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

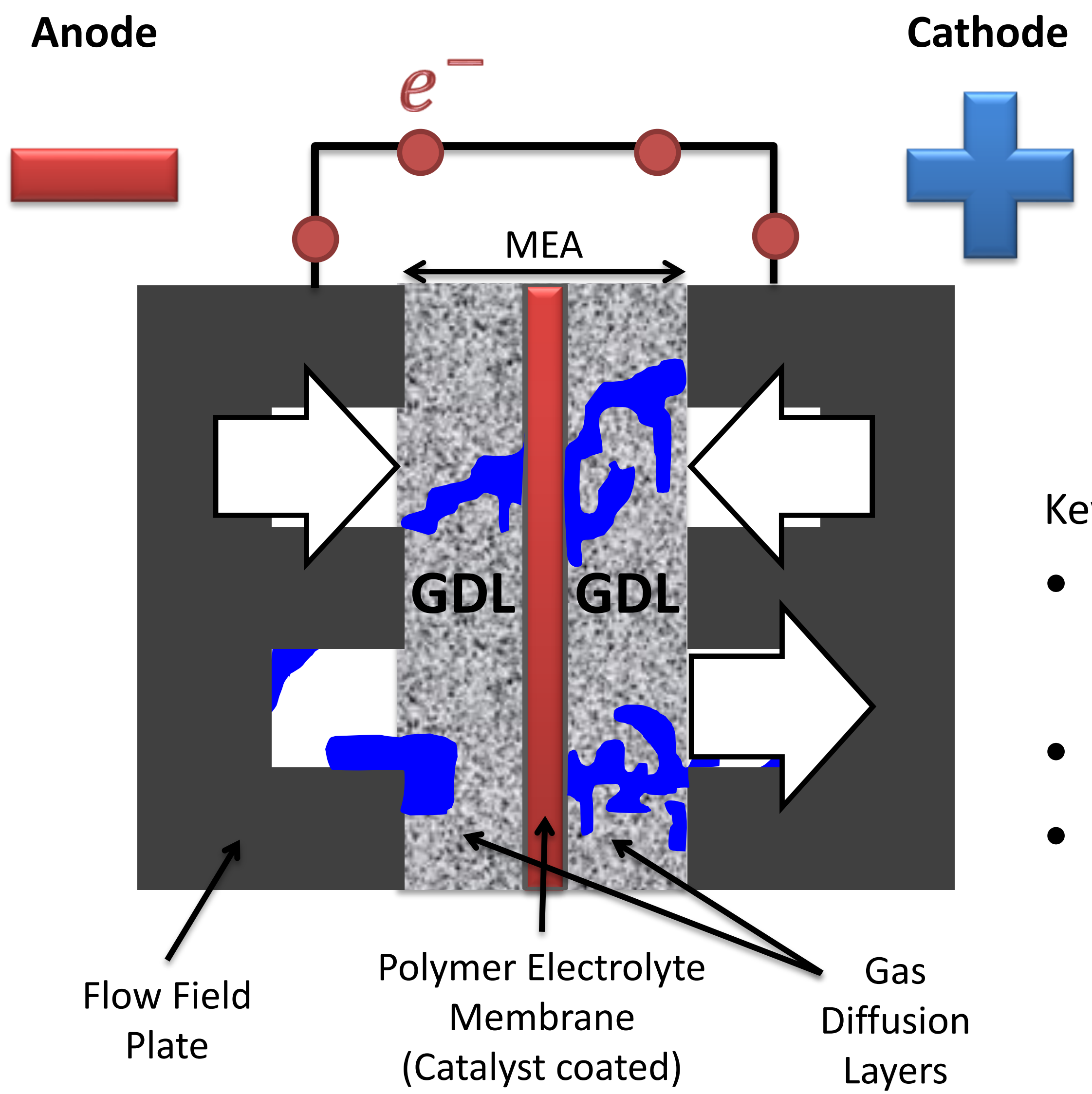
Stéphane Chevalier
Thermofluids for Energy and Advanced Materials (TEAM) Laboratory
Department of Mechanical and Industrial Engineering
University of Toronto

Laboratoire de thermocinétique de Nantes

December 15th, 2014

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

Fuel cell technology



Anode:

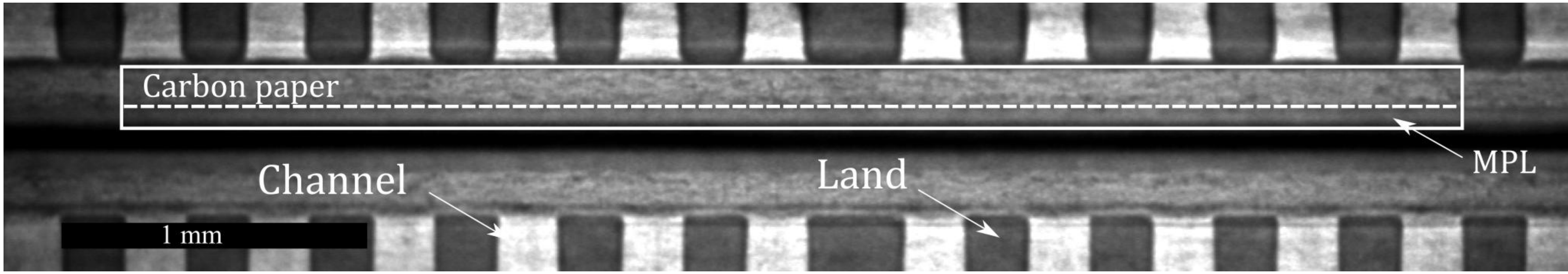
Cathode:

–

Key role playing by the GDL:

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

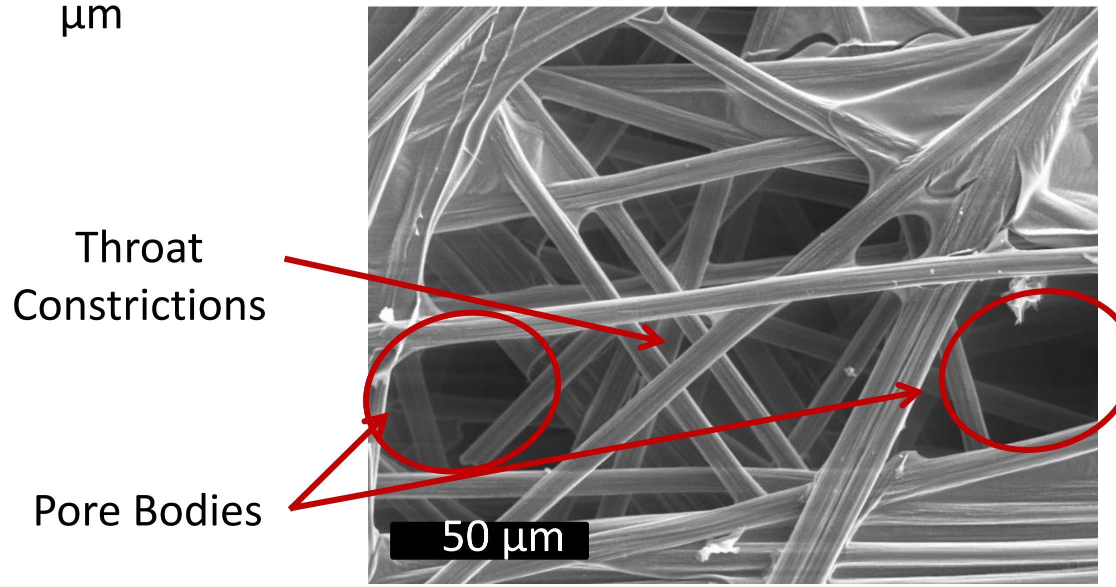
The Gas Diffusion Layer



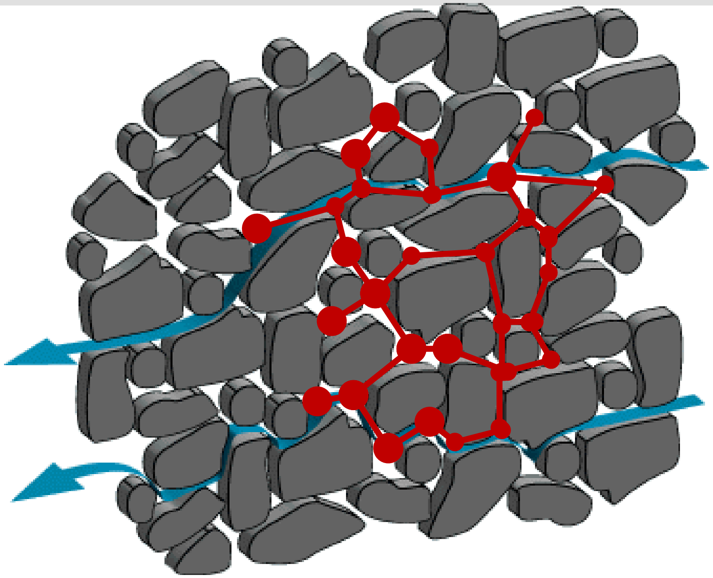
Composed of two porous materials:

