

Modélisation du transport de masse dans les milieux poreux par réseau de pores

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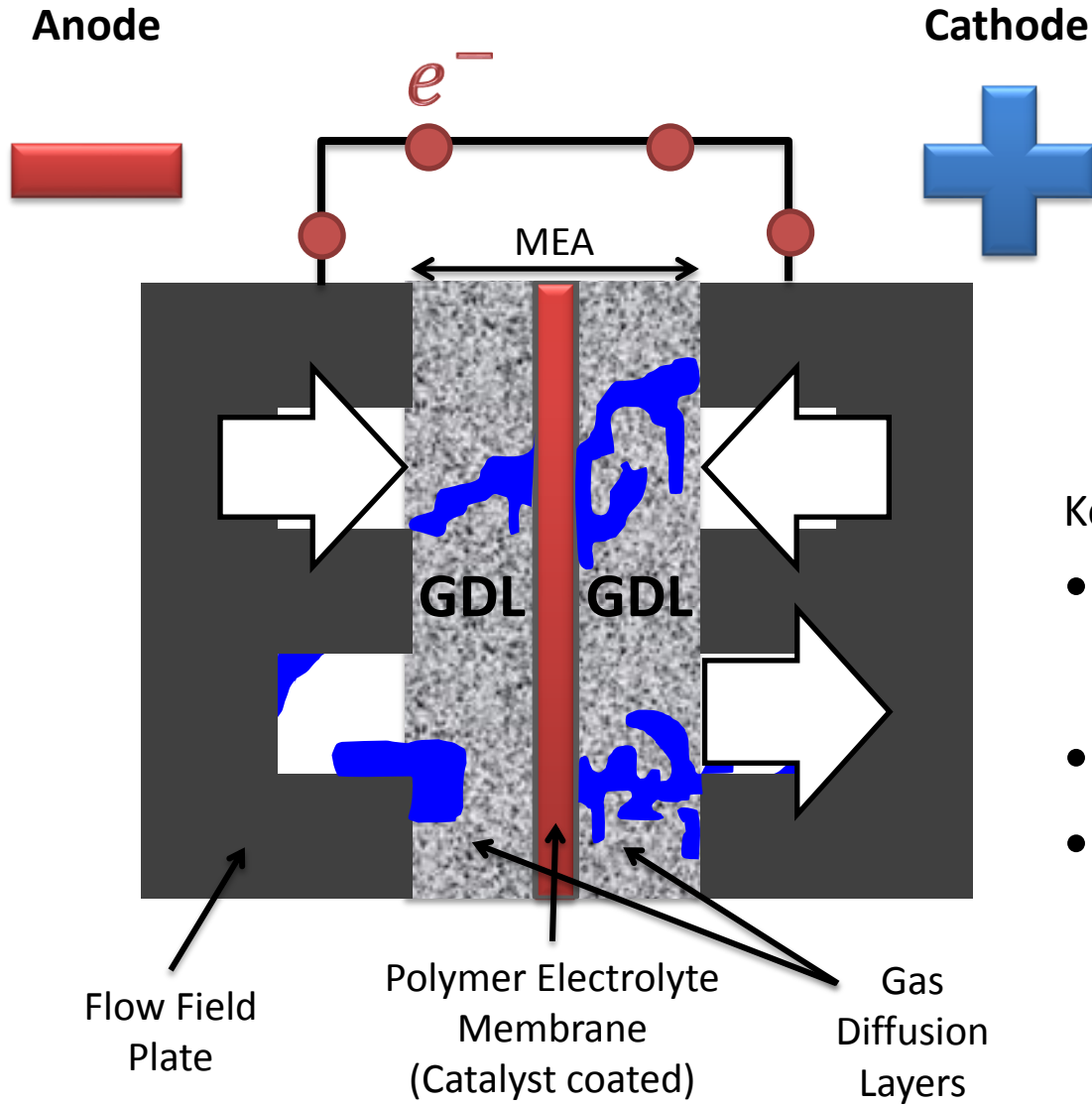
**Laboratoire de
thermocinétique de Nantes**

December 15th, 2014



UNIVERSITY OF TORONTO
FACULTY OF APPLIED SCIENCE & ENGINEERING
Institute for Sustainable Energy

Fuel cell technology



Anode:

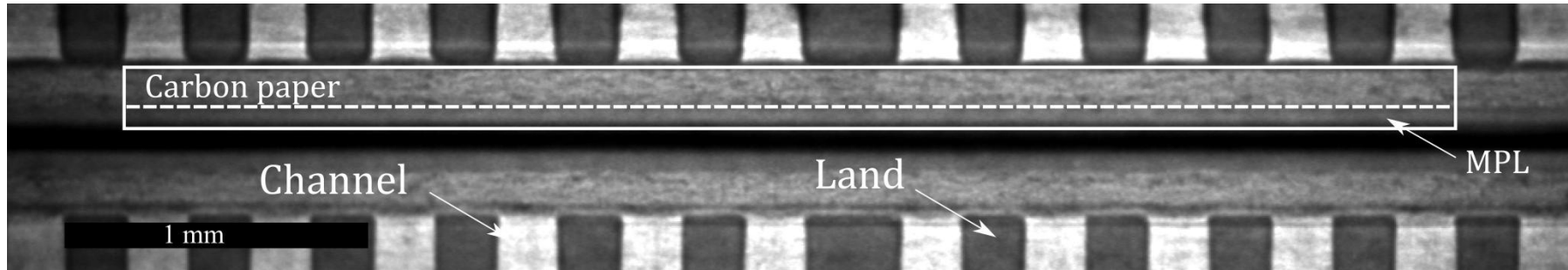
Cathode:

Key role playing by the GDL:

- Diffuse the reactant up to the catalyst layer
- Electrical and thermal conductor
- Remove the water excess



The Gas Diffusion Layer



Composed of two porous materials:

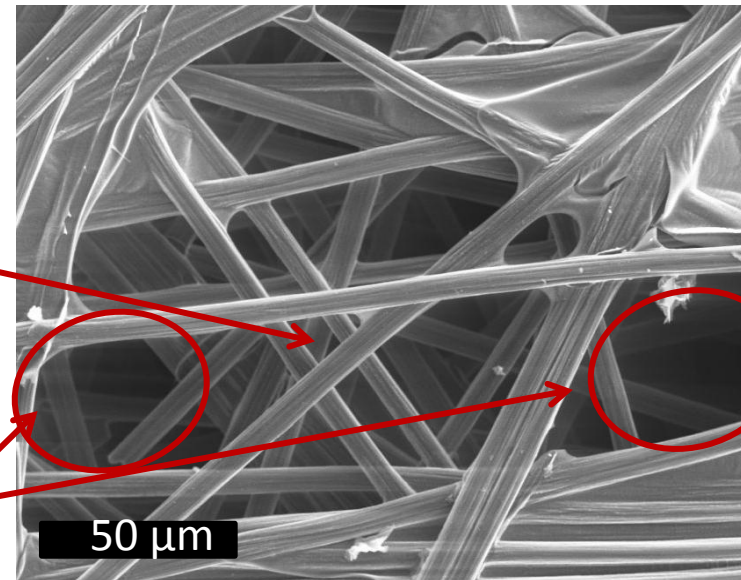
- Carbon fibers, mean pore size μm
- MPL mean pore size nm

What is the optimal design?

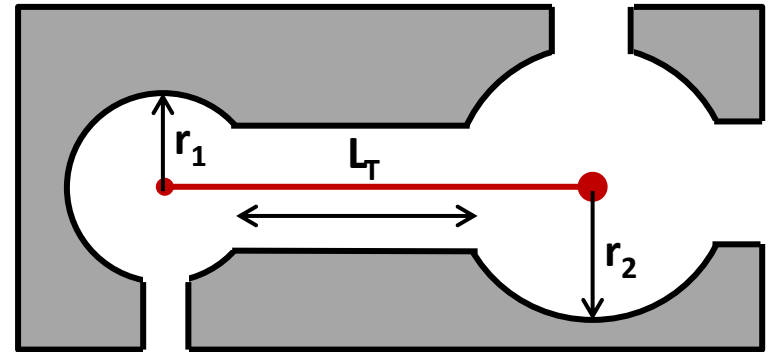
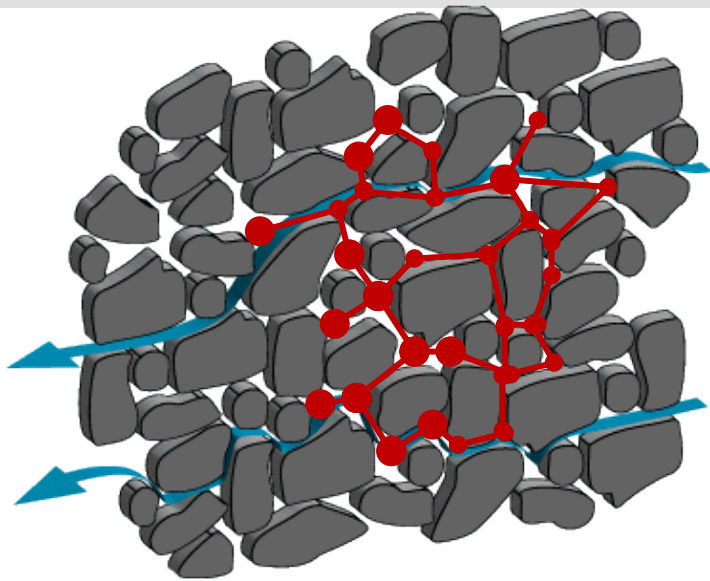
- ➔ Porosity distribution
- ➔ The mean size pore

