# Characterization of the transport properties of gas diffusion layers in polymer electrolyte membrane fuel cells

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**Ulm**

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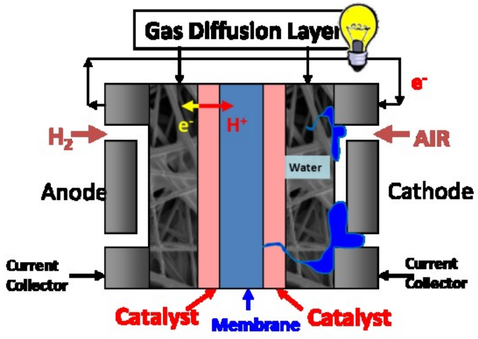
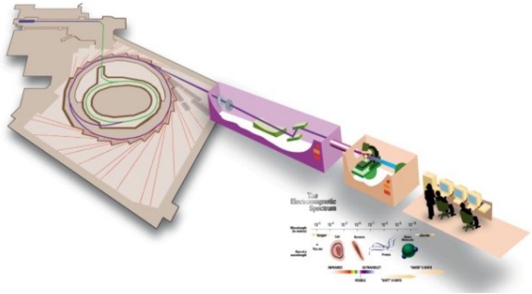
UNIVERSITY OF TORONTO
FACULTY OF APPLIED SCIENCE & ENGINEERING
Institute for Sustainable Energy

# Outlines

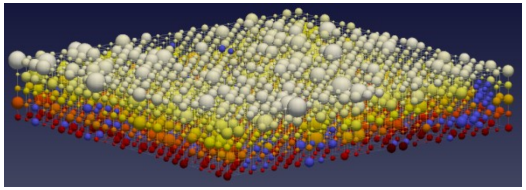
1. Introduction to polymer electrolyte membrane fuel cell




2. Experimental work: X-ray synchrotron radiography of PEMFC in dead-ended anode operation

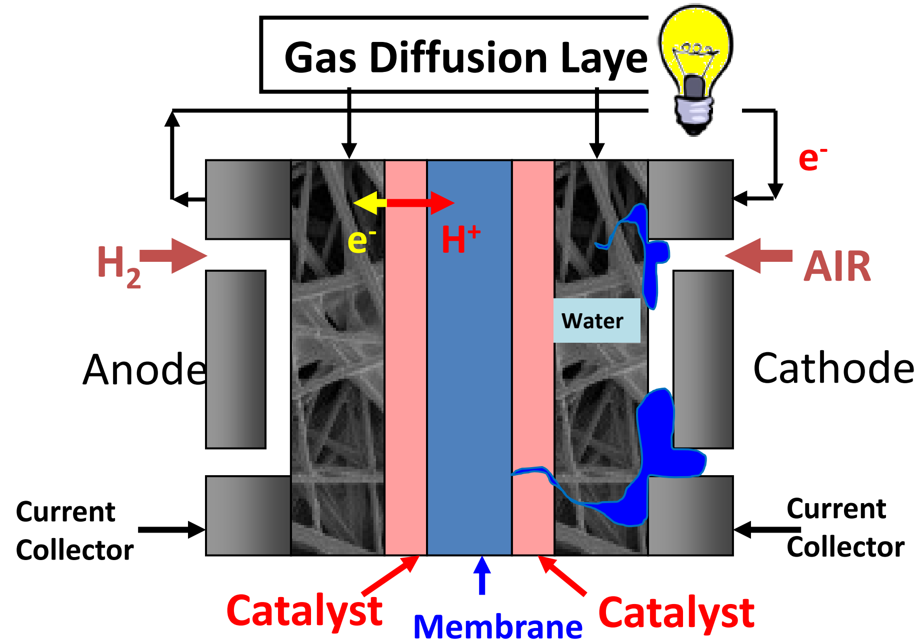


3. Oxygen effective calculation using pore network modeling



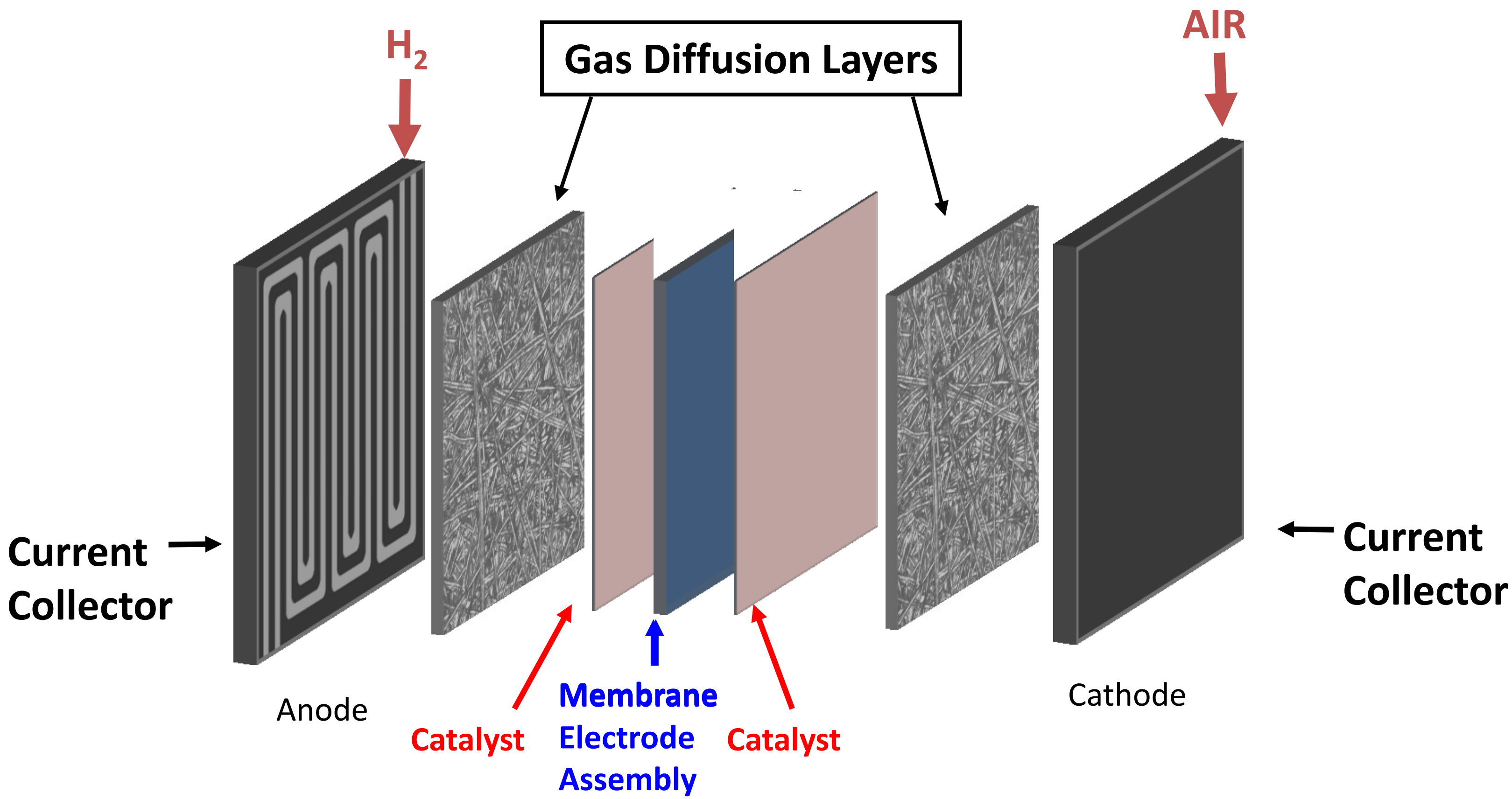
# What is a Polymer Electrolyte Membrane Fuel Cell (PEMFC)?

- A fuel cell is an electrochemical energy conversion device.
- Use Hydrogen and Oxygen to produce electricity
- Water is the only by-product
- Chemical reactions
  - Anode: $H_2 \rightarrow 2H^+ + 2e^-$
  - Cathode: $½.O_2 + 2H^+ + 2e^- \rightarrow H_2O$
  - Overall: $H_2 + ½.O_2 \rightarrow H_2O$