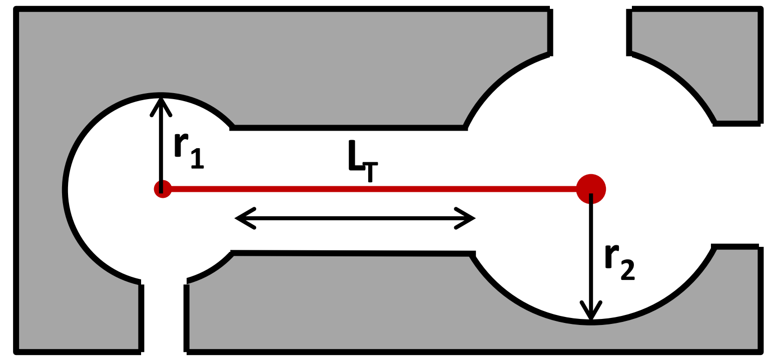
- Carbon fibers, mean pore size µm
- MPL mean pore size nm

What is the optimal design?
➔ Porosity distribution
➔ The mean size pore



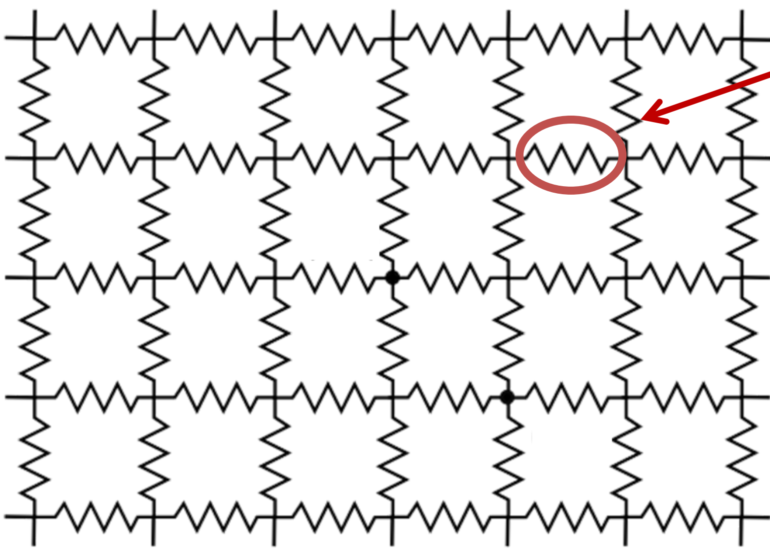
Pore network





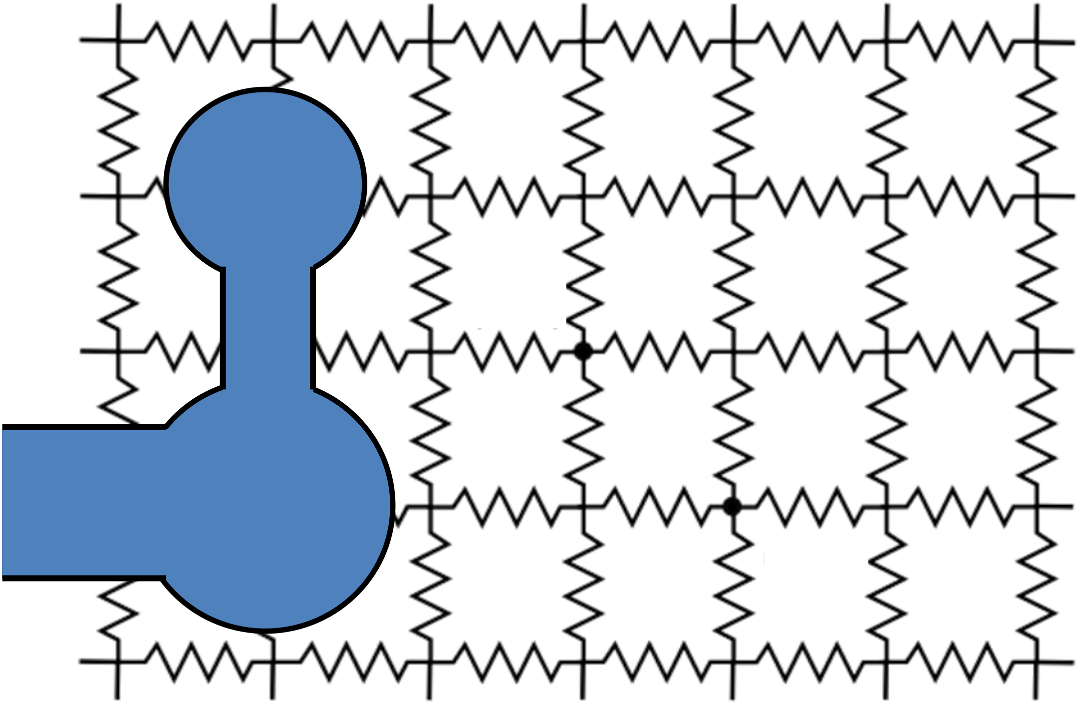
$$Q = \frac{\pi r^4}{8 \mu L} \Delta P_{12}$$

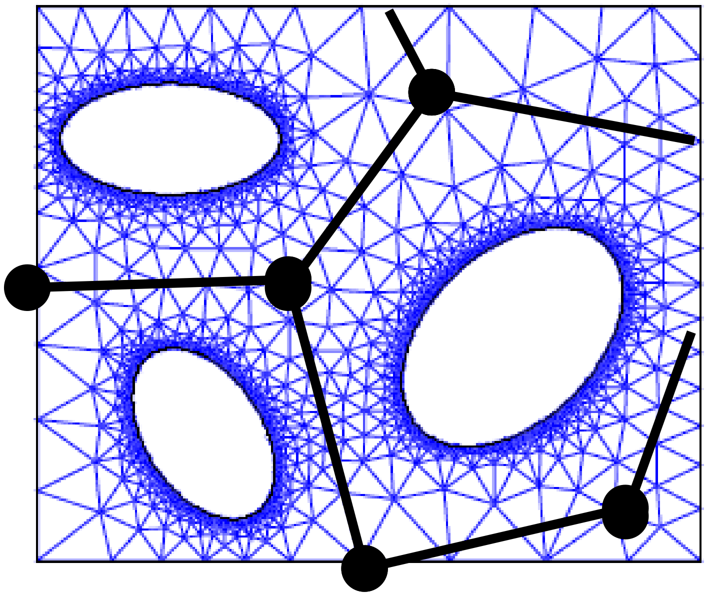
$$P_C = \frac{-2\sigma \cos\theta}{r_T}$$