Throat
Constrictions

Pore Bodies

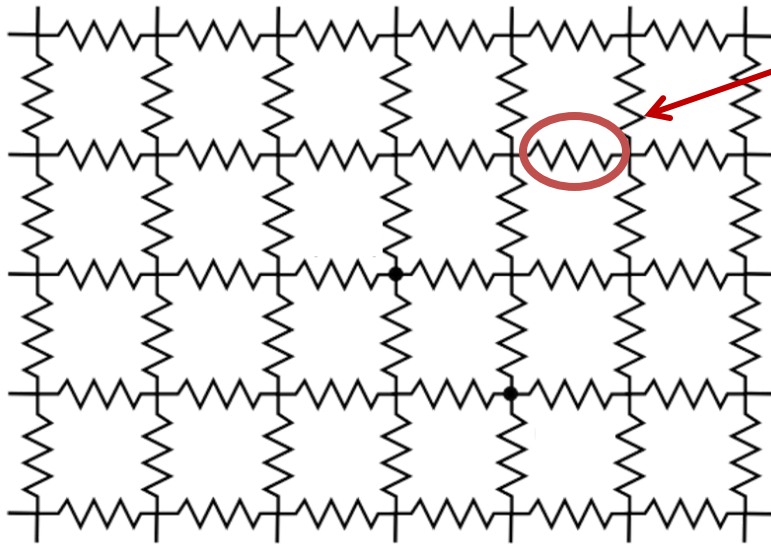


Pore network



$$Q = \frac{\pi r^4}{8\mu L} \Delta P_{12}$$

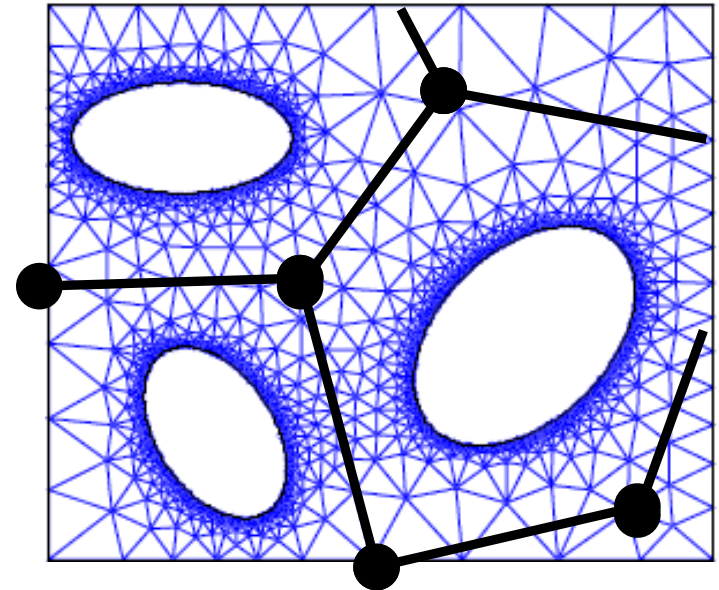
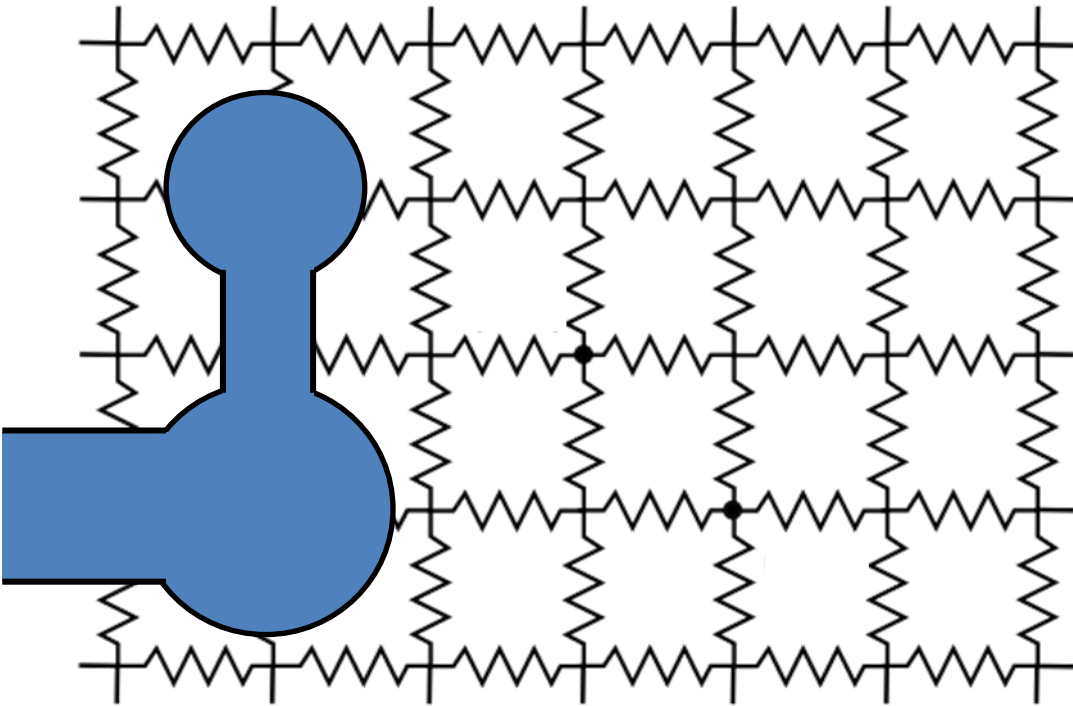
$$P_c = \frac{-2\sigma \cos \theta}{r_T}$$