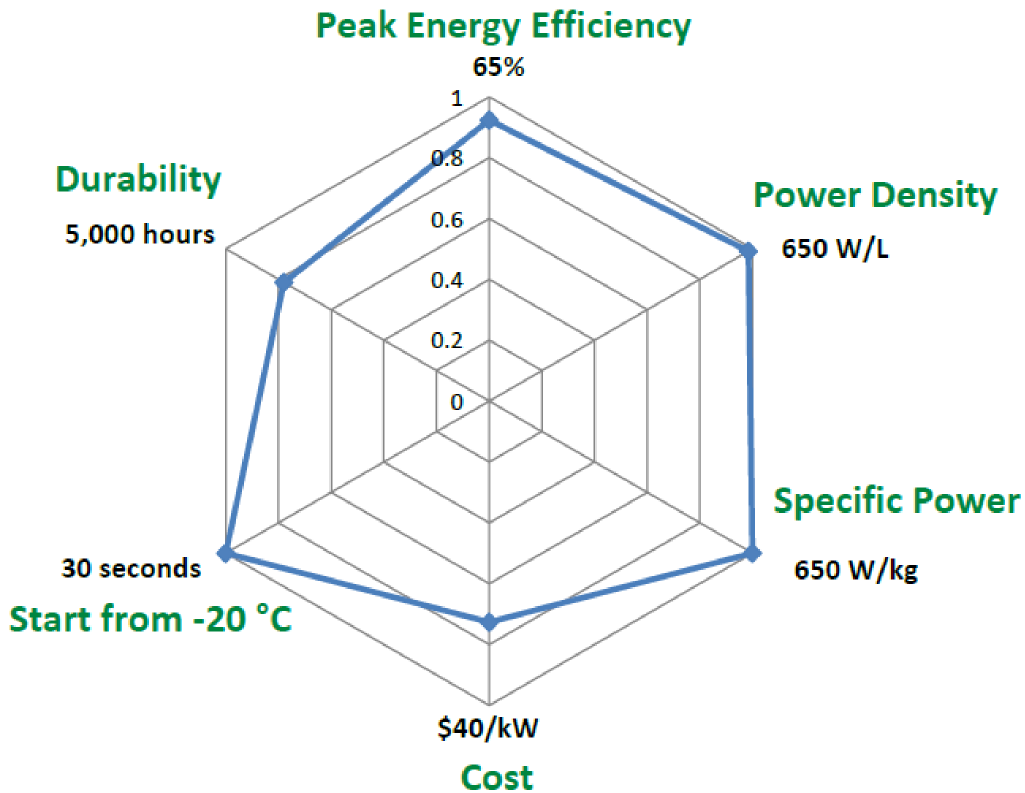

PEMFC Schematic

# Proton Exchange Membrane Fuel Cell (PEMFC) Components




Thicknesses of the layers: between 20 – 200 µm.

# DoE targets by 2020 for the commercial viability of PEMFC



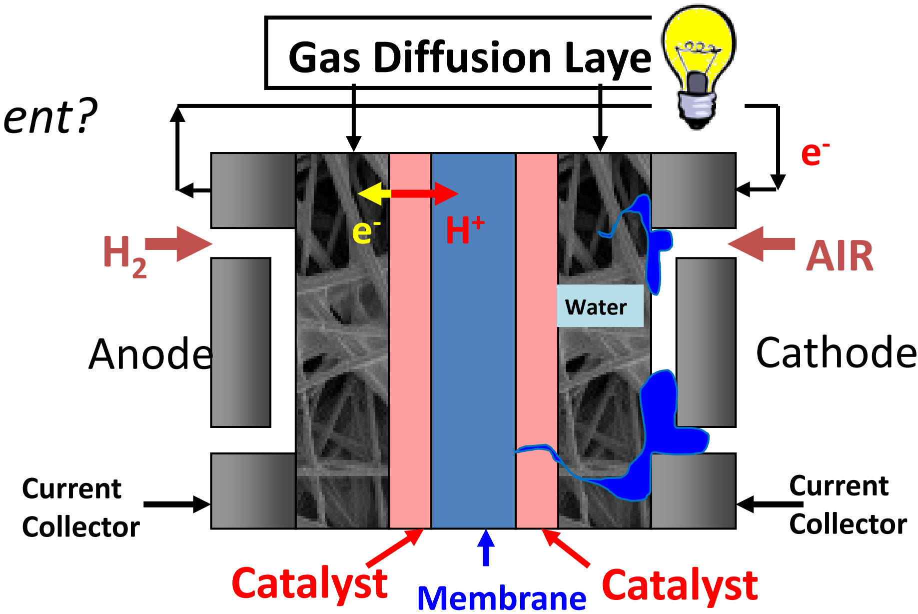

In particular, fuel cell performance and reliability are hindered by non-optimal liquid water management

Figure from *2015 Annual Merit Review and Peer Evaluation Meeting June 8 -12, 2015*

# Fuel cell water management

*What is the optimal fuel cell water management?*

- Let enough liquid water in the fuel cell to hydrate the membrane
- Remove all the liquid water from the GDL




*How to improve it?*

- By obtaining a better understanding of the liquid water transport
- By optimizing the structure of the GDL

These challenges can be tackled by:

➔ visualizing the liquid water in the GDL of an operating fuel cell

➔ modeling the liquid water transport in the GDL

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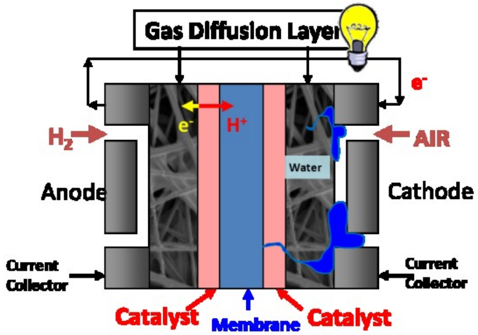


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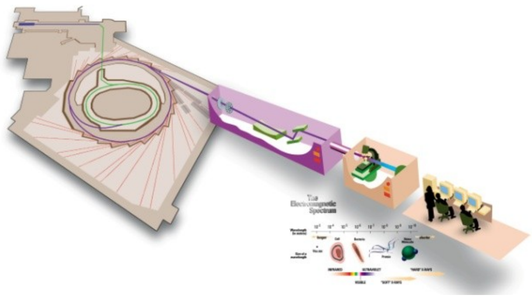

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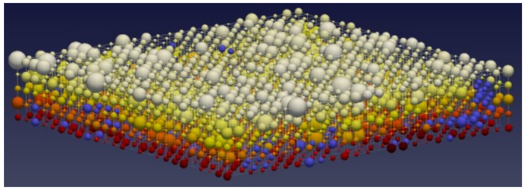
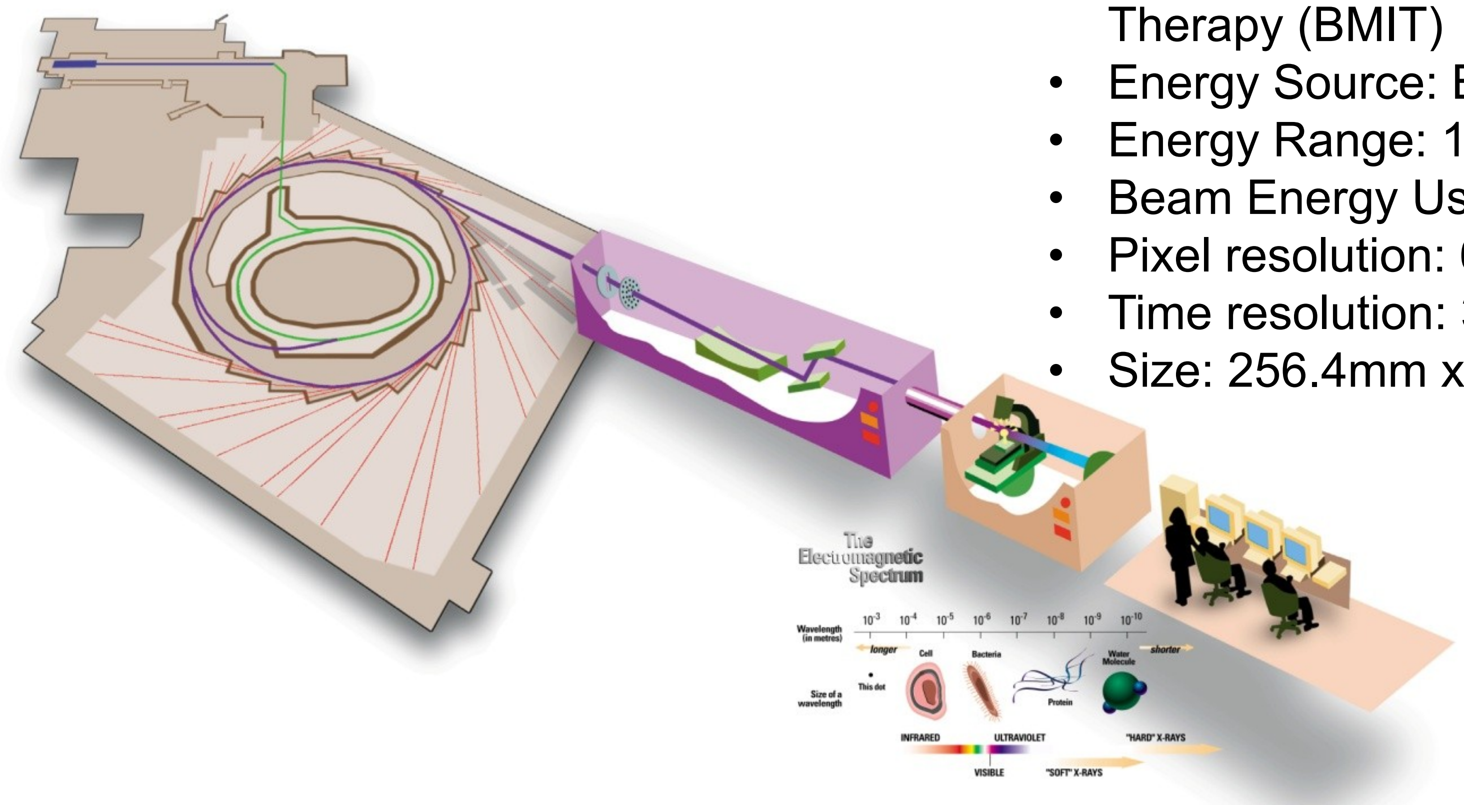