Figures from J. Gostik

Pore network modelling versus continuum modelling



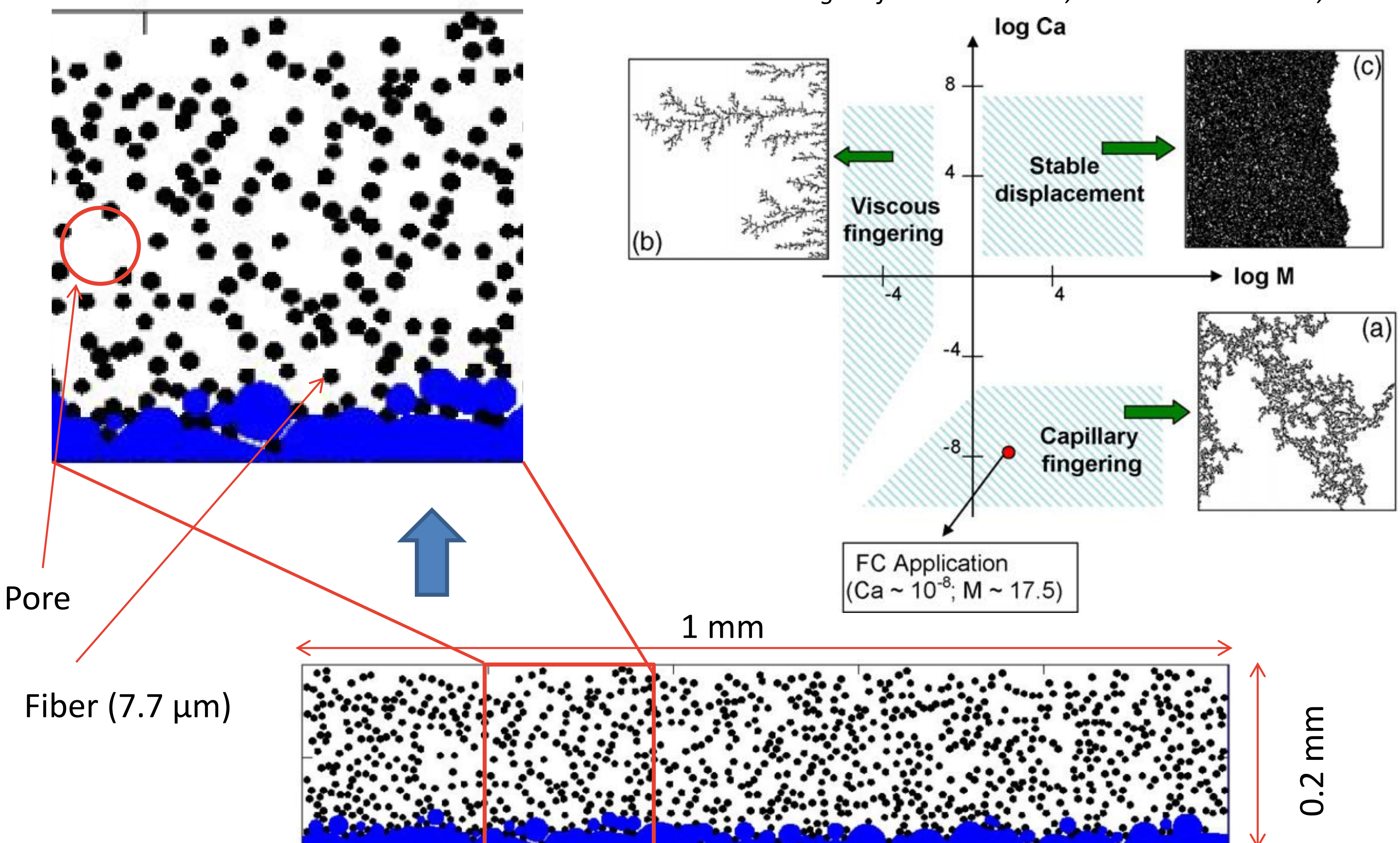


- PNMs track **water fronts** and **two-phase** interfaces by modeling each pore as a junction, and each throat as a resistor
- Combining Multiphase flow with transport is as easy as removing resistors from the network.

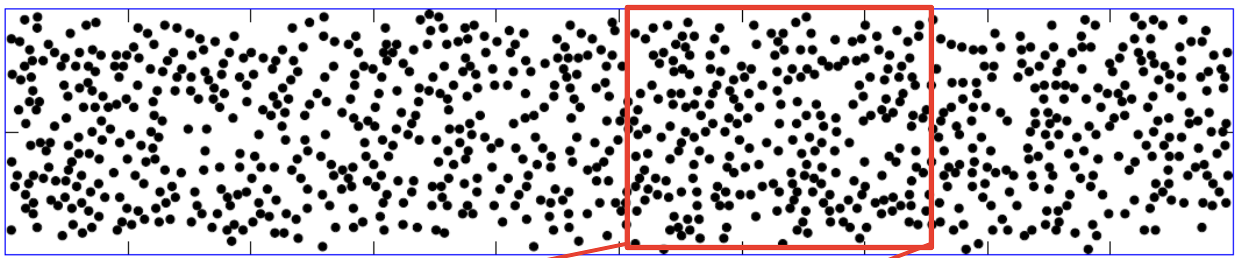
- Despite being 'pore-scale' this approach loses the details within a pore, like streamlines, mixing effects, velocity profiles
- PNMs cannot model transport processes with accuracy comparable to fancy approaches like finite-element analysis

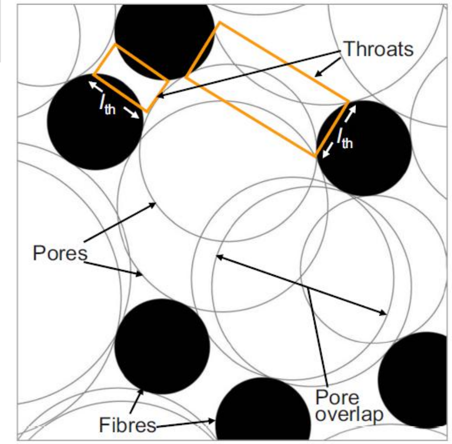
Water invasion of a stochastic porous media

Figure from Sinha et al., Electrochemica Acta, 2007



Invasion percolation





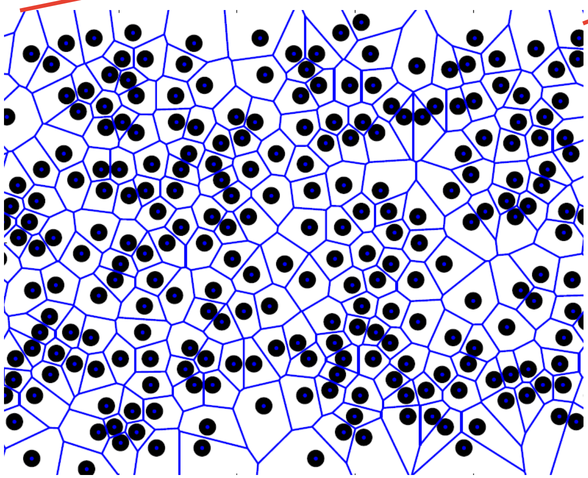
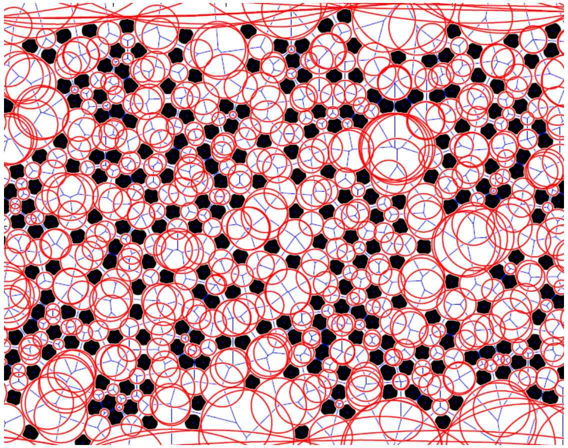
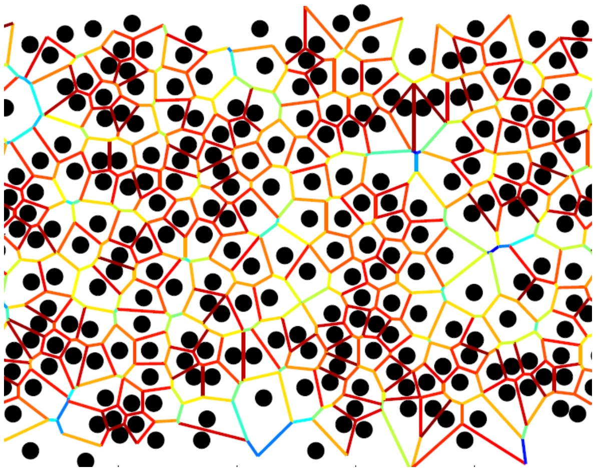