Figures from J. Gostik



Pore network modelling versus continuum modelling

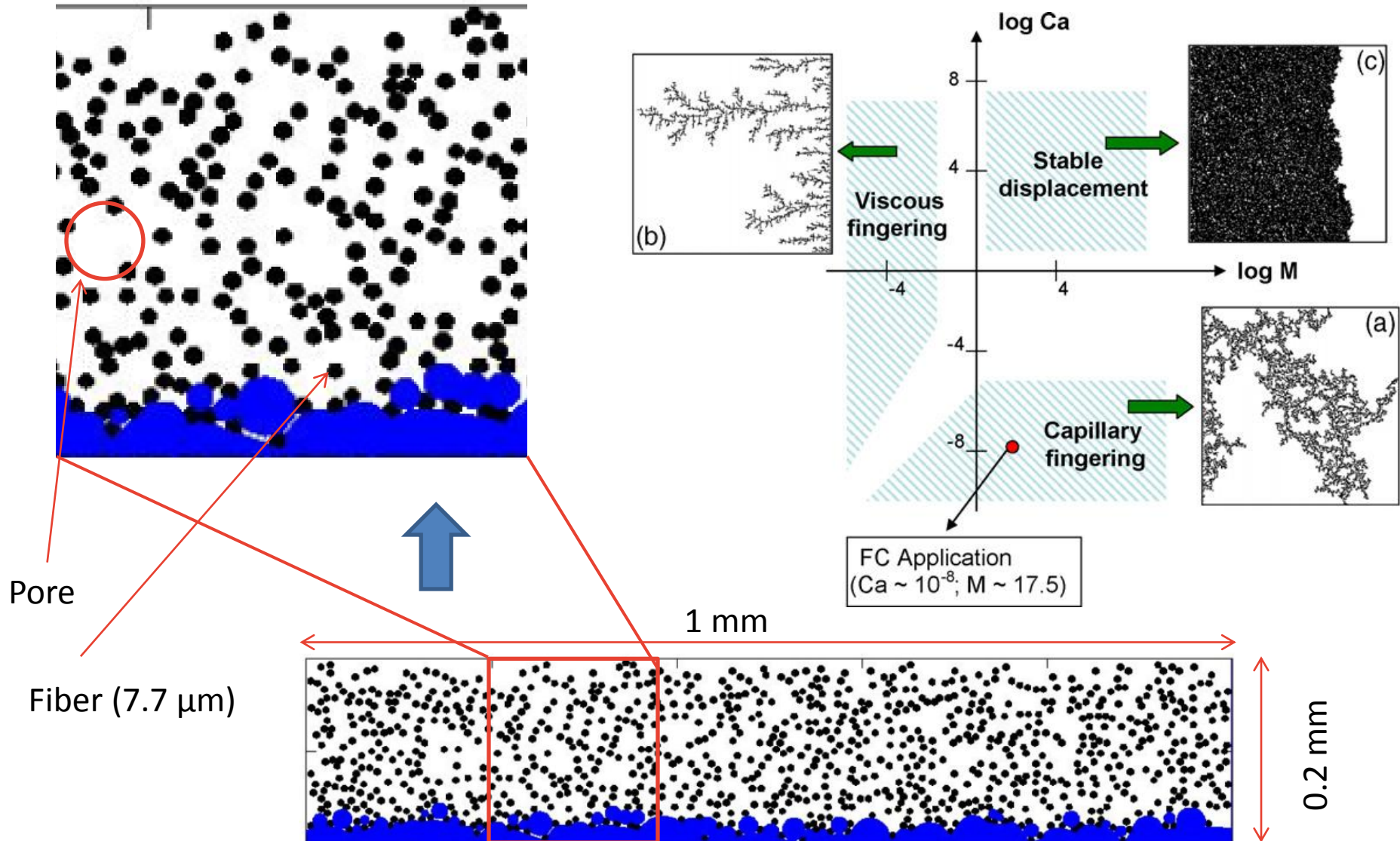


- PNMs track **water fronts** and **two-phase** interfaces by modeling each pore as a junction, and each throat as a resistor
- Combining Multiphase flow with transport is as easy as removing resistors from the network.
- Despite being 'pore-scale' this approach loses the details within a pore, like streamlines, mixing effects, velocity profiles
- PNMs cannot model transport processes with accuracy comparable to fancy approaches like finite-element analysis



Water invasion of a stochastic porous media

Figure from Sinha et al., *Electrochimica Acta*, 2007



Invasion percolation

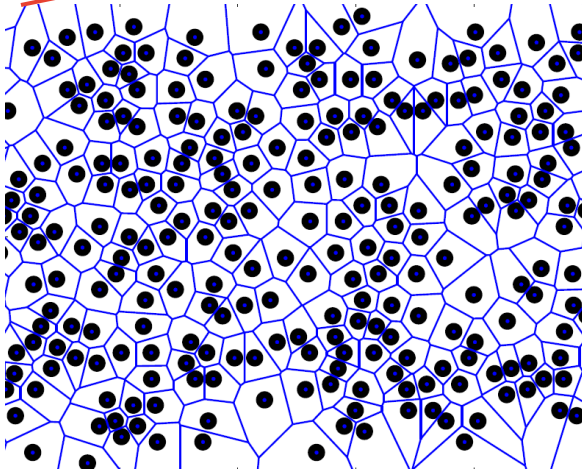
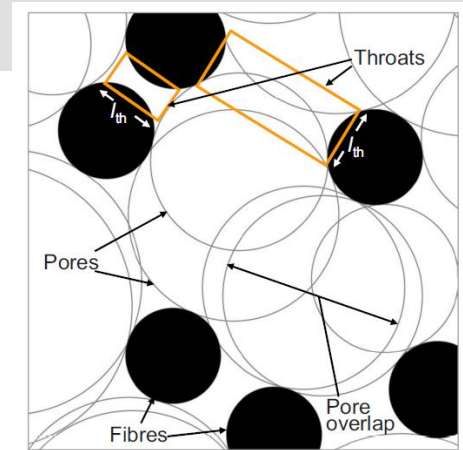
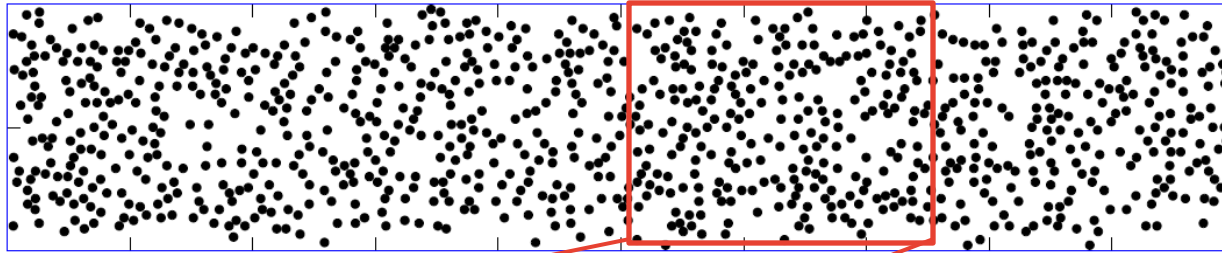
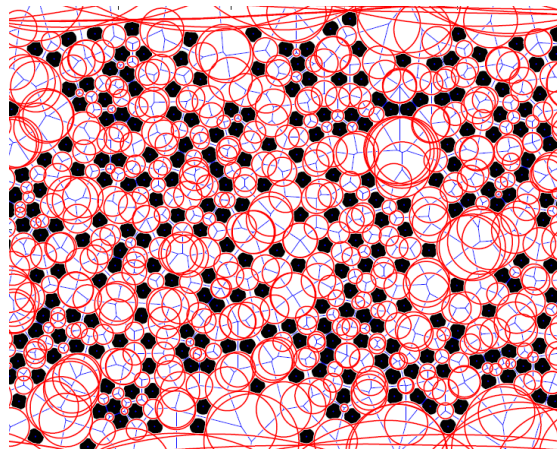
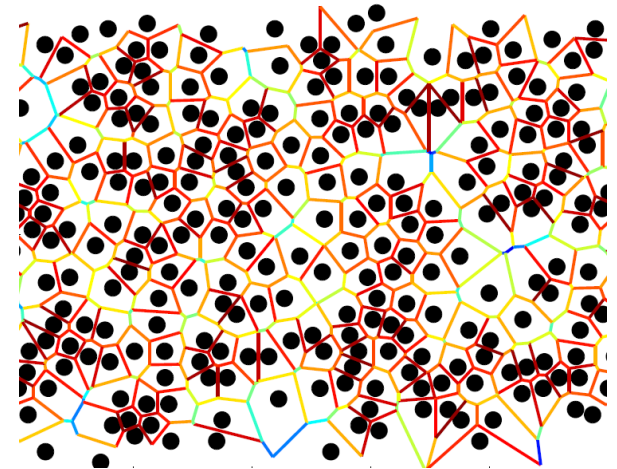