# Fuel cell imaging at the Canadian light source (CLS)

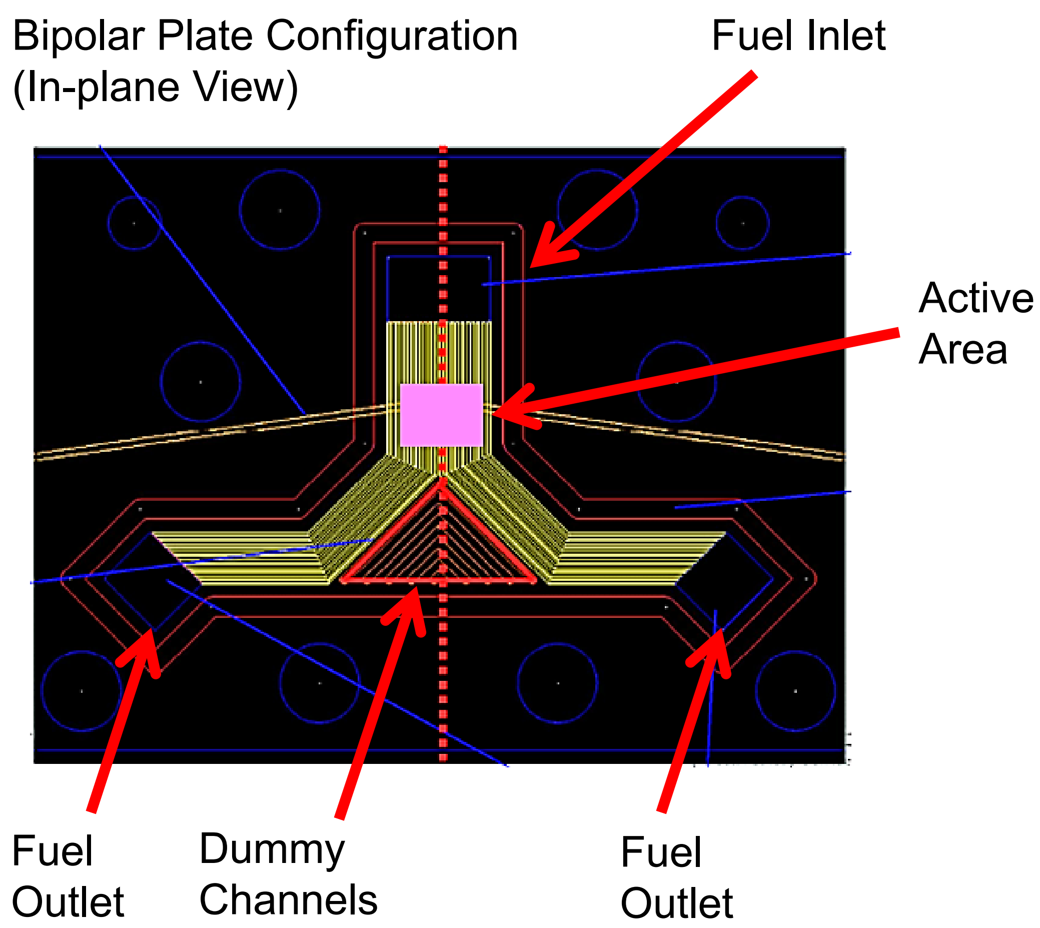
Employing high intensity, monochromatic, and collimated X-rays to facilitate imaging at with high spatial and temporal resolutions.

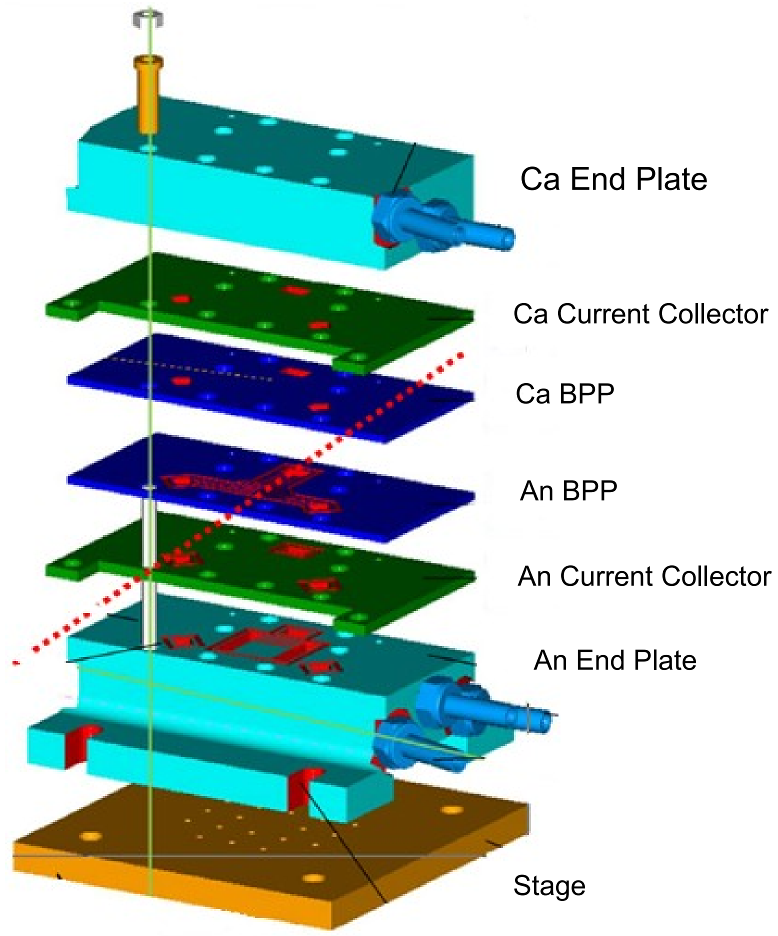
<u>Canadian Light Source Inc.</u>

- Beamline: BioMedical Imaging & Therapy (BMIT)
- Energy Source: Bending Magnet
- Energy Range: 15-40 keV
- Beam Energy Used: 24 keV
- Pixel resolution: 6.5 µm/pixel
- Time resolution: 3 s/image
- Size: 256.4mm x 8.7 mm @ 26m



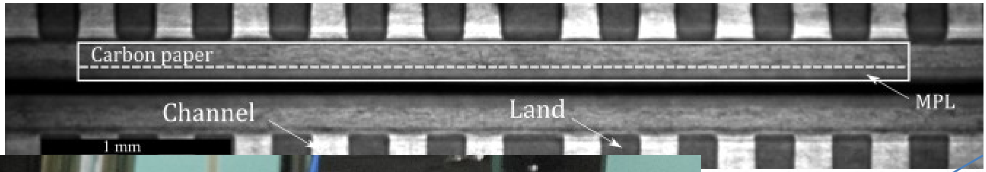
# Miniature fuel cell was specifically designed for synchrotron X-ray radiography