Diagram de Voronoi



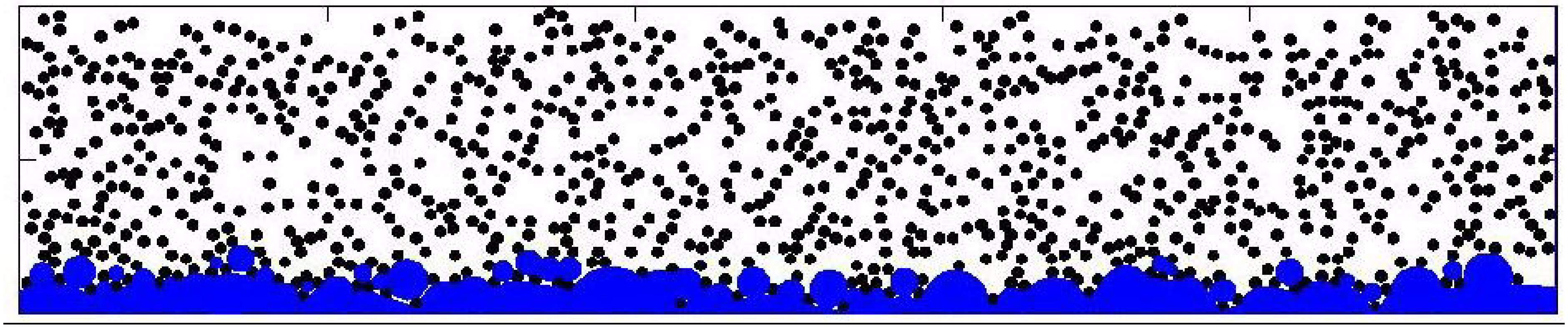
Creation of pores



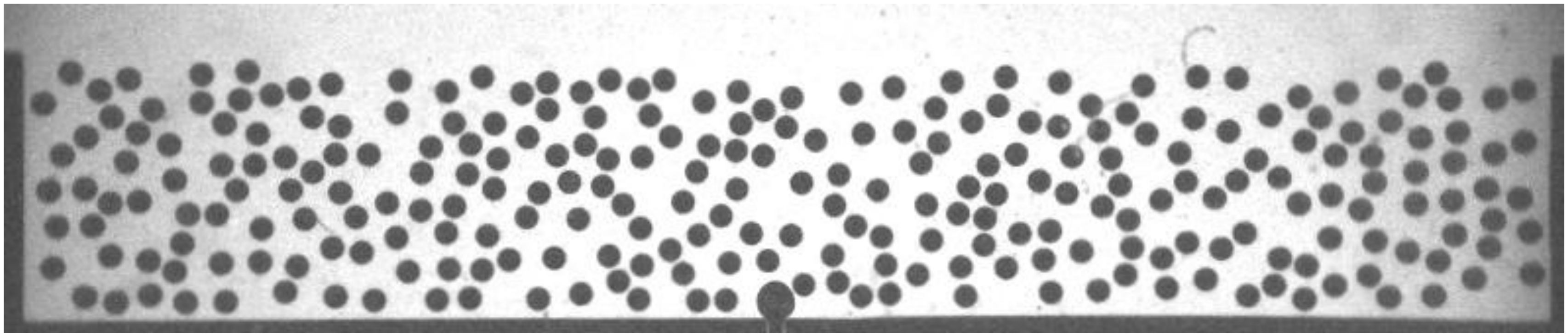
Weighting of the throats

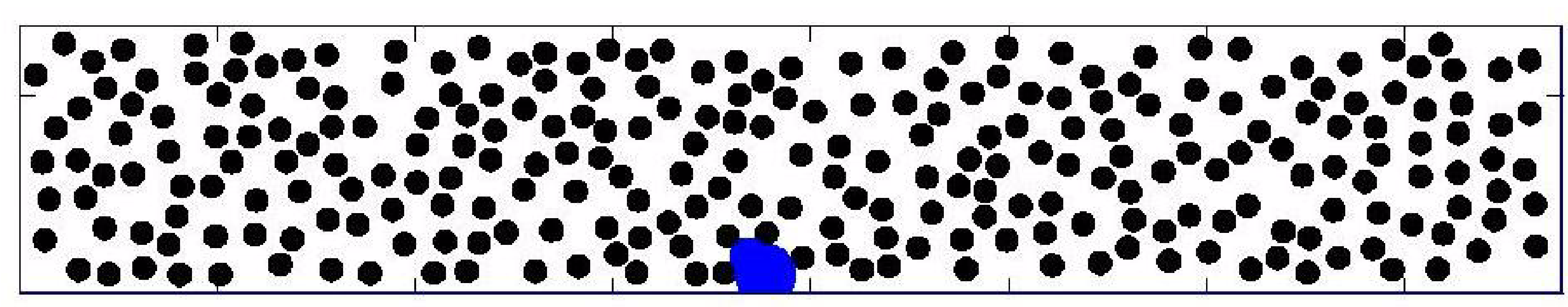
Invasion percolation

Wilkinson et al., 1983
Chapuis et al., 2008



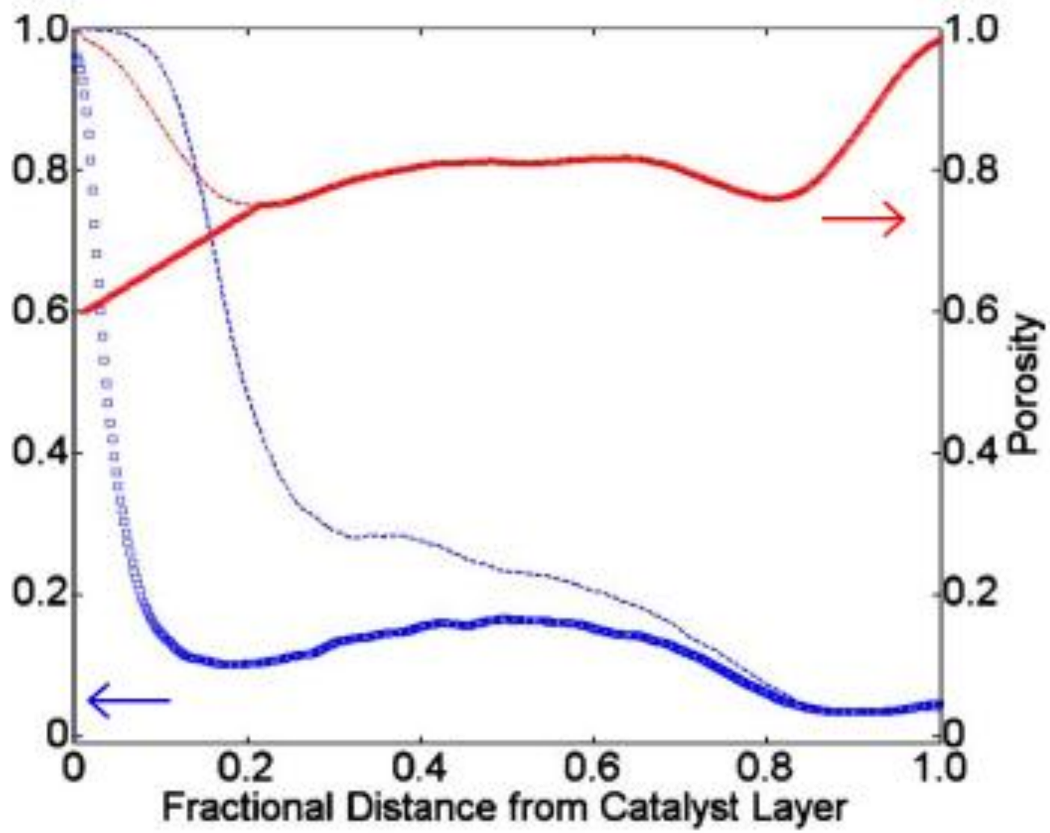
Invasion percolation





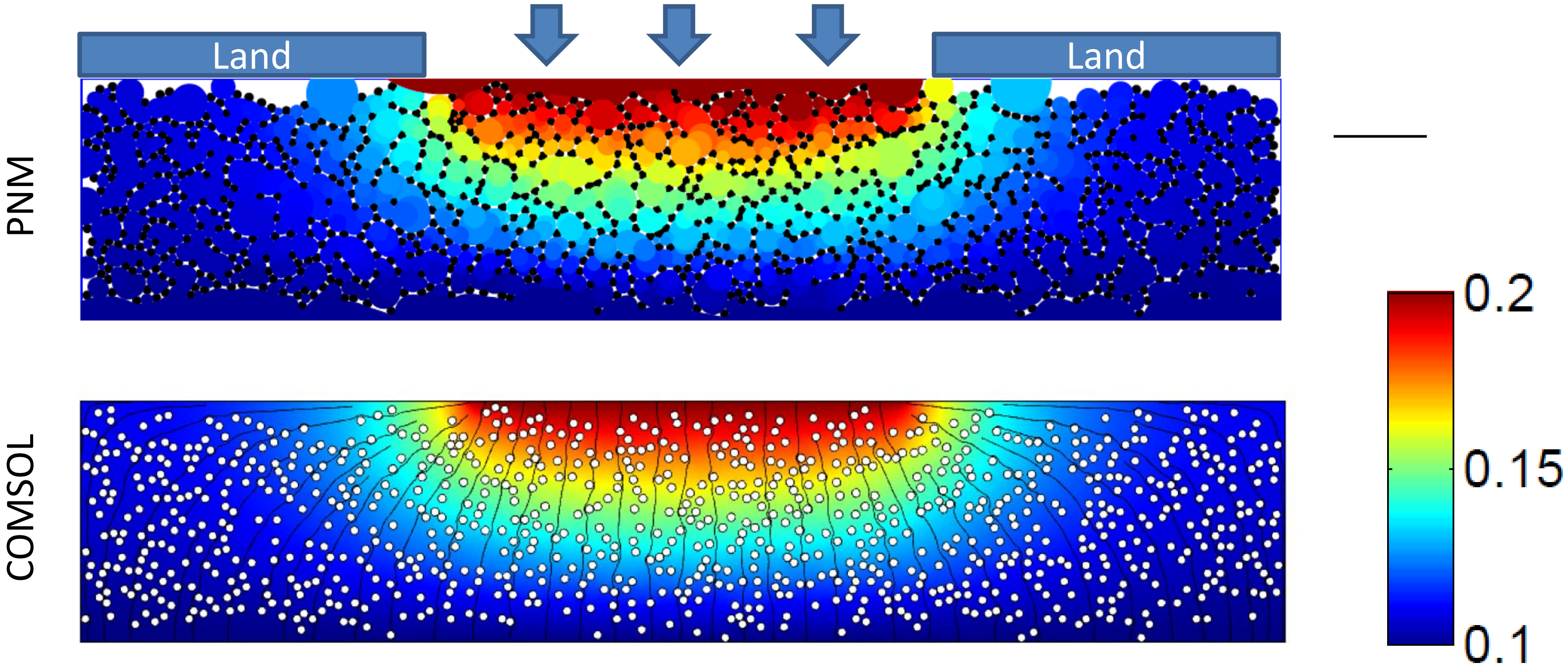
Results from 2D stochastic networks

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



Solving Laplace equation