Diagram de Voronoi



Creation of pores



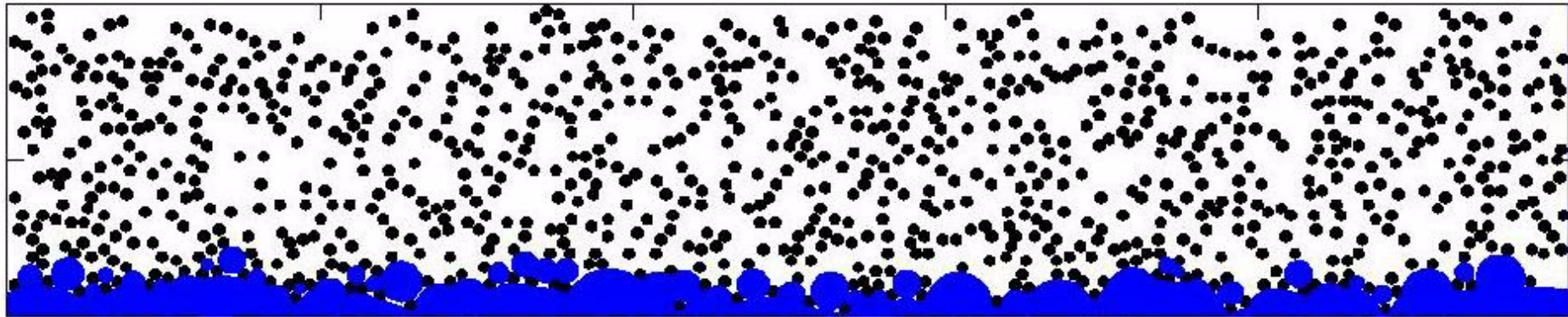
Weighting of the throats



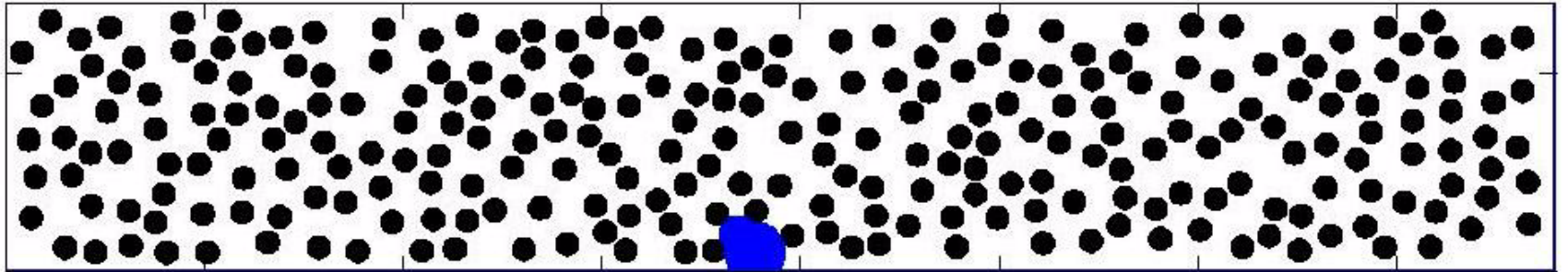
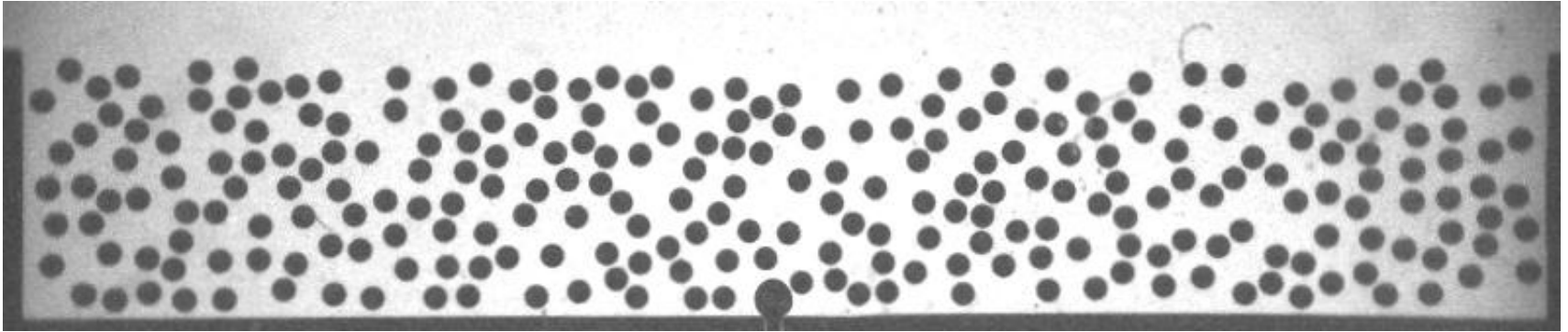
Invasion percolation

Wilkinson et al., 1983

Chapuis et al., 2008

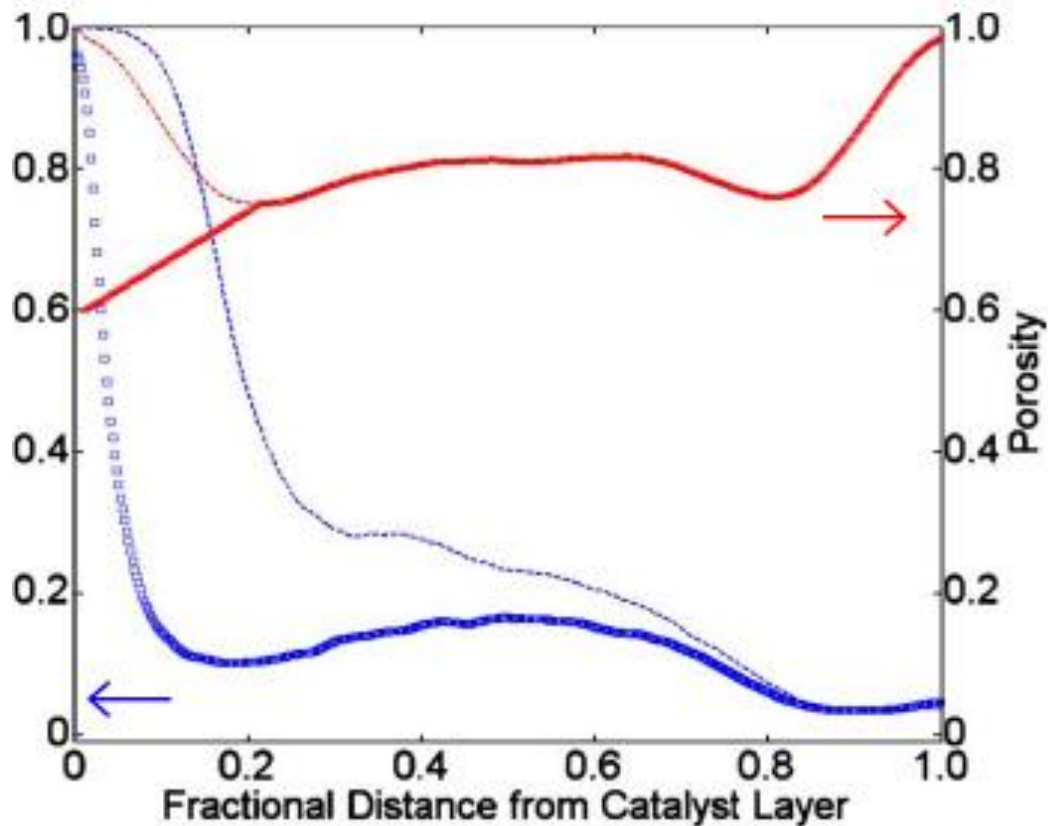


Invasion percolation



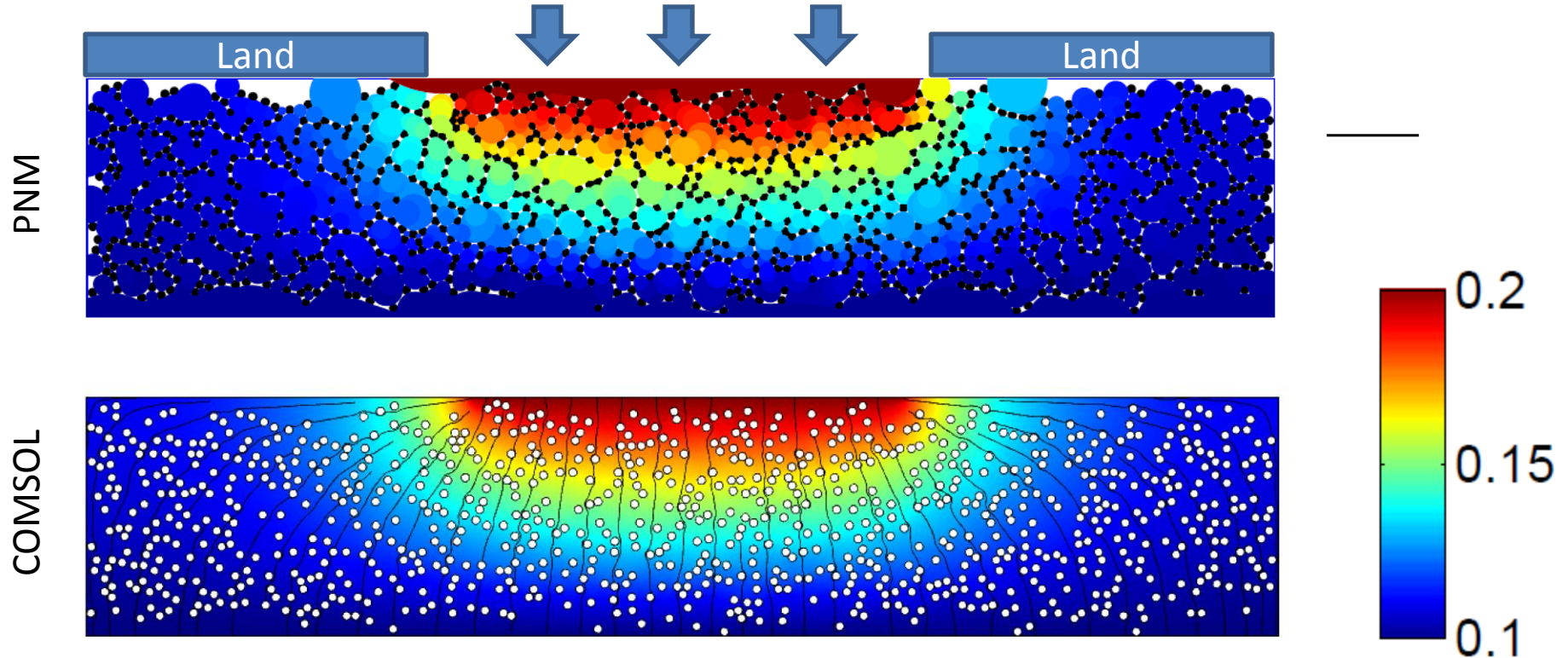
Results from 2D stochastic networks

Study of the correlation between the local porosity distribution of the saturation
- 100 simulations (600 x 200 μm) -



Solving Laplace equation

Transport Modelling: $(\vec{})$ \longrightarrow Characterisation of the effective properties



PNM Summary

PNM advantages:

- **Very fast resolution** compare to continuum models → high numbers of stochastic geometry can be studied
- Can handle **large geometry** with small pores

Issues:

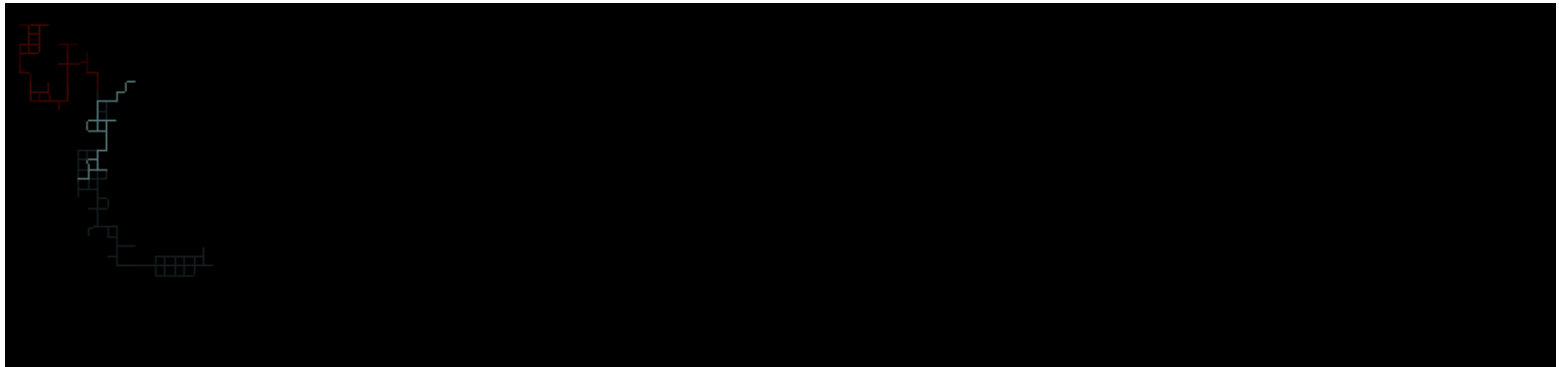
- Build the equivalent network

→ All this concept are embedded in the free software **OpenPNM**



Integration of all the PNM concepts in one open source software:

- 3D geometry
- Structured and unstructured network
- **Multiphysics**: invasion percolation and transport equations
- Python library



Main partners involve in OpenPNM framework:

- Mc Gill University (J. Gostick, Montreal)
- University of Toronto
- University of Leeds (UK)
- University of Jülich (Germany)
- American Fuel Cell Consortium



```

1 import OpenPNM
2 '==== Build Topological Network ====='
3 pn = OpenPNM.Network.Cubic(shape=[50,50,10],spacing=0.0001,name='net',loglevel=20)
4
5 '==== Build Geometry ====='
6 Ps = pn.pores('boundary',mode='not')
7 Ts = pn.find_neighbor_throats(pores=Ps,mode='intersection',flatten=True)
8 geom = OpenPNM.Geometry.Toray990(network=pn,pores=Ps,throats=Ts)
9
10 '==== Build Phases ====='
11 air = OpenPNM.Phases.Air(network=pn,name='air')
12 water = OpenPNM.Phases.Water(network=pn,name='water')
13
14 '==== Build Physics ====='
15 phys_water = OpenPNM.Physics.Standard(network=pn,phase=water,pores=pn.Ps,throats=pn.Ts)
16 phys_water.add_model(model=OpenPNM.Physics.models.capillary_pressure.washburn)
17 phys_air = OpenPNM.Physics.Standard(network=pn,phase=air,pores=pn.Ps,throats=pn.Ts)
18 phys_air.add_model(model=OpenPNM.Physics.models.diffusive_conductance.bulk_diffusion)
19
20 '==== Begin Simulations ====='
21 # Perform a Drainage Experiment (OrdinaryPercolation)
22 OP_1 = OpenPNM.Algorithms.OrdinaryPercolation(network=pn,invading_phase=water)
23 Ps = pn.pores(labels=['bottom_boundary'])
24 OP_1.run(inlets=Ps)
25 OP_1.update_results(Pc=7000)
26
27 '==== Perform Fickian Diffusion ====='
28 alg = OpenPNM.Algorithms.FickianDiffusion(loglevel=20, network=pn,phase=air)
29 # Assign Dirichlet boundary conditions to top and bottom surface pores
30 BC1_pores = pn.pores('top_boundary')
31 alg.set_boundary_conditions(bctype='Dirichlet', bcvalue=0.6, pores=BC1_pores)
32 BC2_pores = pn.pores('bottom_boundary')
33 alg.set_boundary_conditions(bctype='Dirichlet', bcvalue=0.4, pores=BC2_pores)
34 #Add new model to air's physics that accounts for water occupancy
35 phys_air.add_model(model=OpenPNM.Physics.models.multiphase.conduit_conductance)
36 propname='throat.conduit_diffusive_conductance'
37 throat_conductance='throat.diffusive_conductance')
38 #Use newly defined diffusive conductance in the diffusion calculation
39 alg.run(conductance='throat.diffusive_conductance')
40 alg.update_results()
41 Deff = alg.calc_eff_diffusivity()
42

```

OpenPNM

03_PoreNetworkModelling
01_OpenPNM
03_OpenPNM...aster_version
OpenPNM

Raccourcis

Récents
Dossier personnel
Bureau
Documents
Images
Musique
Téléchargements
Vidéos
Corbeille
Périphériques
XP
Ordinateur
Signets
PostDoc
Dropbox
Réseau
Parcourir le réseau
Connexion à un se...

Figures

Nom

Taille

Type

Dernière modification

Algorithms
12 éléments
Dossier
21 oct.

Base
4 éléments
Dossier
15 oct.

Geometry
11 éléments
Dossier
15 oct.

Materials
3 éléments
Dossier
30 sept.

Network
9 éléments
Dossier
15 oct.

Phases
8 éléments
Dossier
15 oct.

Physics
6 éléments
Dossier
15 oct.

models
8 éléments
Dossier
27 oct.

__pycache__
7 éléments
Dossier
27 oct.

capillary_pressure.py
3,6 ko
Texte
29 sept.

diffusive_conductance.py
3,3 ko
Texte
23 oct.

electrical_conductance.py
1,9 ko
Texte
29 sept.

hydraulic_conductance.py
3,1 ko
Texte
23 oct.

__init__.py
537 octets
Texte
29 sept.

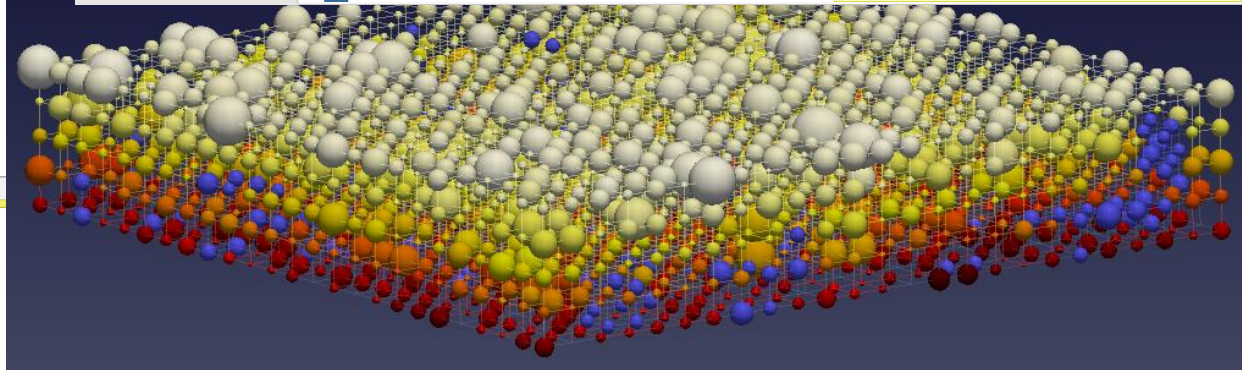
multiphase.py
4,4 ko
Texte
29 sept.

thermal_conductance.py
2,0 ko
Texte
29 sept.

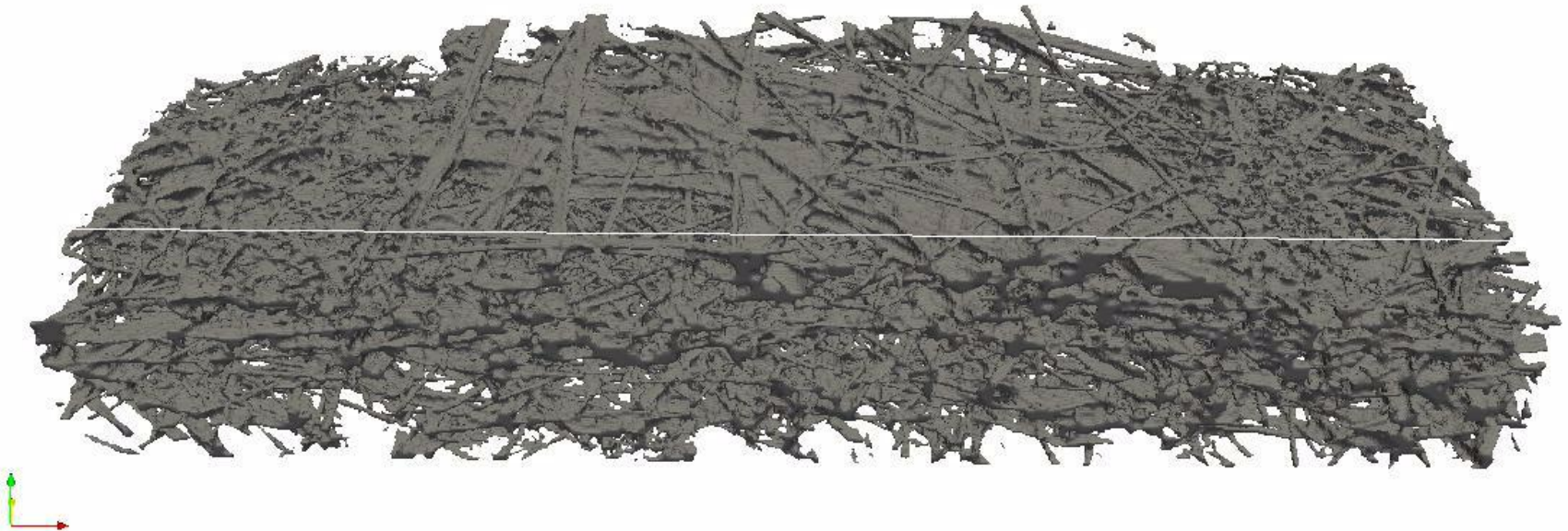
__pycache__
4 éléments
Dossier
15 oct.