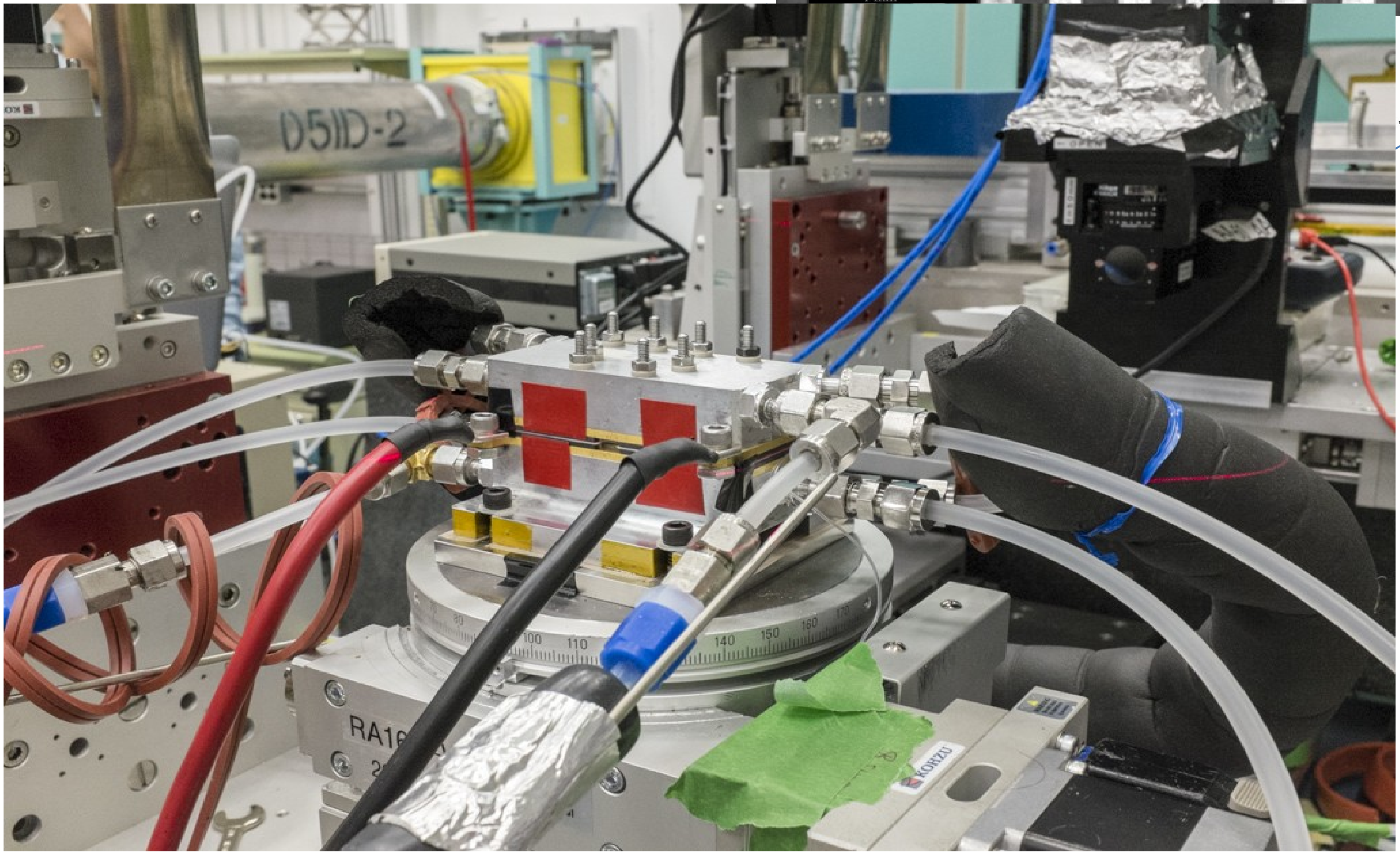


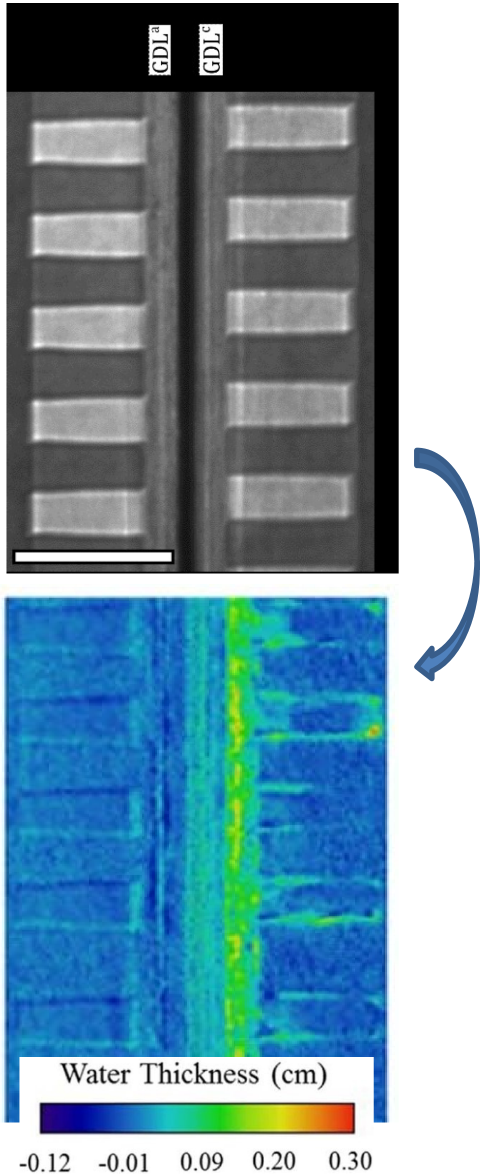

This fuel cell was designed in collaboration with Nissan Motor, Japan

# Experimental setup



# Image processing



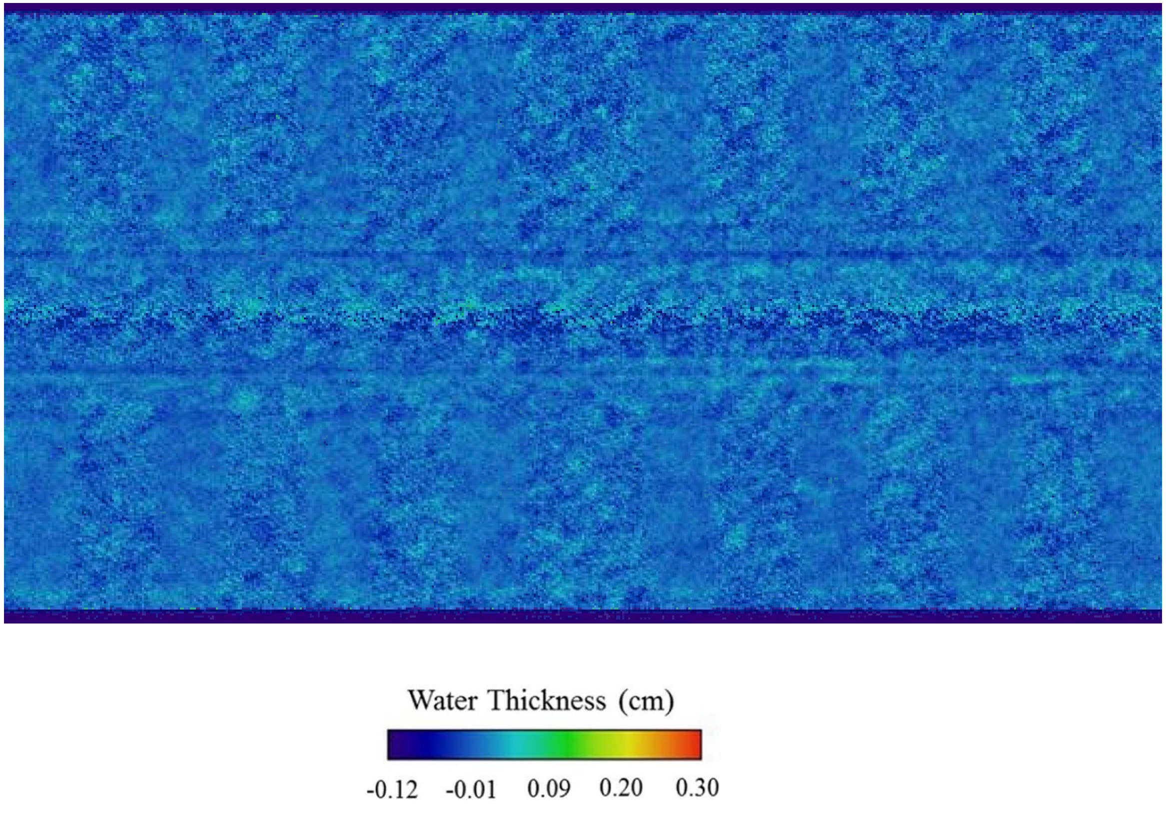

1. Subtract dark image from stack (eliminates stationary artifacts in detector)
2. Compensate for intensity decrease over time
3. Correct images micro-movements
4. Apply Beer-Lambert Law

$$X_w = \frac{1}{\mu_w} \ln\left(\frac{I_d}{I_w}\right)$$

- $X_w$: Liquid water thickness
- $\mu_w$: X-ray attenuation coefficient of water
- $I_d$: Dry image: fuel cell without liquid water
- $I_w$: Wet image: when liquid water has accumulated in the cell

# Results

Liquid water in an operating fuel cell

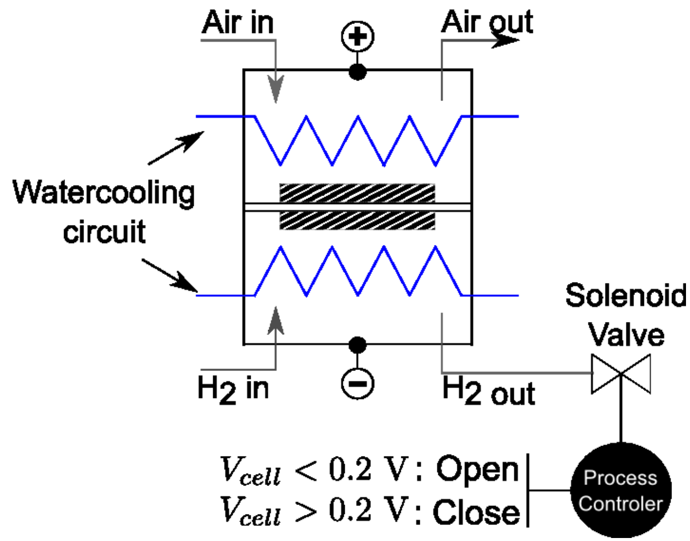


# In situ analysis of voltage degradation in a polymer electrolyte membrane fuel cell with a dead-ended anode

Dead-ended anode operation = Anode outlet closed by a solenoid valve

Benefit: it reduces the hydrogen consumption and therefore increases the car mileage