Transport Modelling: (→) → Characterisation of the effectives 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**

OpenPNM

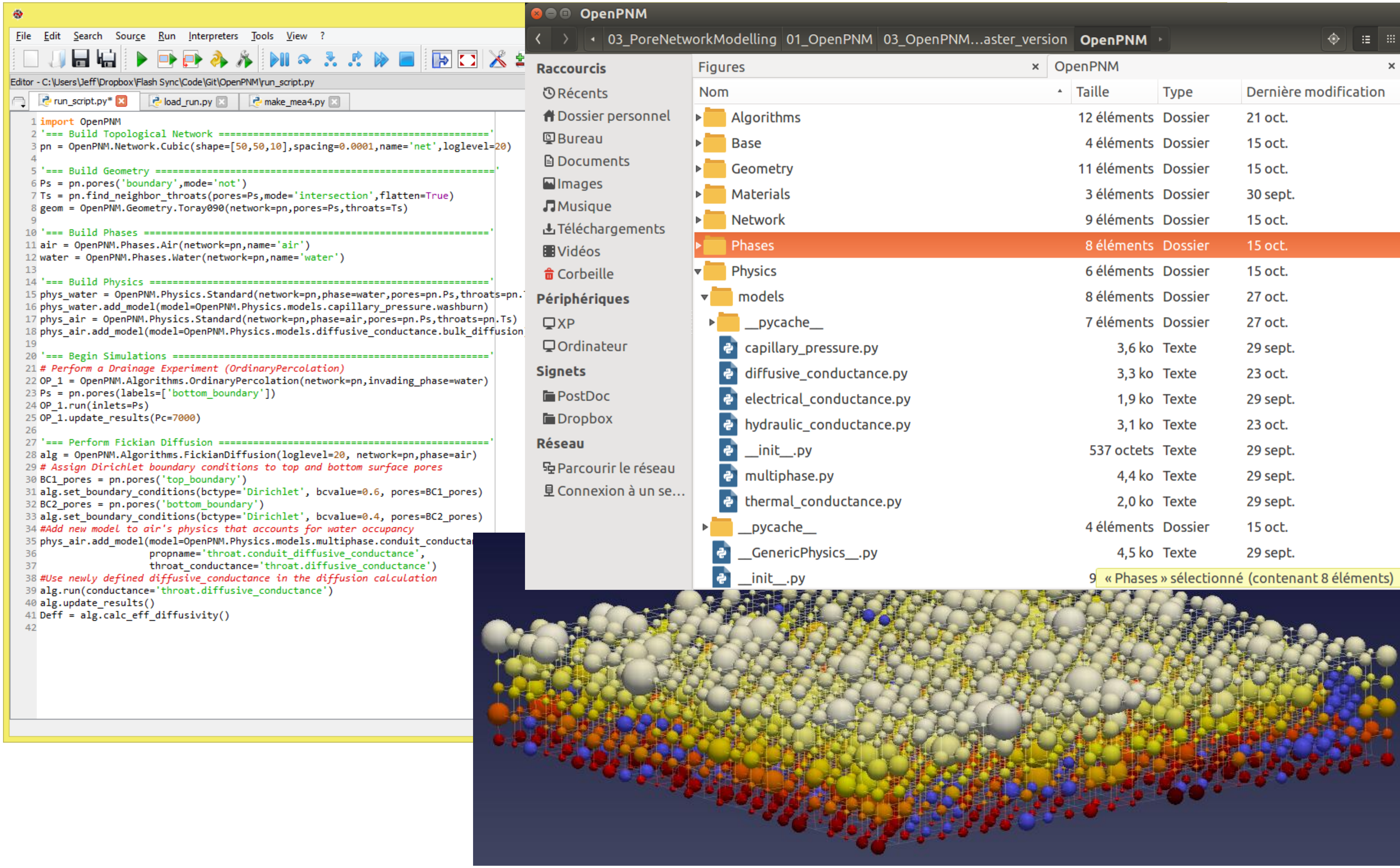
Integration of all the PNM concepts in one open source software:

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

Main partners involve in OpenPNM framework:

- Mc Guill University (J. Gostick, Monteral)
- University of Toronto
- University of Leeds (UK)
- University of Julich (Germany)
- American Fuel Cell Consortium