__GenericPhysics__.py
4,5 ko
Texte
29 sept.

__init__.py
9 « Phases » sélectionné (contenant 8 éléments)



3D invasion percolation



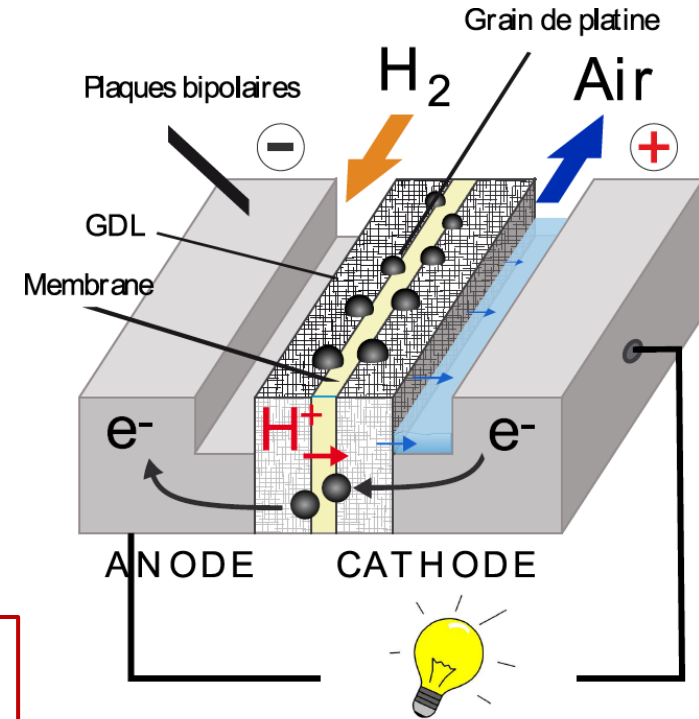
Characterisation of GDL oxygen effective diffusivity

Fuel cell **performance** and **oxygen diffusivity**:

— (At one given voltage)

Ex-situ GDL characterization in four steps:

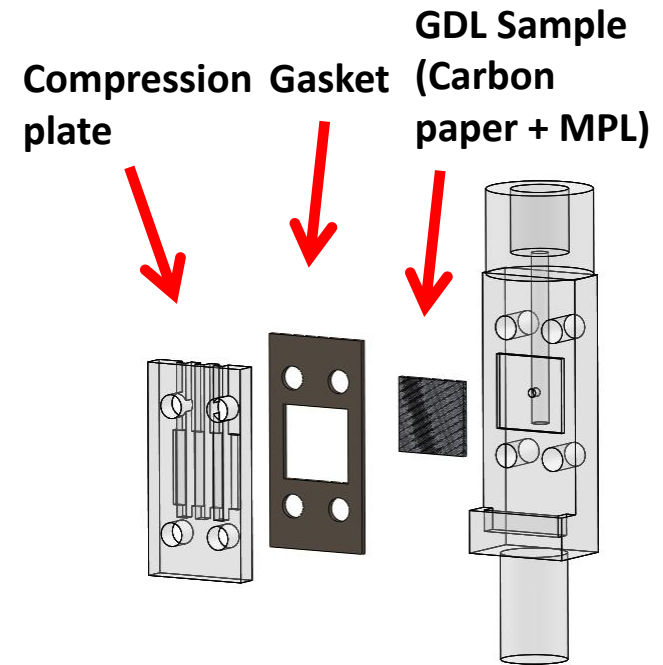
1. 3D scans of compressed GDL
2. Segmentation
3. Extraction of the equivalent network
4. Modeling of the gas transport



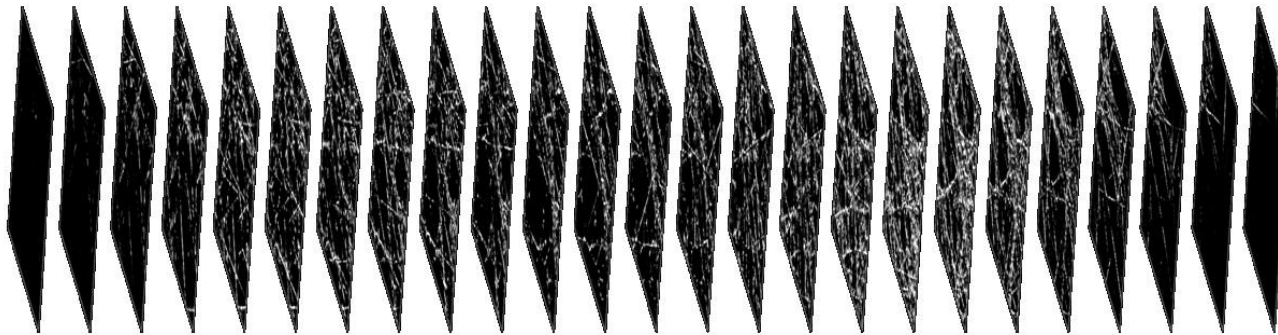
Micro-compute tomography



- System: Skyscan 1172.
- 11 mega-pixels X-Ray camera.
- Up to 8000 pixels x 8000 pixels in every slice.
- Down to 0.7 μm detail detectability.
- Achievable spatial resolution of 5 μm .



Compressed GDL (25%)



