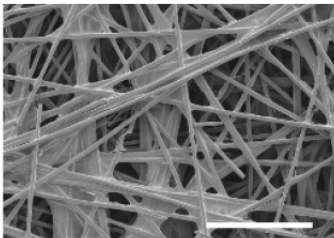
Pore Network Model (PNM)

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

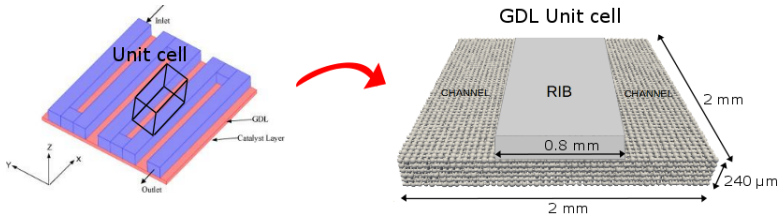


Ceballos et al., Phys. Rev. E 84, 056311 (2011)

- 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 : $\Theta = 110^\circ$

Outline

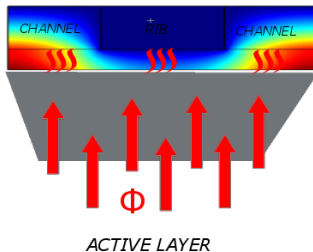
- 1 Introduction
- 2 Pore Network Model
- 3 Water transfer ($\Delta T \neq 0$)
 - Temperature field
 - Hypothesis
 - Pore Network Model with condensation and evaporation
 - Results
- 4 Conclusion

Introduction

Introduction

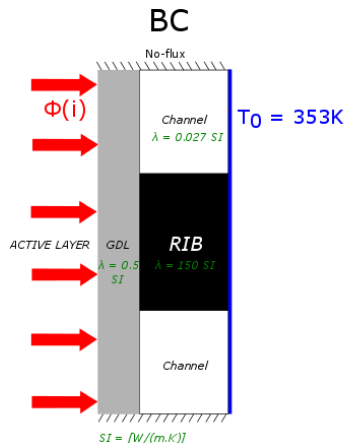
Electrolysis \Rightarrow Heat flux Φ at the GDL/active layer interface

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



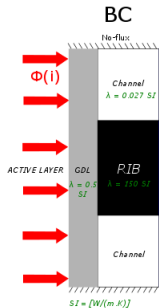
$\lambda \text{ (W/(m.K))}$

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

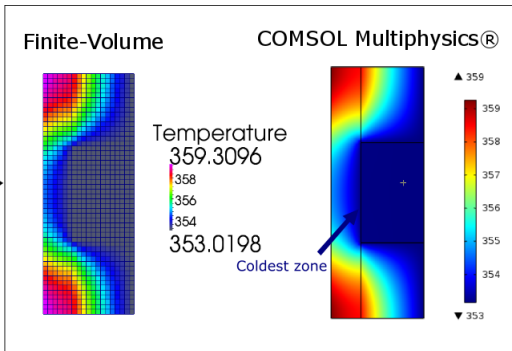
Anisotropy

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

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

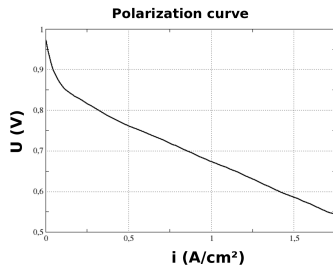
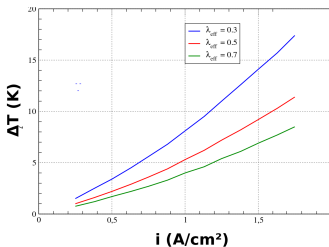
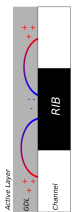
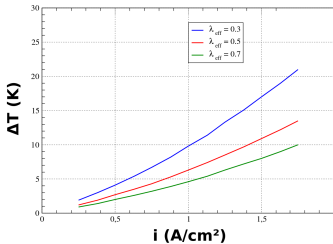
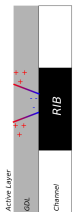