Drawback: it decreases the reliability of the fuel cell performance



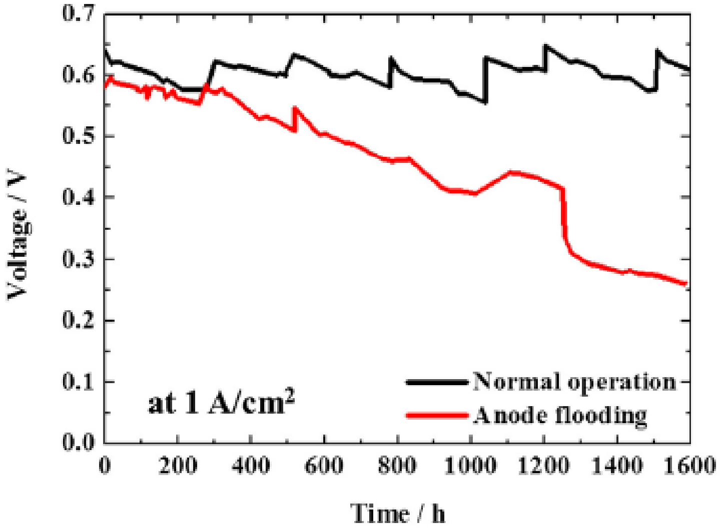
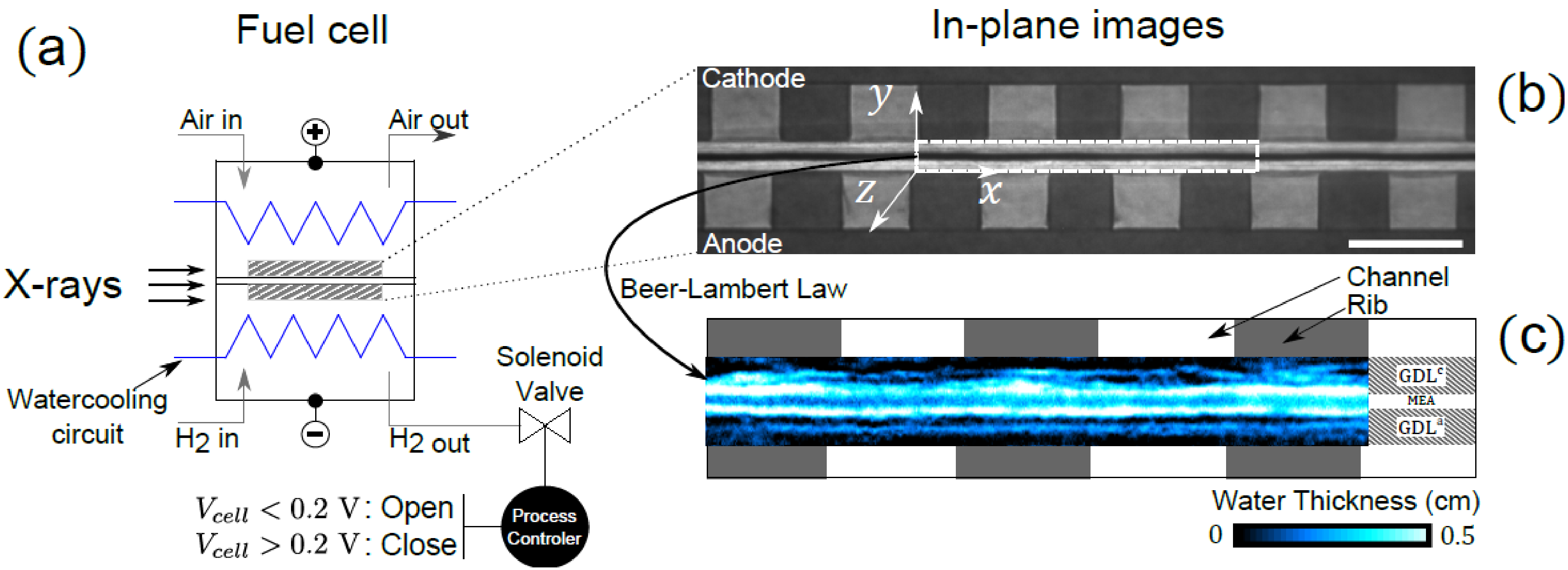




Figure: M. Kim et al., Effects of anode flooding on the performance degradation of polymer electrolyte membrane fuel cells, J. Power Sources. 266 (2014) 332–340.

# Experimental setup

Objective: visualizing the liquid water while the fuel cell was operating in DEA mode

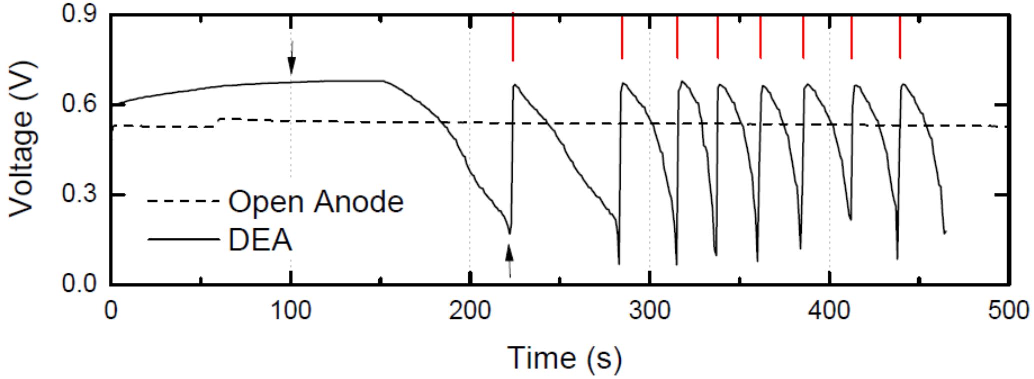


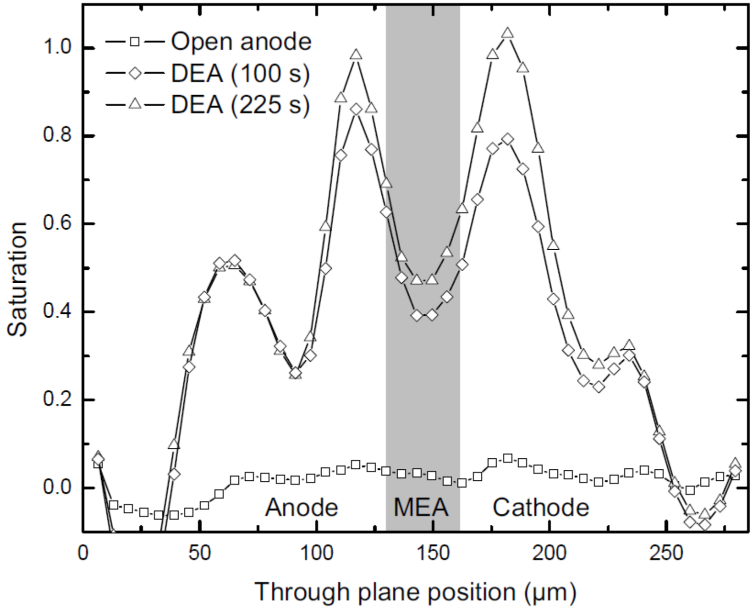

(a): fuel cell in DEA

(b): raw radiograph

(c): liquid water thickness after the post processing

# Origin of the unsteady performance



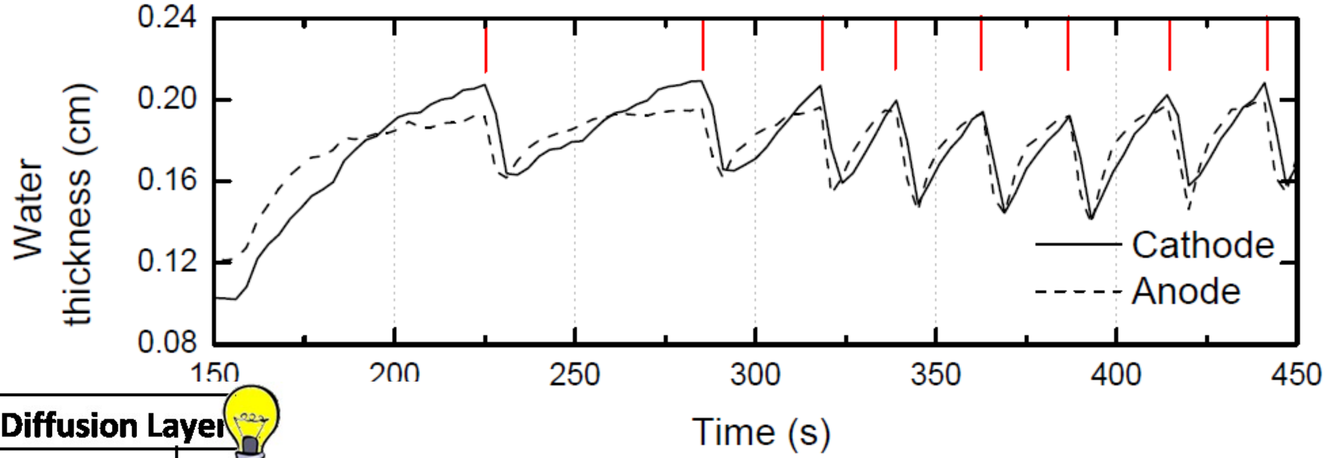



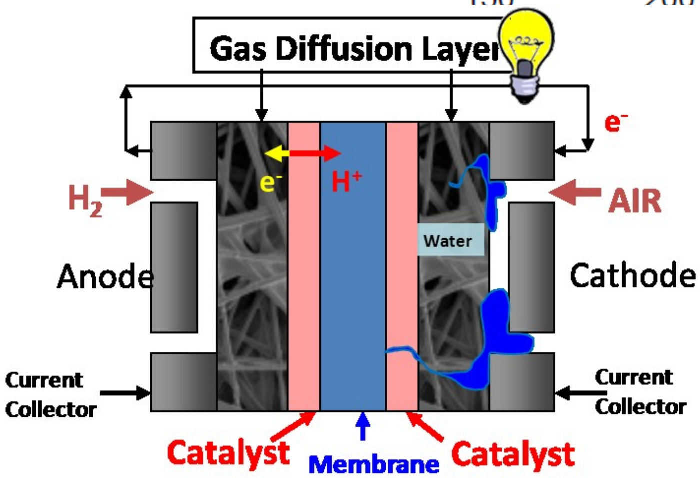

1. The DEA mode induced unsteady performance.
2. The saturation in the GDL increases until 100% in both anode and cathode
3. The oxygen and hydrogen cannot reach the catalyst layer which decrease the performance

Fuel cell performance degradations came from both anode and cathode flooding.