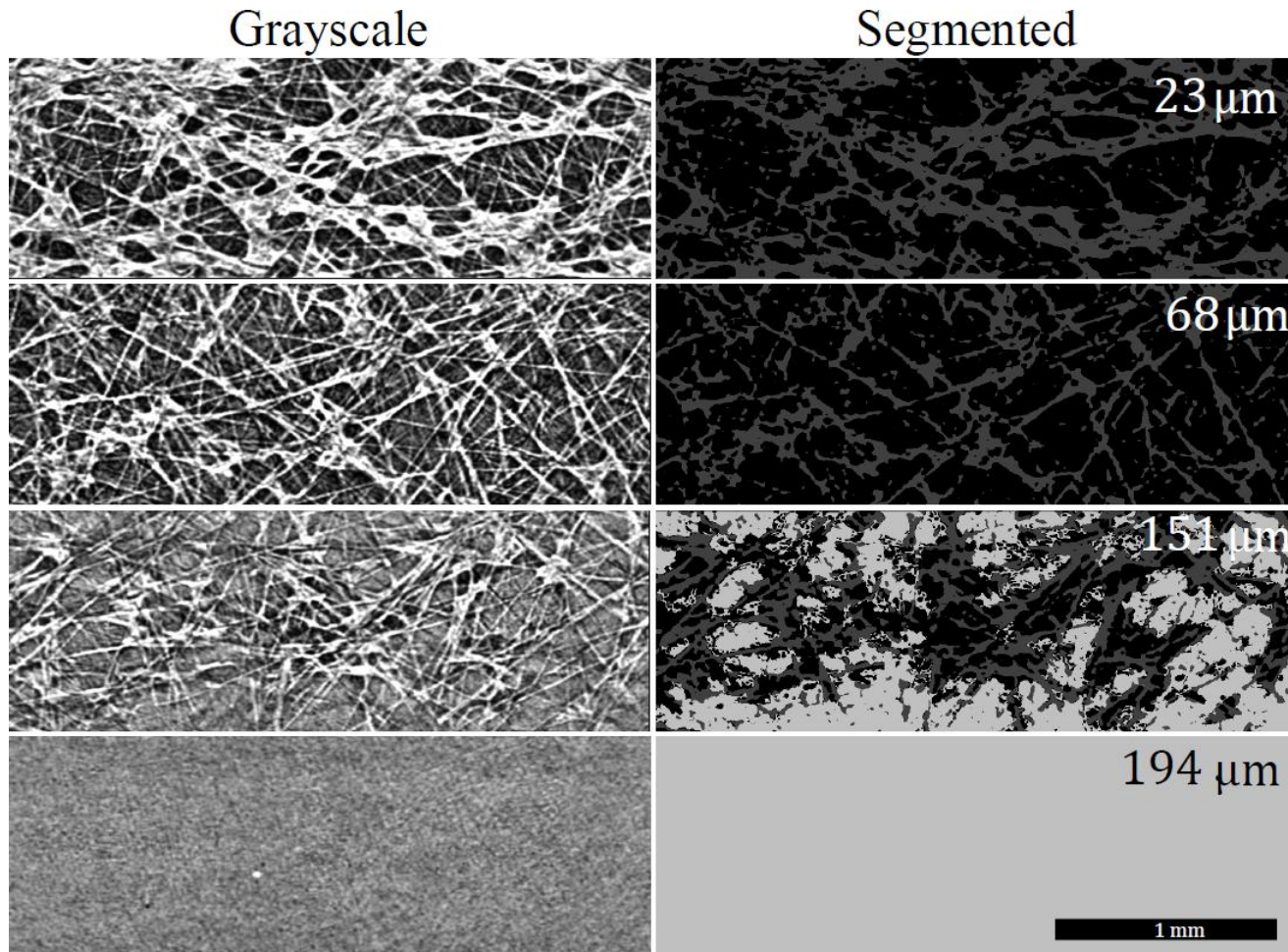
Series of in-plane
GDL slices



Grayscale image segmentation

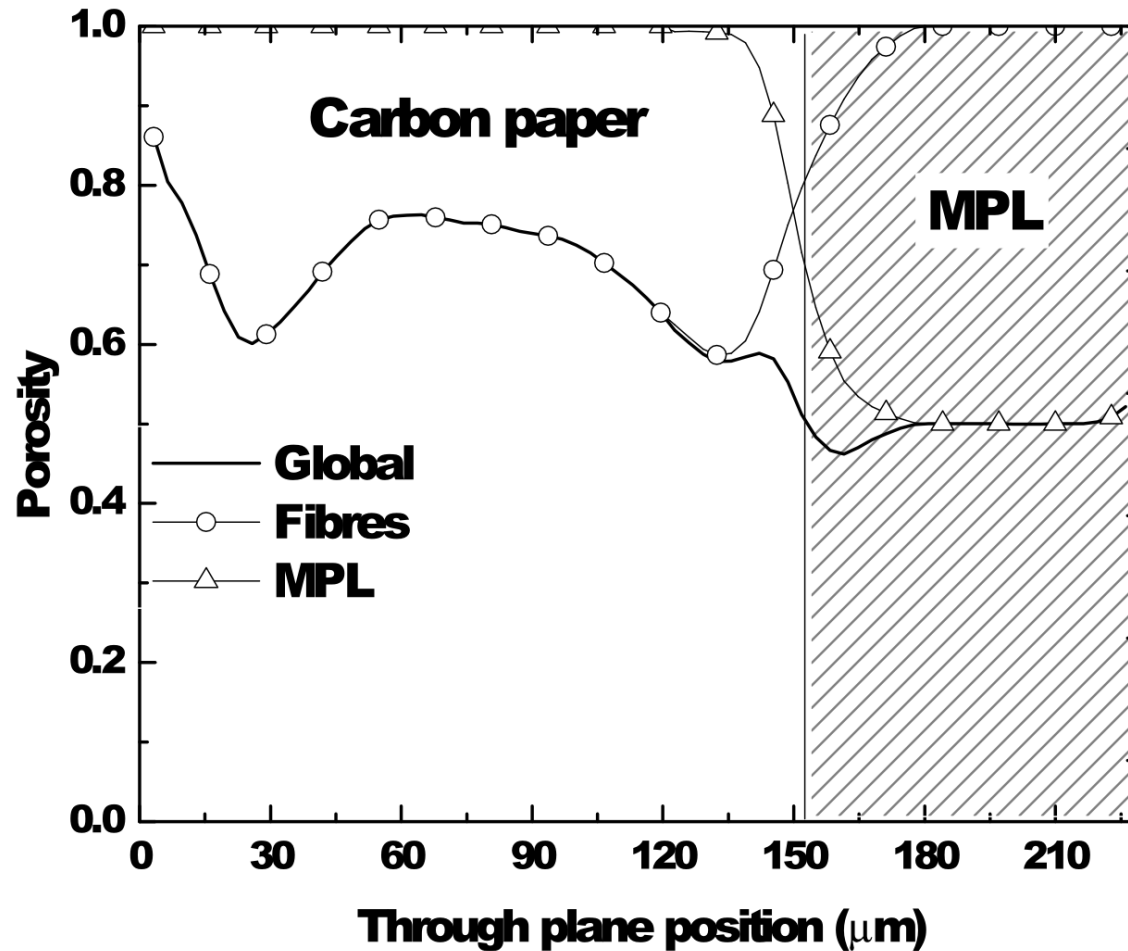
Thresholding of 3 phases:

1. Void (black)
2. Fibers (bright)
3. MPL (light gray)



Through plan porosity distribution

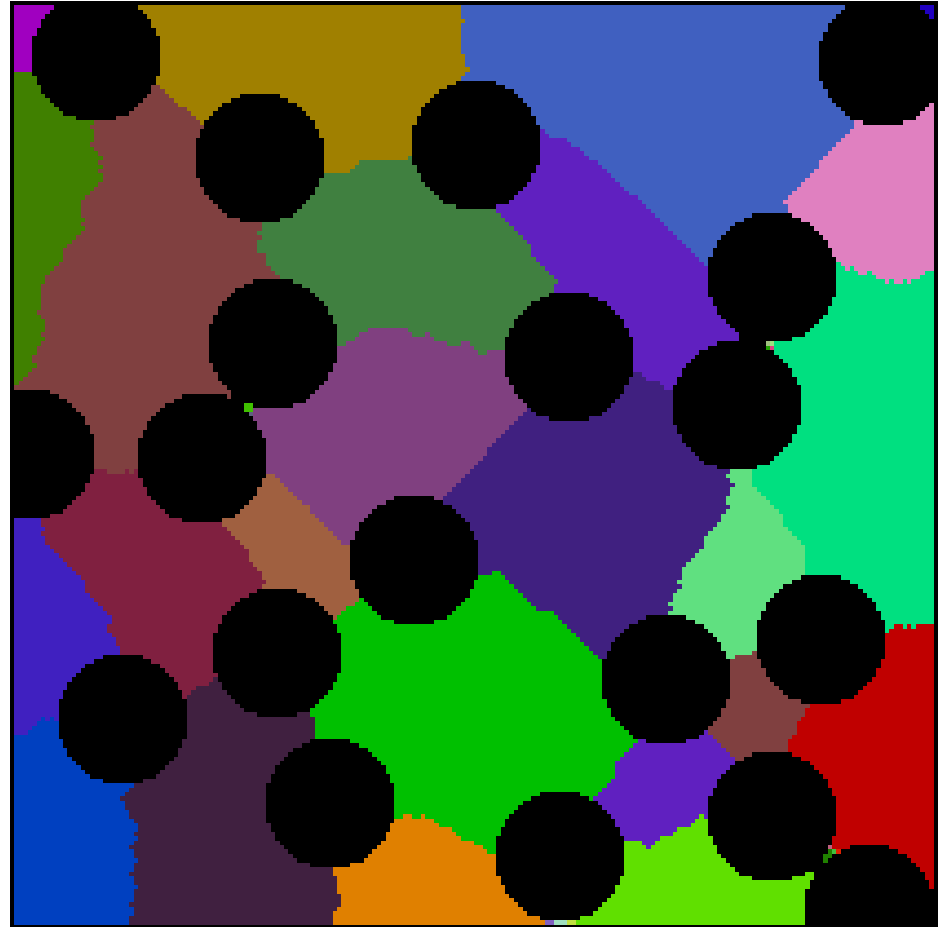
From the segmented images, the porosity of each slices is computed as:



Extraction of the equivalent pore network

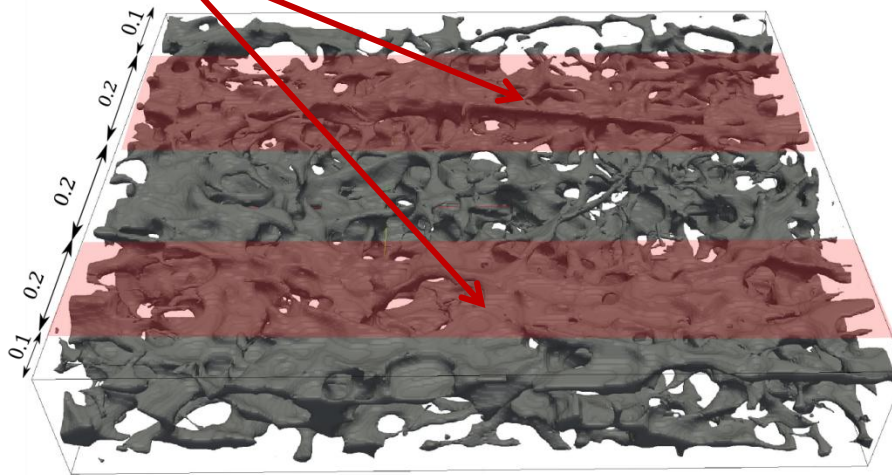
In house C++ code extracts the pores

- Pore volume
- Pore surface
- Pore hydraulic diameter
- Throat diameters
- Throat length (based on the adjacent fiber diameters)