$$\Phi(i) = (\Delta H_{\text{liq}}/2F - U) i$$

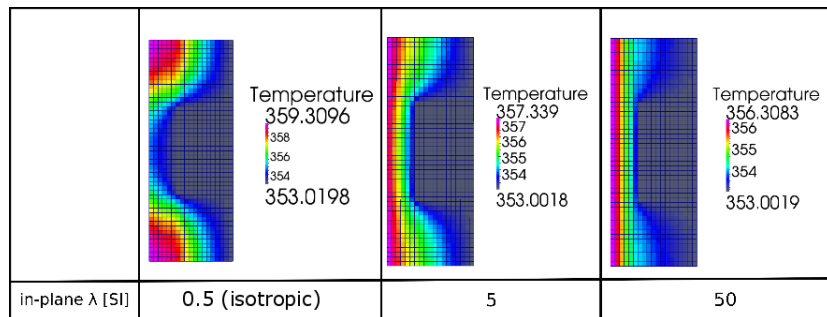


Temperature field

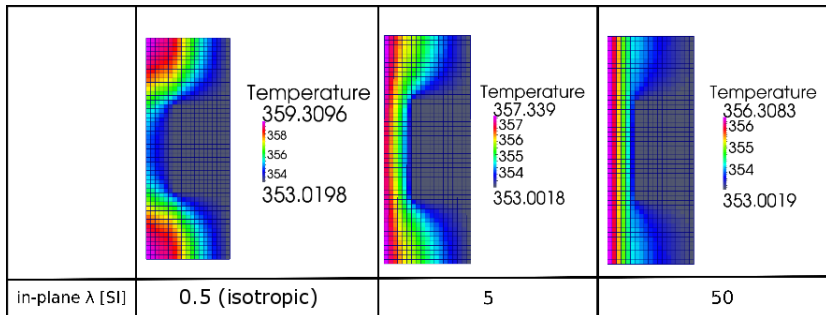
At 80°C, $\frac{\Delta H_{liq}}{2F} = 1,48$. U and i are taken from the polarisation curve below.



b) **Thermal anisotropy** in the GDL $\rightarrow \lambda = 0.5W/(m.K)$ in through-plane direction and $\lambda = 5$ or $50W/(m.K)$ in in-plane direction (for $i = 1 A/cm^2$)

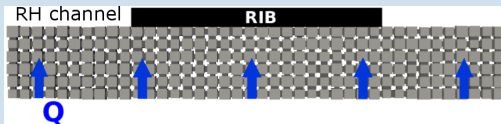


b) **Thermal anisotropy** in the GDL $\rightarrow \lambda = 0.5W/(m.K)$ in through-plane direction and $\lambda = 5$ or $50W/(m.K)$ in in-plane direction (for $i = 1 A/cm^2$)



☞ Anisotropy tends to make the in-plane temperature uniform

Water production rate



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

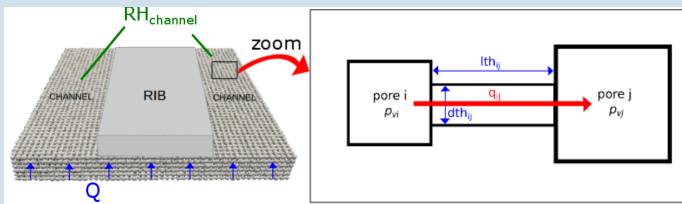
- i : current density
- A : cross-sectional area
- F : Faraday constant

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 : $\sum_{j=1}^{nb_{neighbours}} q_{ij} = 0$

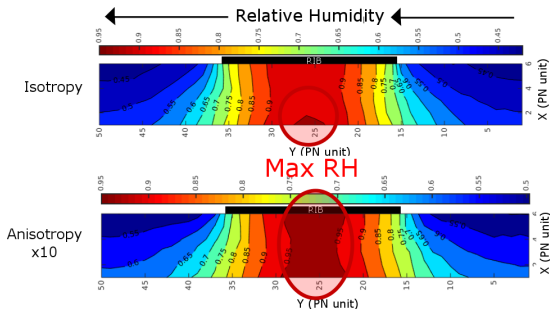
$q_{ij} = g_{ij}(x_{vi} - x_{vj})$ is the local vapor flux from pore i to pore j

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

- 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 $i = 1 \text{ A/cm}^2$ - RH channel = 50 %

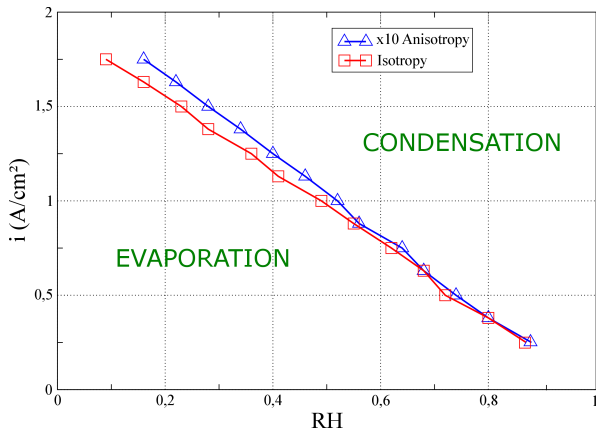
$$RH_{local} = \frac{p_v(x,y,z)}{p_{vs}(T(x,y,z))}$$