This phenomenon was observed for the first time.

# Impact of the anode purge




1. The purge of anode impacts both anode and cathode liquid water contents
2. Anode and Cathode liquid water increase and decrease accordingly.

Our visualizations revealed a strong coupling between the cathode and the anode liquid water

S. Chevalier et al., In situ analysis of voltage degradation in a polymer electrolyte membrane fuel cell with a dead-ended anode, Electrochem. Commun. 59 (2015) 16–19

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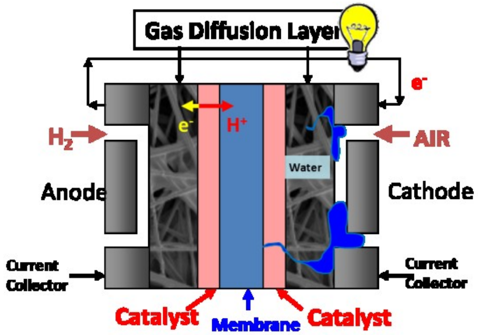


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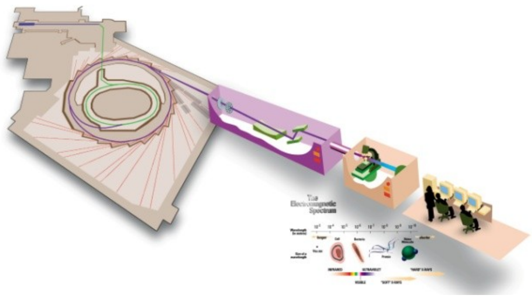

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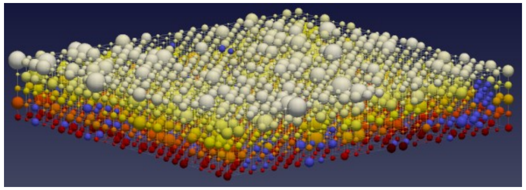
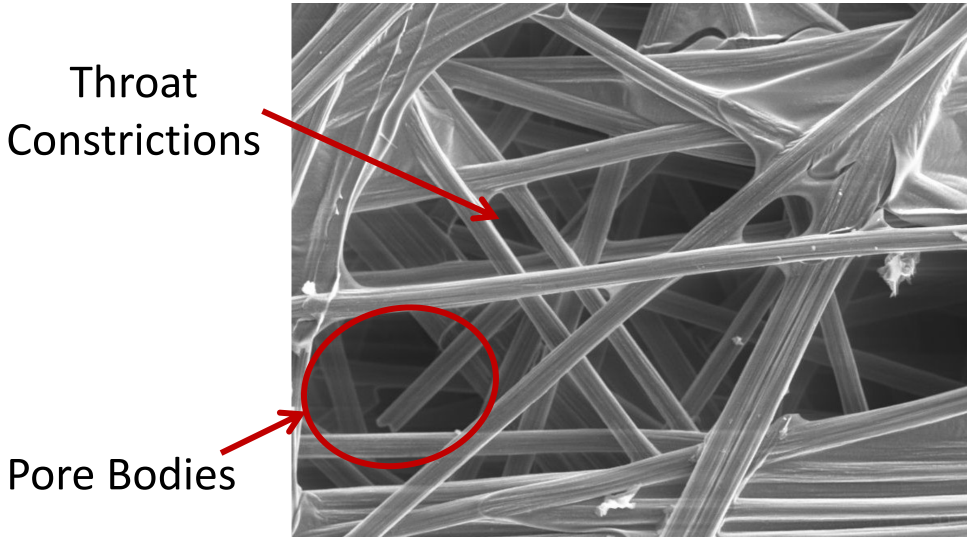
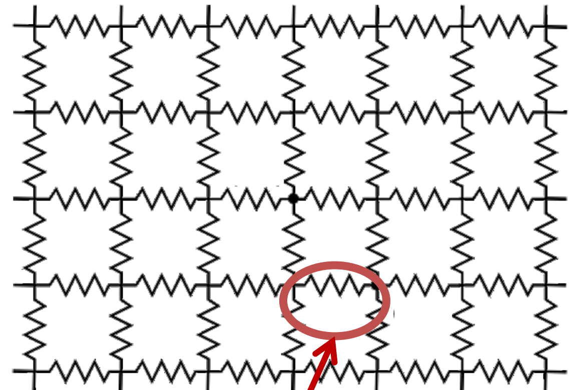
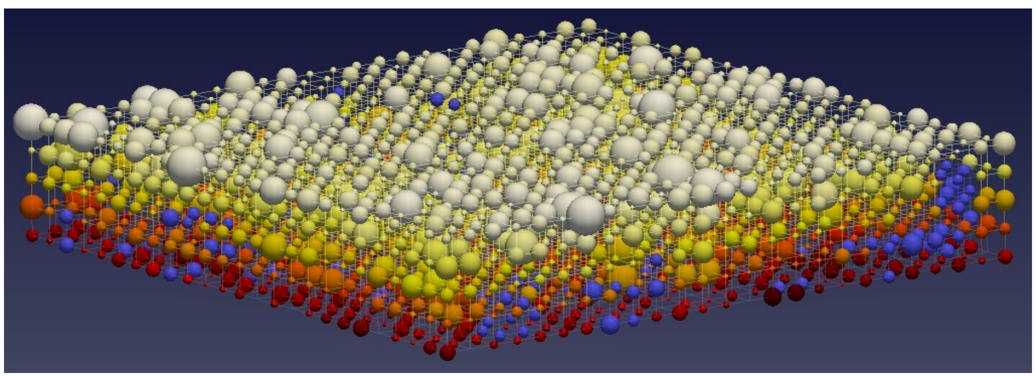


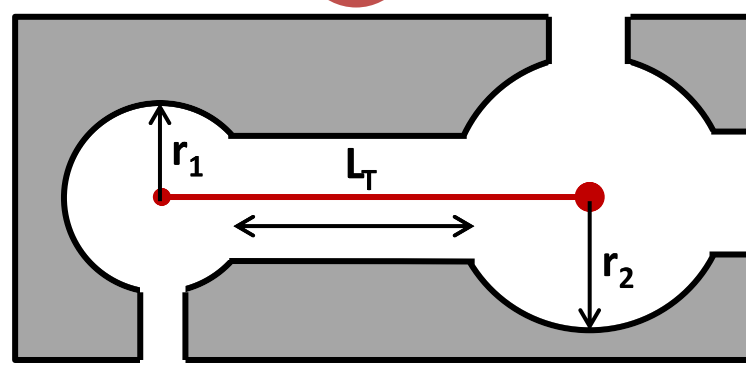
# Pore Network Modelling



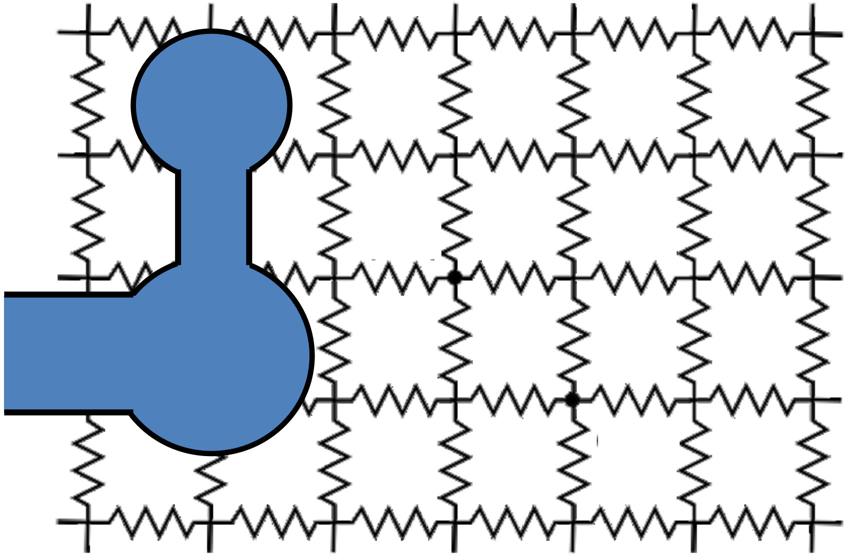
$$Q = \frac{\pi r^4}{8 \mu L} \Delta P_{12}$$