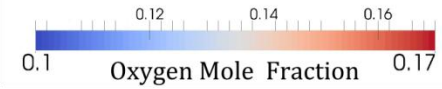


Effective diffusivity characterization via OpenPNM

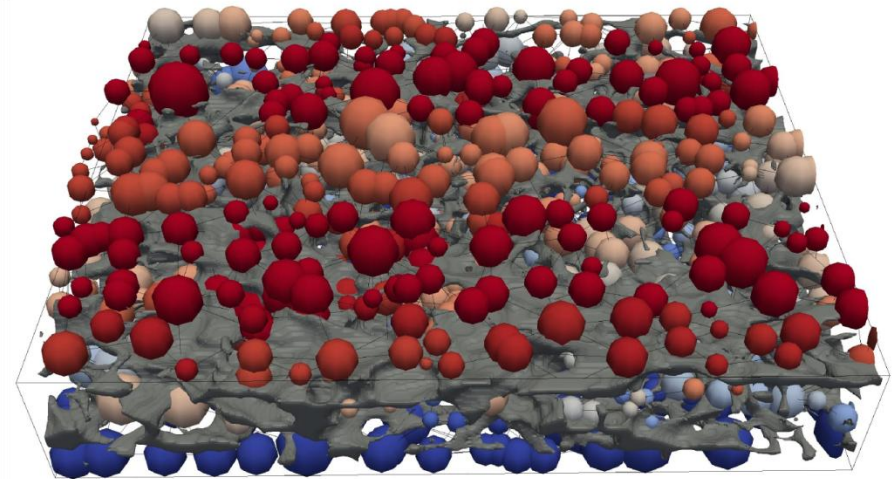
Inlets



(a)

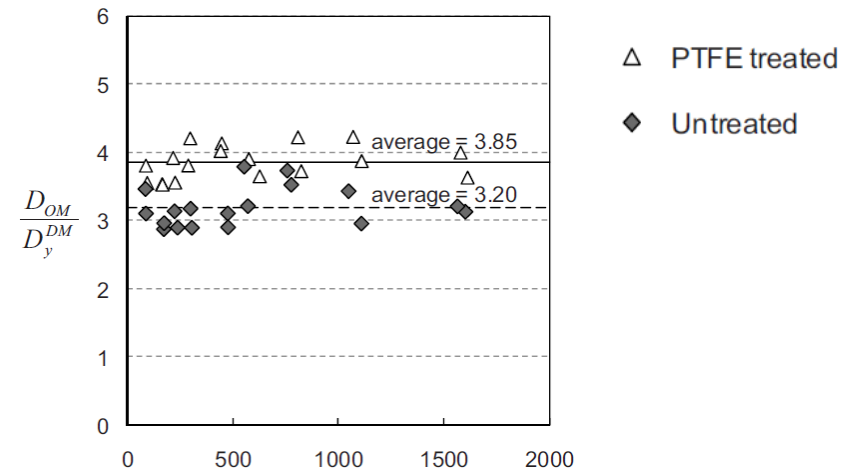


(b)



Results

Toray 060, 5% PTFE:

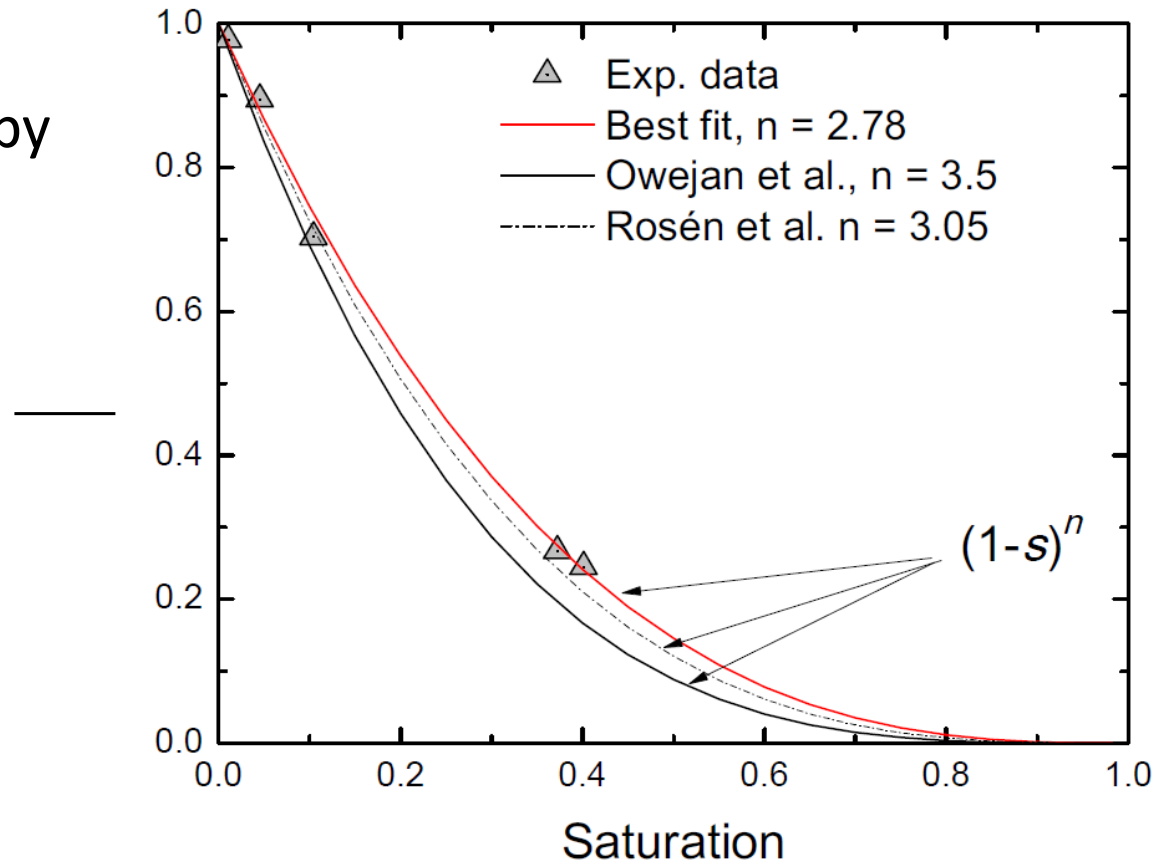


In-situ experimental measures by Baker et al., 2009



Coupling Pore Network and In-situ visualization technic

- X-rays imaging
- Impedance spectroscopy
- PNM

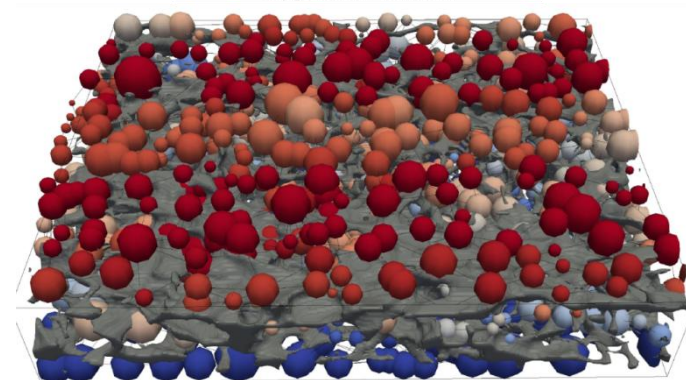
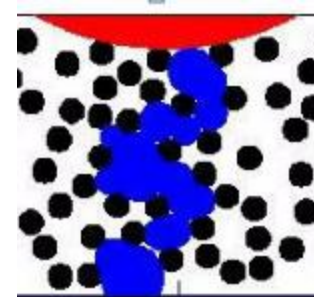
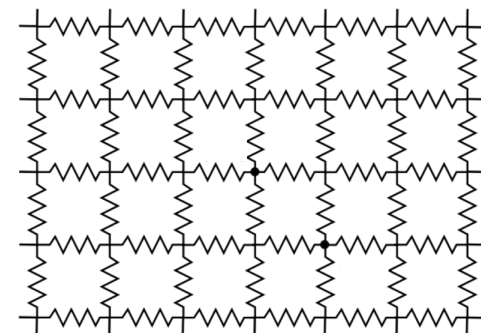


Characterization of the GDL oxygen diffusivity at liquid water different saturation



Summary

- ✓ Porous material can be view as **resistor network**
- ✓ **Multiphasic modeling** in fingering regime can be achieved via **Invasion Percolation algorithm** on pore network handle realistic result
- ✓ **OpenPNM** is opensource package for 3D multiphasic modelling and porous material characterization
- ✓ Ex-situ **characterization of oxygen diffusivity** compressed GDL



(b)



Thank You.



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