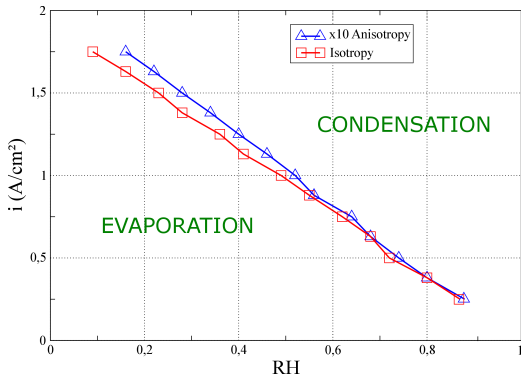
- ⇒ Isotropy : Maximum of local Relative Humidity at the GDL/AL interface
- ⇒ Anisotropy : Maximum of local Relative Humidity under the rib and at the GDL/AL interface
- ⇒ No condensation as long as local RH < 1 in the GDL

Phase diagram

From many simulations varying i and RH channel



Pore Network Model with condensation and evaporation

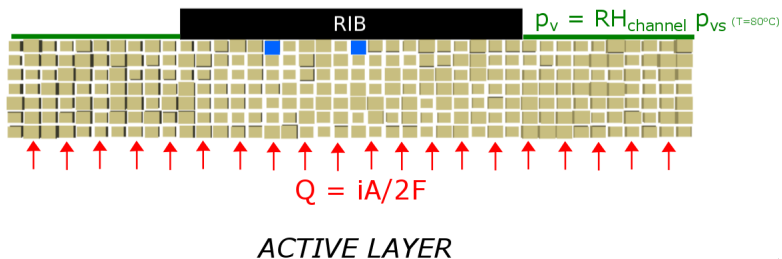


If condensation is possible \Rightarrow 2 steps : nucleation and growth of liquid clusters

Step 1 : Nucleation

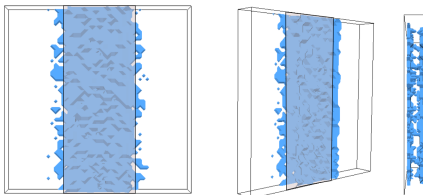
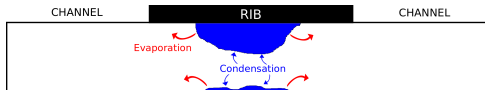
Identification of nucleation spots

- 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

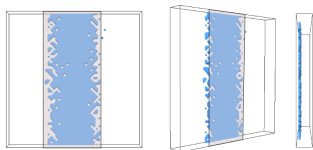


Step 2 : Pore Network Simulation of liquid cluster growth due to condensation

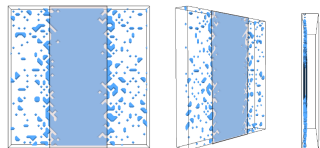
Growth stops when evaporation rate = condensation rate for each liquid cluster



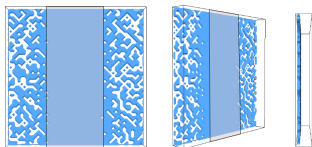
Results (I) Isotropic Thermal Conductivity & $i = 1 \text{ A/cm}^2$



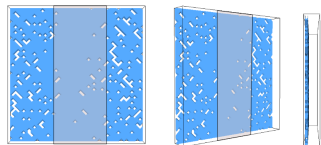
RH = 65%



RH = 75%

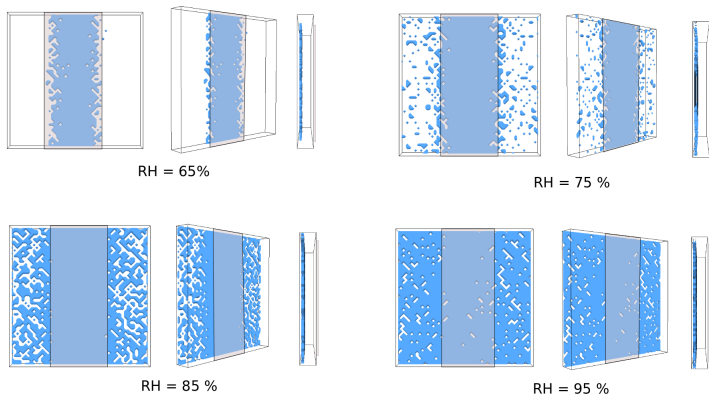


RH = 85%

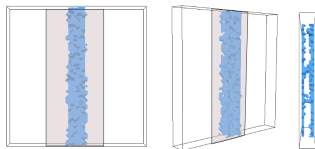


RH = 95%

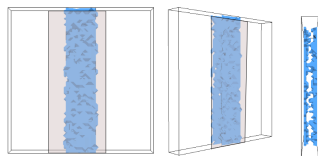
Results (I) Isotropic Thermal Conductivity & $i = 1 \text{ A/cm}^2$