OpenPNM

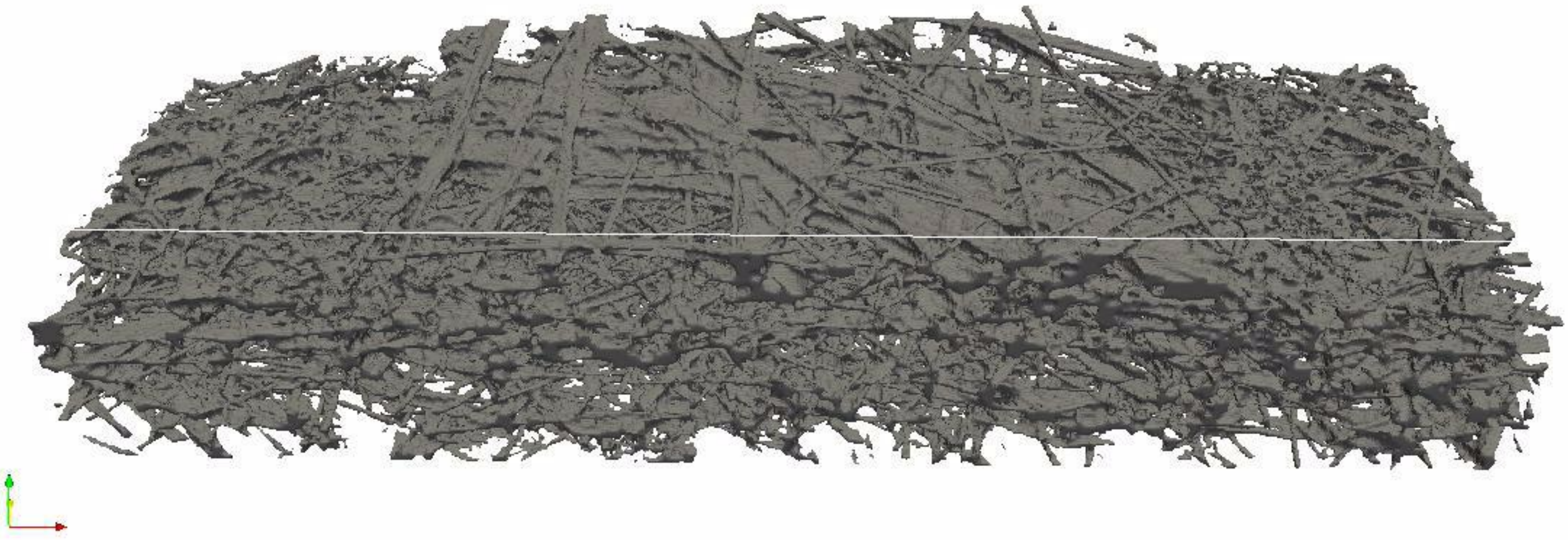


Thermofluids for Energy and
Advanced Materials Laboratory

Stéphane Chevalier
schevali@mie.utoronto.ca

UNIVERSITY OF TORONTO

3D invasion percolation

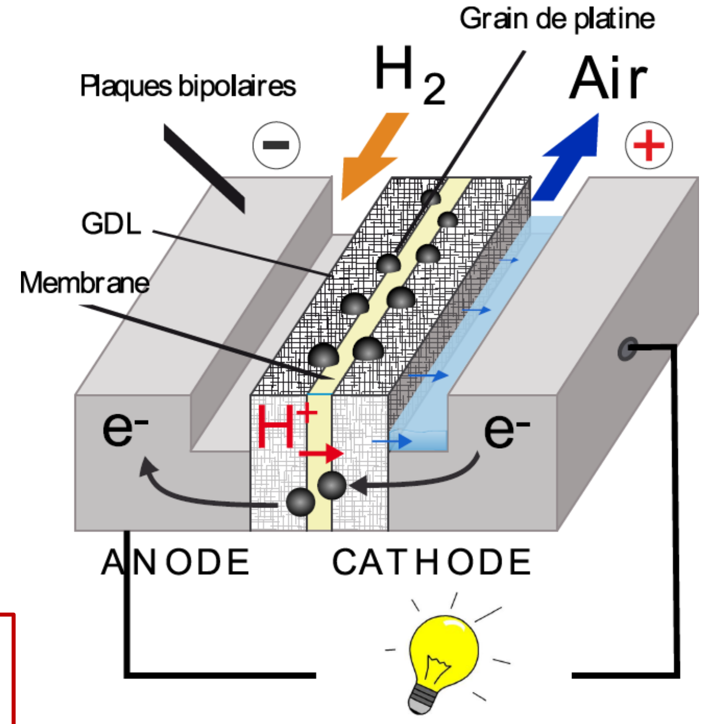


Stéphane Chevalier
schevali@mie.utoronto.ca

Characterisation of GDL oxygen effective diffusivity

Fuel cell performance and oxygen diffusivity:

— (At one given voltage)

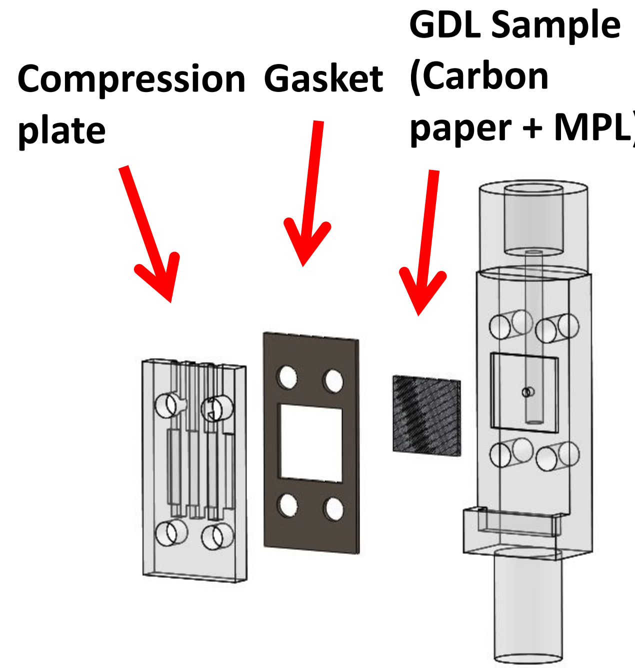


Ex-situ GDL characterization in four steps:

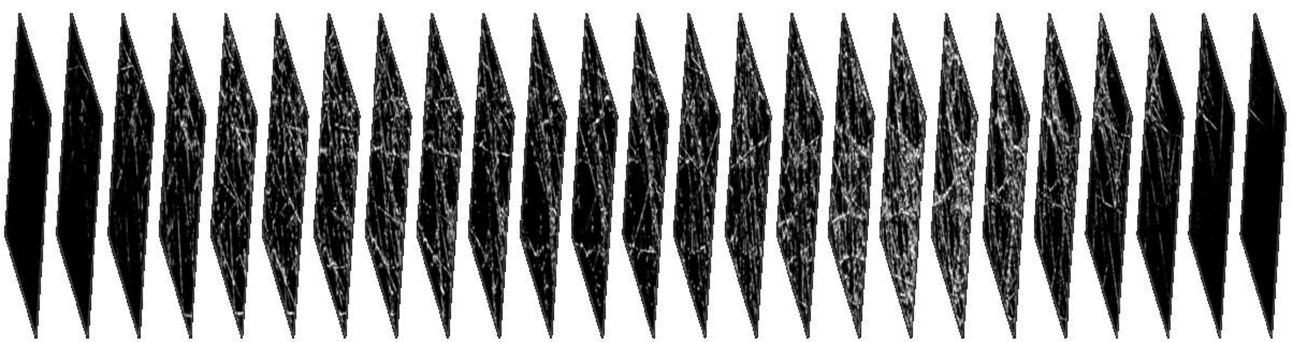
1. 3D scans of compressed GDL
2. Segmentation
3. Extraction of the equivalent network
4. Modeling of the gas transport

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%)