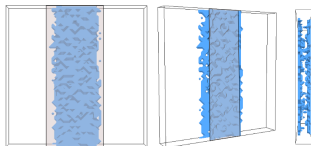
→ Condensation happens at the AL/GDL interface and water spreads over the whole AL/GDL interface

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

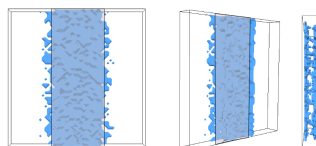
RH = 65%



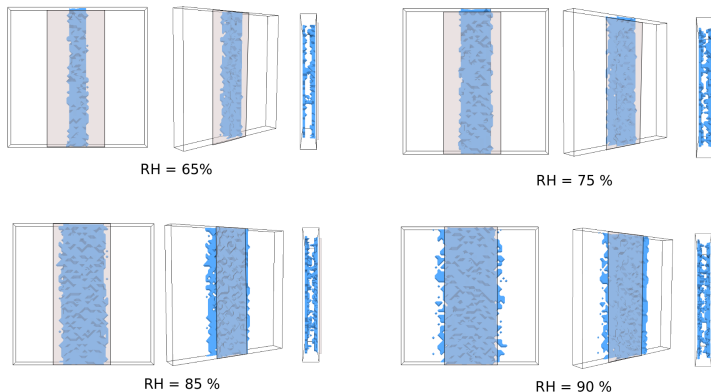
RH = 75%



RH = 85%

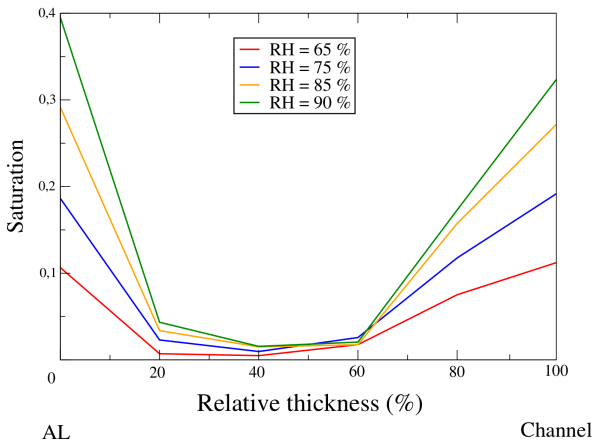


RH = 90%

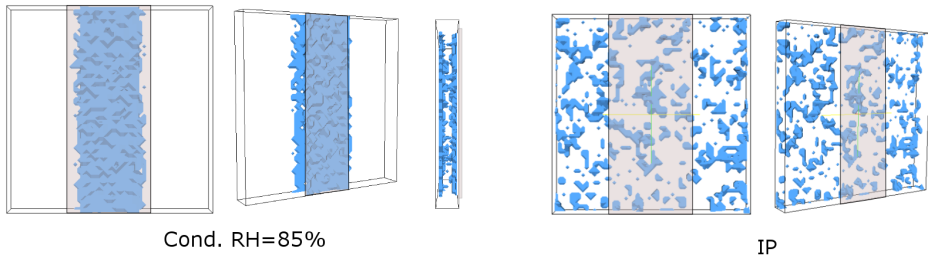
Results (II) $\times 10$ Anisotropy & $i = 1 \text{ A/cm}^2$ 

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

Results (III) Slice saturation (Anisotropic case)

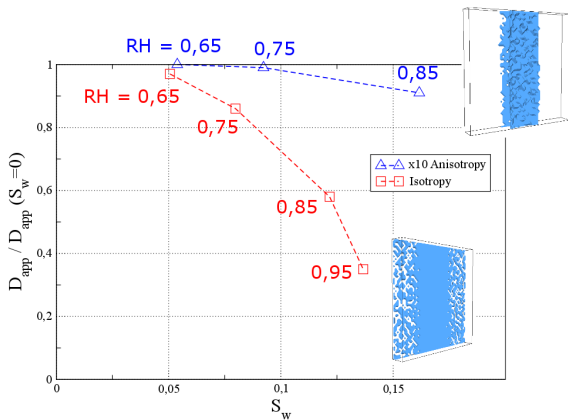


Comparison with previous works (PNM)



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

Apparent O_2 diffusion coefficient

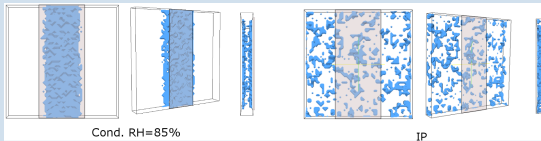


Outline

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

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 visualisations 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 ?