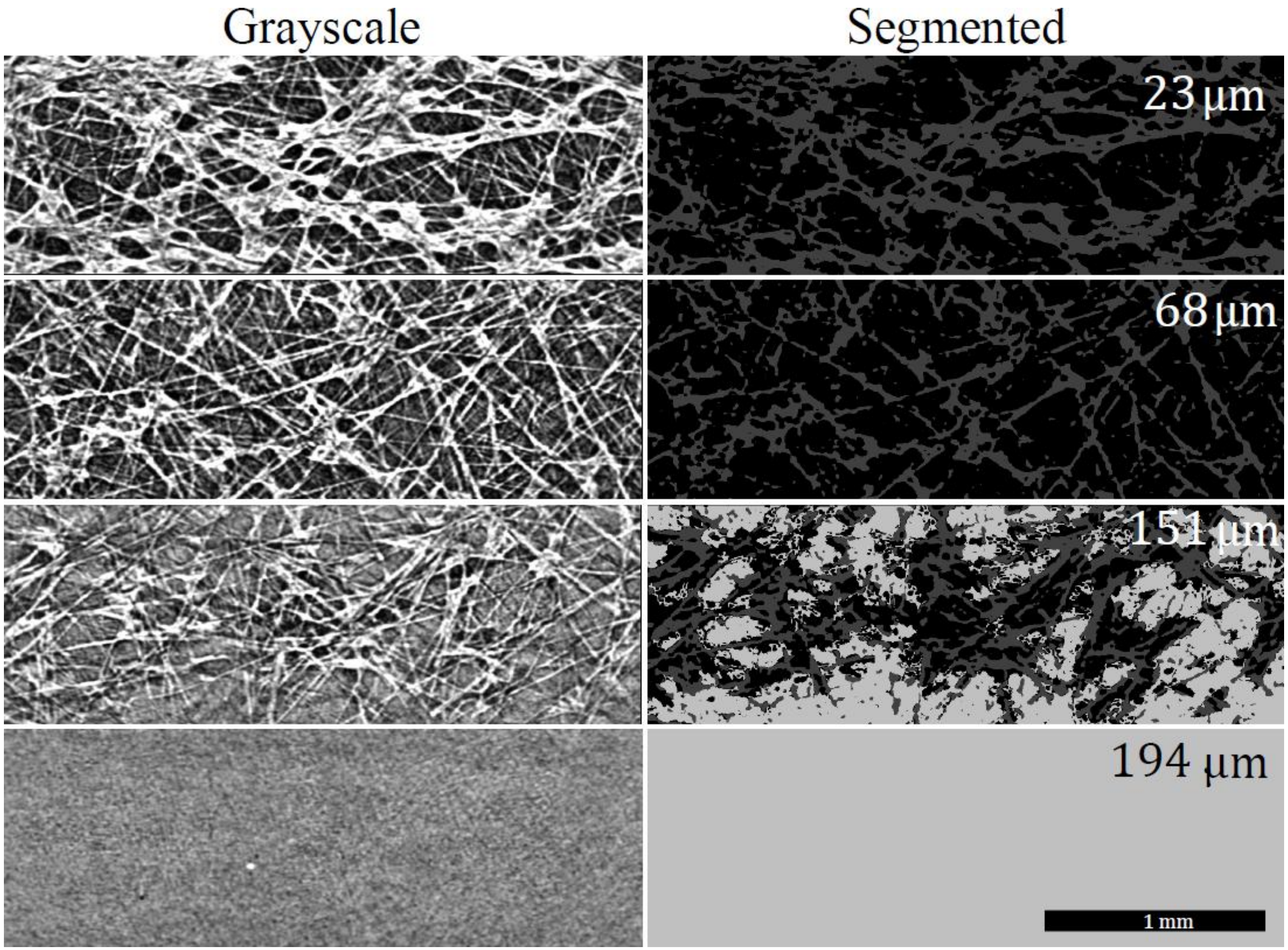


Series of in-plane GDL slices

Grayscale image segmentation

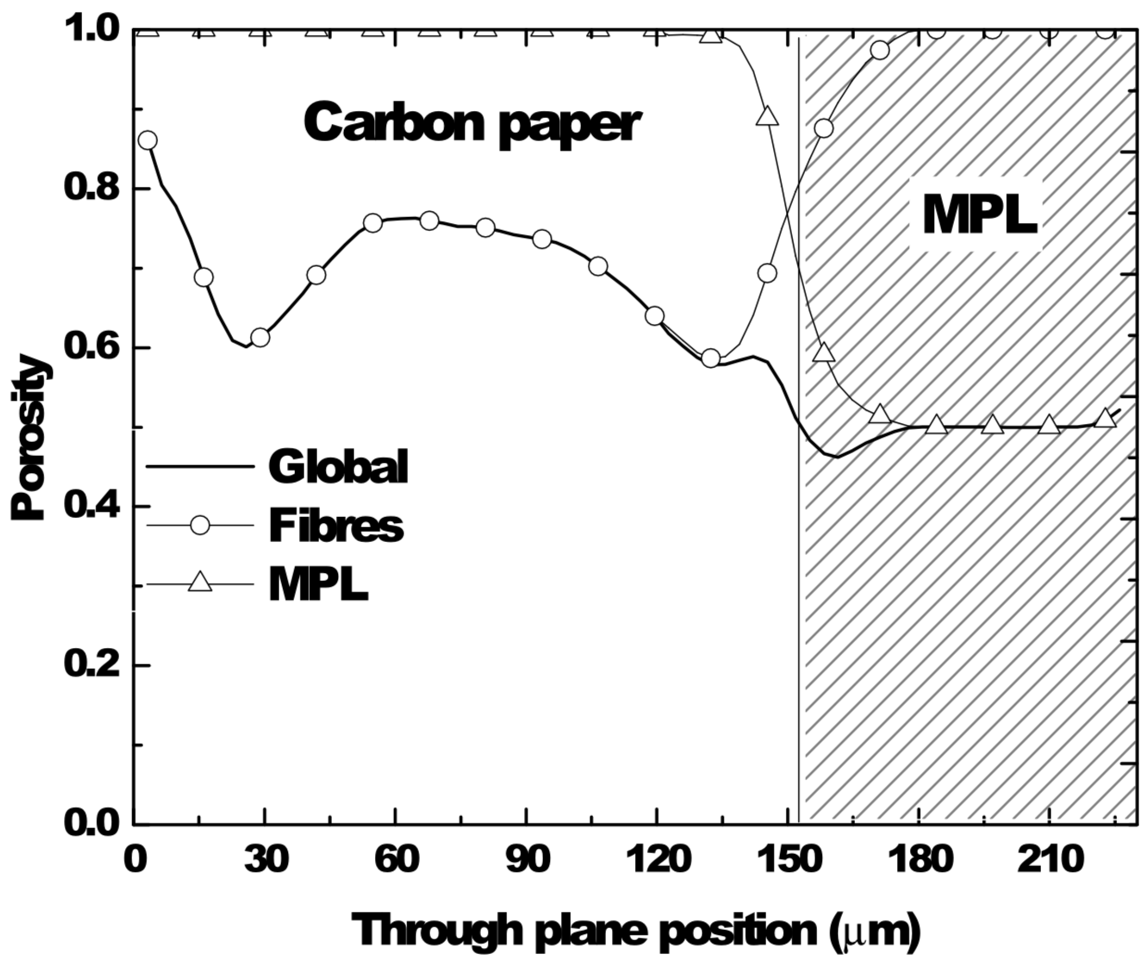
Thresholding of 3 phases:

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



Through plan porosity distribution

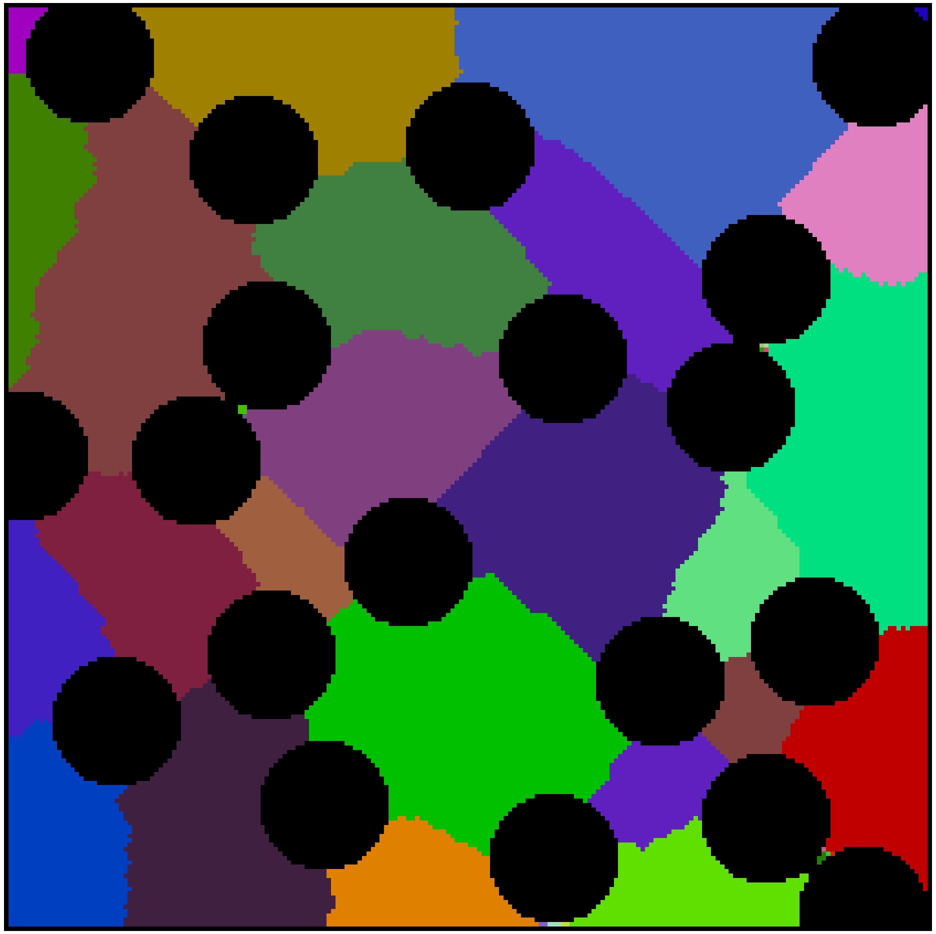
From the segmented images, the porosity of each slices is computed as:



Extraction of the equivalent pore network

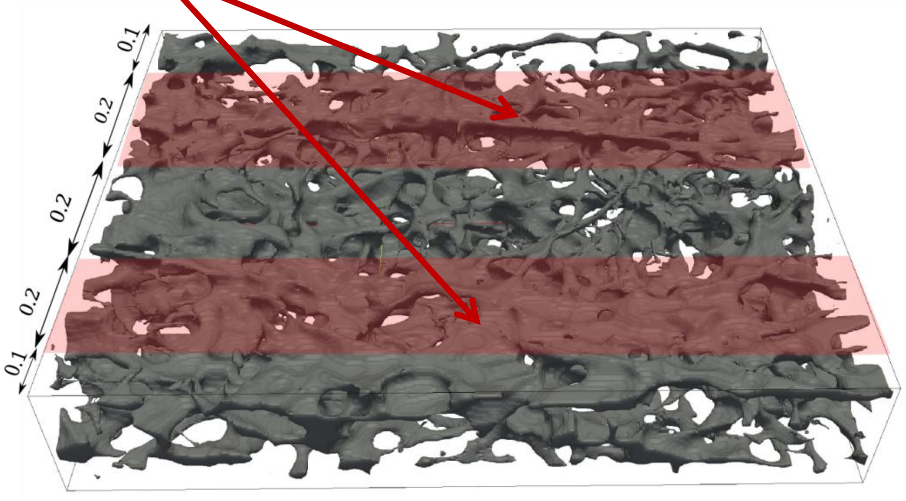
In house C++ code extracts the pores

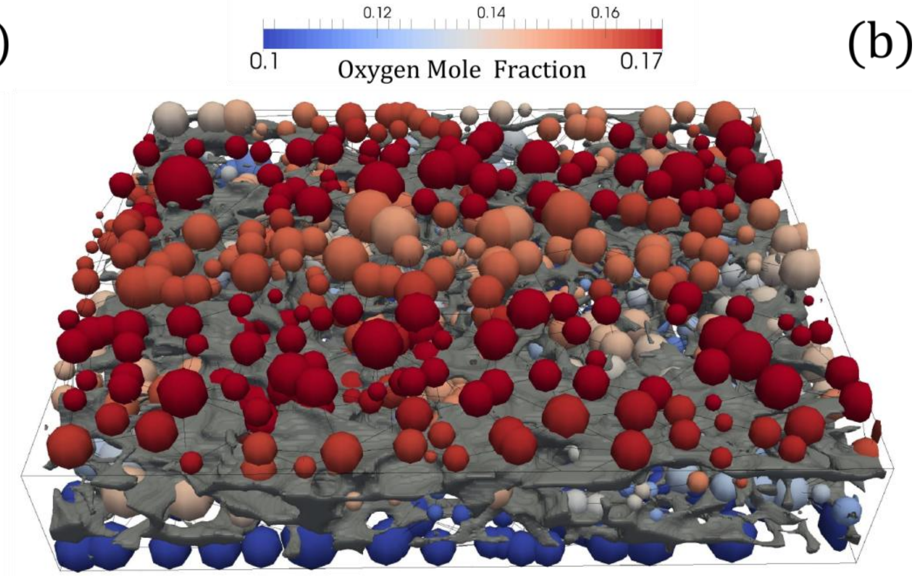
- Pore volume
- Pore surface
- Pore hydraulic diameter
- Throat diameters
- Throat length (based on the adjacent fiber diameters)



Effective diffusivity characterization via OpenPNM

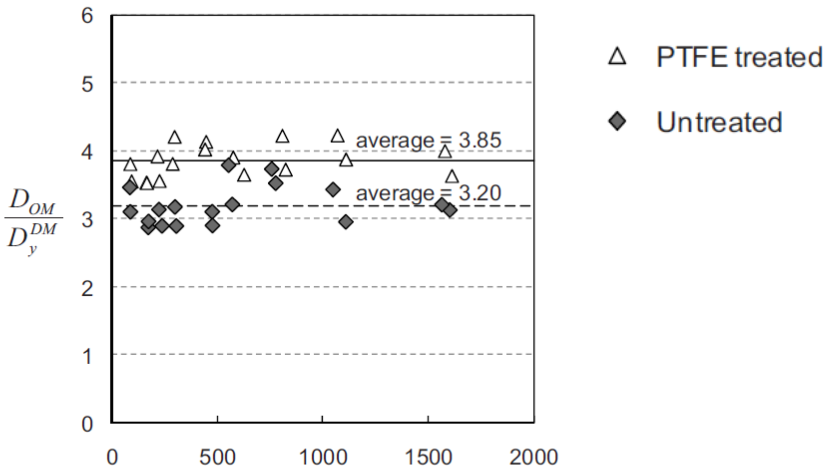
Inlets





Results

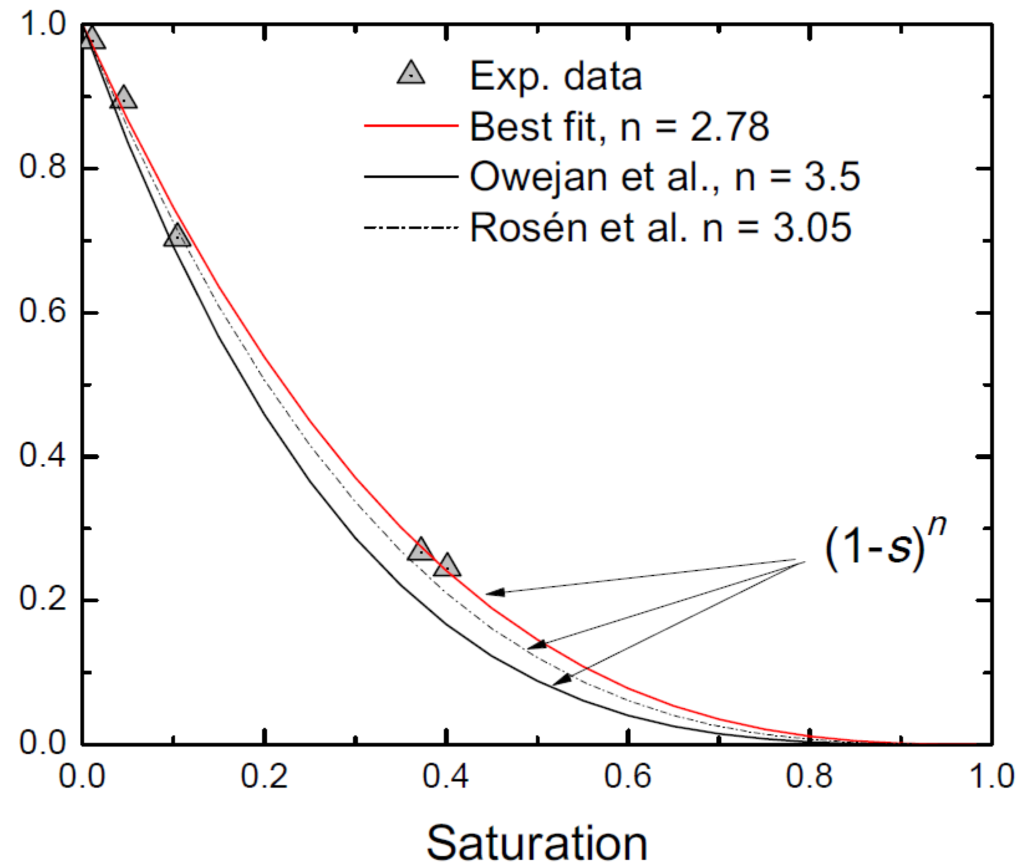
Toray 060, 5% PTFE:



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

Coupling Pore Network and In-situ visualization technic

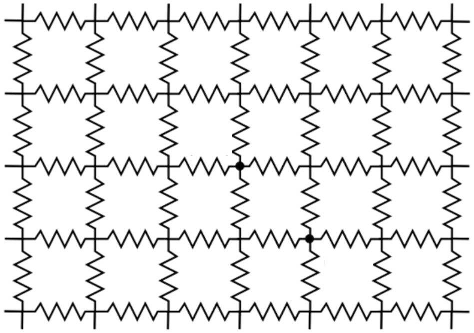
- X-rays imaging
- Impedance spectroscopy
- PNM



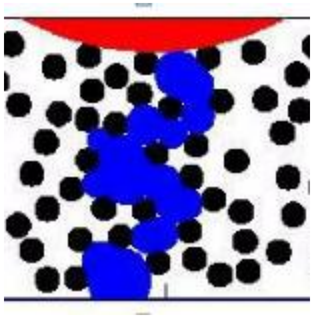
Characterization of the GDL oxygen diffusivity at liquid water different saturation

Summary

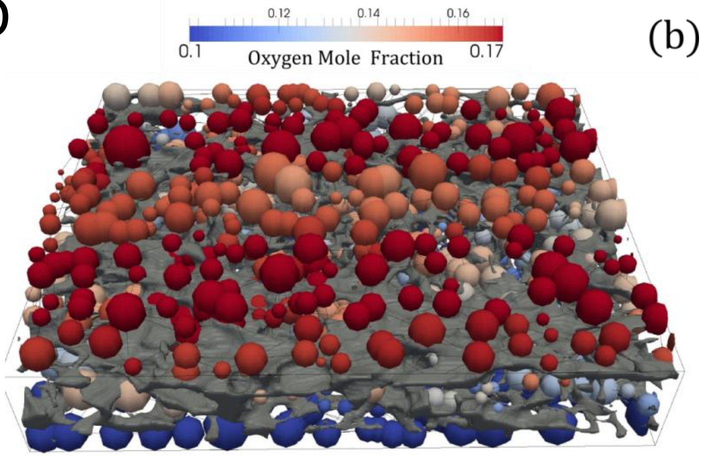
- ✓ Porous material can be view as resistor network



- ✓ 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

Thank You.

Mechanical & Industrial Engineering
UNIVERSITY OF TORONTO

NISSAN

NSERC
CRSNG

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

Canadian Light Source
Centre canadien de rayonnement synchrotron

Contact Info:

Chevalier Stéphane
Dept. of Mechanical & Industrial Engineering
University of Toronto

Email: schevali@mie.utoronto.ca
Website: http://bazylak.mie.utoronto.ca/
Phone: 416-946-5031