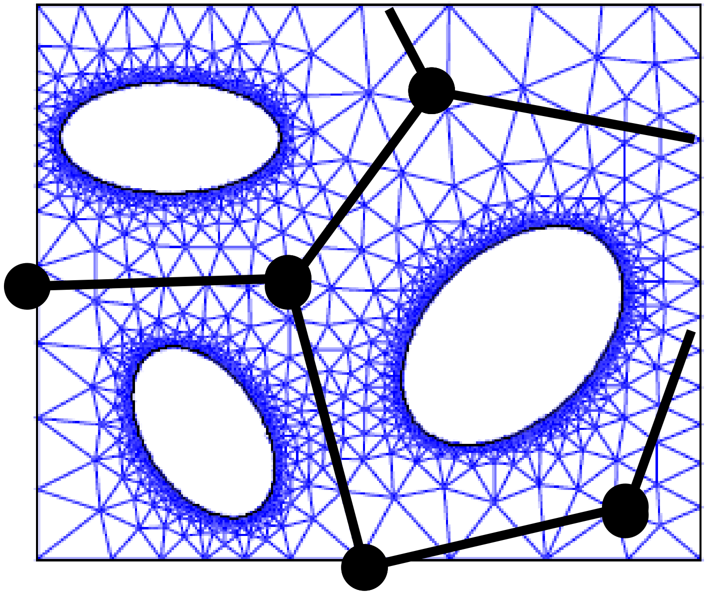





*Figures from J. Gostik*

# 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 approaches like finite-element analysis

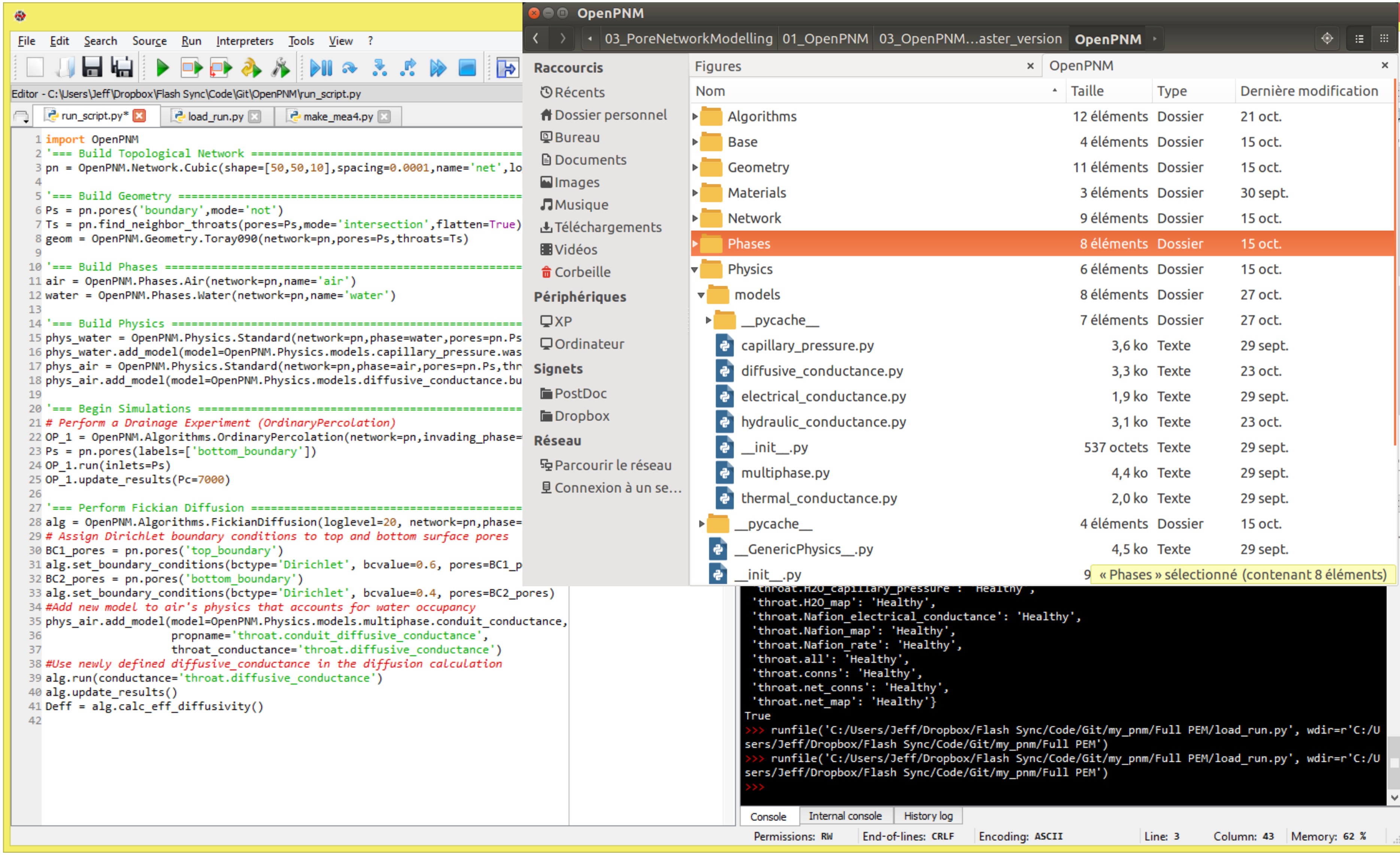
# OpenPNM: http://openpnm.org/

- Work any network lattice, random, 2D/3D
- Fully **Flexible** to any scientific pursuit (not just Fuel Cells)
- **Accessible** for non-computer scientists
- Professional, well **Documented**
- **Free** using Python

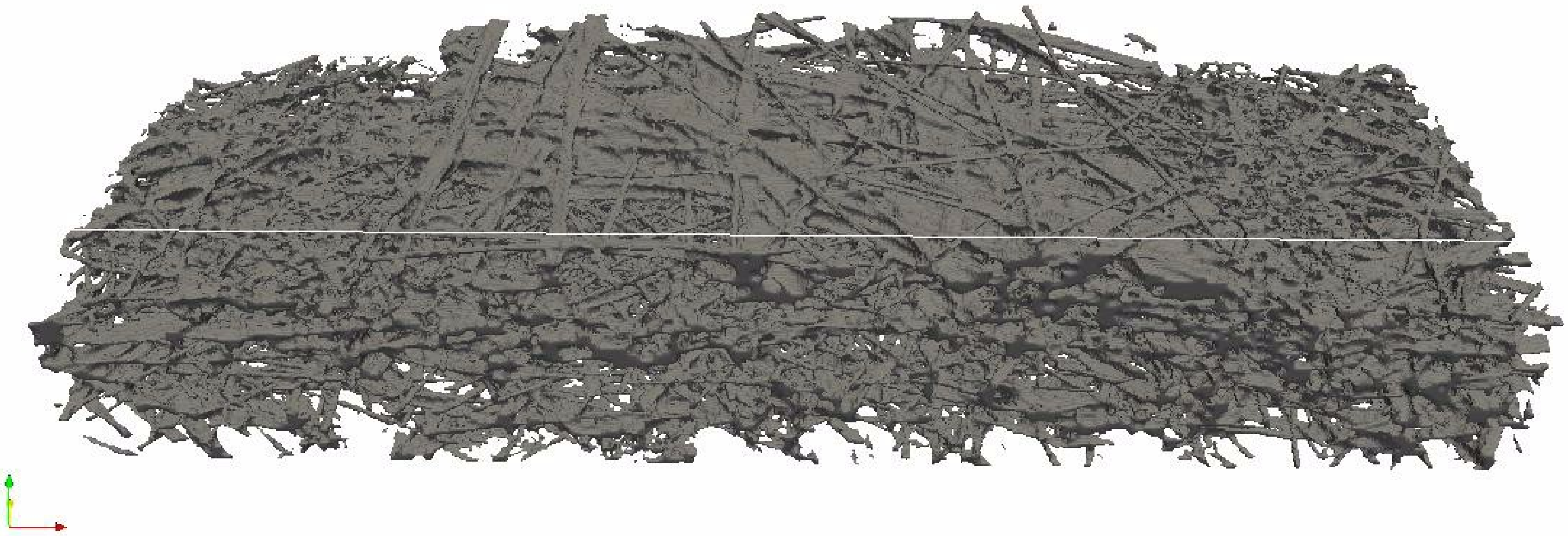
Main partners involve in OpenPNM framework:

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

# OpenPNM


File Edit Search Source Run Interpreters Tools View ?
Editor - C:\Users\Jeff\Dropbox\Flash Sync\Code\Git\OpenPNM\run_script.py
run_script.py* load_run.py make_mea4.py
import OpenPNM
'=== Build Topological Network ===
pn = OpenPNM.Network.Cubic(shape=[50,50,10],spacing=0.0001,name='net',lo
'=== Build Geometry ===
Ps = pn.pores('boundary',mode='not')
Ts = pn.find_neighbor_throats(pores=Ps,mode='intersection',flatten=True)
geom = OpenPNM.Geometry.Toray090(network=pn,pores=Ps,throats=Ts)
'=== Build Phases ===
air = OpenPNM.Phases.Air(network=pn,name='air')
water = OpenPNM.Phases.Water(network=pn,name='water')
'=== Build Physics ===
phys_water = OpenPNM.Physics.Standard(network=pn,phase=water,pores=pn.Ps
phys_water.add_model(model=OpenPNM.Physics.models.capillary_pressure.was
phys_air = OpenPNM.Physics.Standard(network=pn,phase=air,pores=pn.Ps,thr
phys_air.add_model(model=OpenPNM.Physics.models.diffusive_conductance.bu
'=== Begin Simulations ===
# Perform a Drainage Experiment (OrdinaryPercolation)
OP_1 = OpenPNM.Algorithms.OrdinaryPercolation(network=pn,invading_phase=
Ps = pn.pores(labels=['bottom_boundary'])
OP_1.run(inlets=Ps)
OP_1.update_results(Pc=7000)
'=== Perform Fickian Diffusion ===
alg = OpenPNM.Algorithms.FickianDiffusion(loglevel=20, network=pn,phase=
# Assign Dirichlet boundary conditions to top and bottom surface pores
BC1_pores = pn.pores('top_boundary')
alg.set_boundary_conditions(bctype='Dirichlet', bcvalue=0.6, pores=BC1_p
BC2_pores = pn.pores('bottom_boundary')
alg.set_boundary_conditions(bctype='Dirichlet', bcvalue=0.4, pores=BC2_pores)
#Add new model to air's physics that accounts for water occupancy
phys_air.add_model(model=OpenPNM.Physics.models.multiphase.conduit_conductance,
propname='throat.conduit_diffusive_conductance',
throat_conductance='throat.diffusive_conductance')
#Use newly defined diffusive_conductance in the diffusion calculation
alg.run(conductance='throat.diffusive_conductance')
alg.update_results()
Deff = alg.calc_eff_diffusivity()
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
OpenPNM
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
« Phases » sélectionné (contenant 8 éléments)
'throat.H2O_map': 'Healthy',
'throat.Nafion_electrical_conductance': 'Healthy',
'throat.Nafion_map': 'Healthy',
'throat.Nafion_rate': 'Healthy',
'throat.all': 'Healthy',
'throat.conns': 'Healthy',
'throat.net_conns': 'Healthy',
'throat.net_map': 'Healthy'}
True
>>> runfile('C:/Users/Jeff/Dropbox/Flash Sync/Code/Git/my_pnm/Full PEM/load_run.py', wdir=r'C:/Users/Jeff/Dropbox/Flash Sync/Code/Git/my_pnm/Full PEM')
>>> runfile('C:/Users/Jeff/Dropbox/Flash Sync/Code/Git/my_pnm/Full PEM/load_run.py', wdir=r'C:/Users/Jeff/Dropbox/Flash Sync/Code/Git/my_pnm/Full PEM')
>>>
Console Internal console History log
Permissions: RW End-of-lines: CRLF Encoding: ASCII Line: 3 Column: 43 Memory: 62 %

# 3D invasion percolation



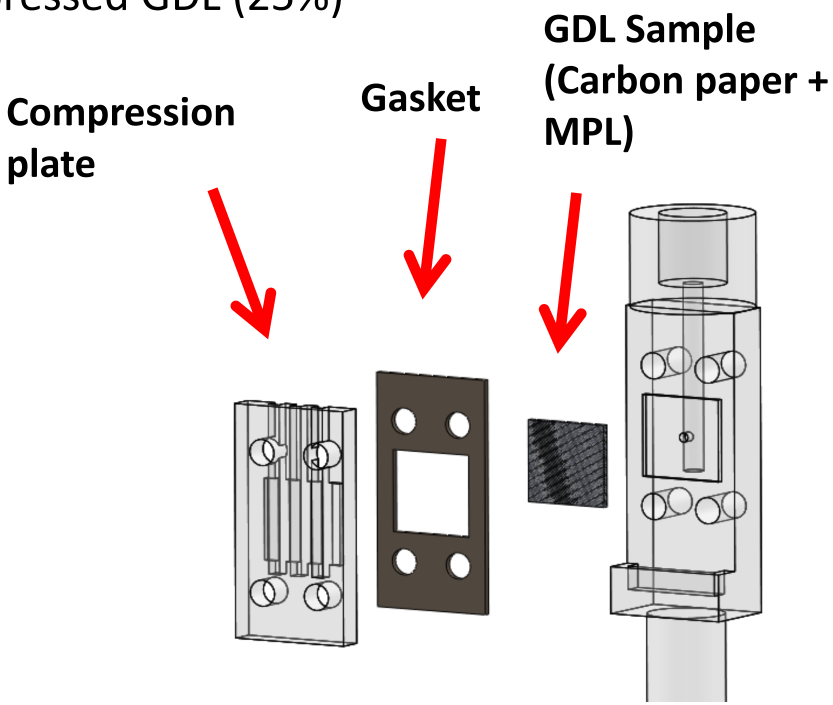
# Oxygen diffusivity calculation by PNM

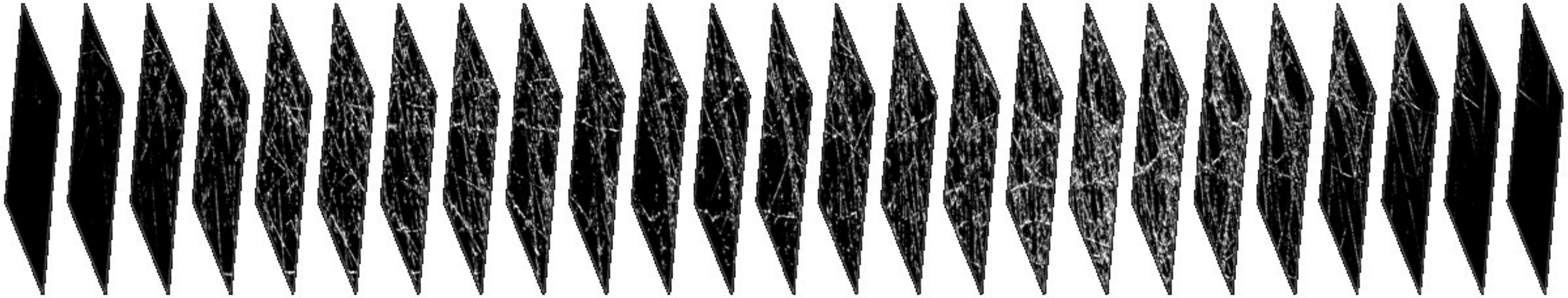
1. Characterization of the GDL 3D structure by microcomputed tomography
2. Segmentation (binarisation) of the images
3. Extraction of the equivalent pore network based on the segmented images
4. Pore network modeling of the diffusive gas transport (Fick's law)
5. Calculation of the effective diffusivity

# Micro-compute tomography

3D Characterization of Compressed GDL (25%)

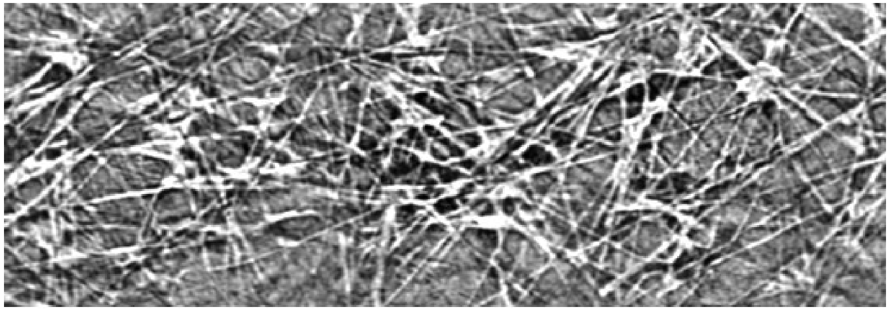
- X-rays micro tomography
- Down to 0.7 µm detail detectability.
- Achievable spatial resolution of 5 µm.



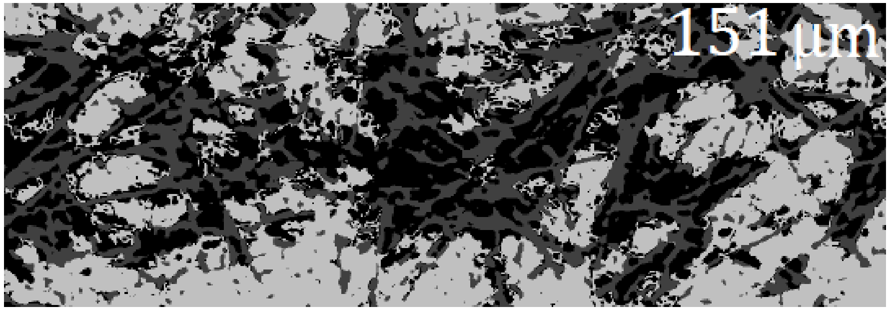



# Image segmentation

Greyscale value

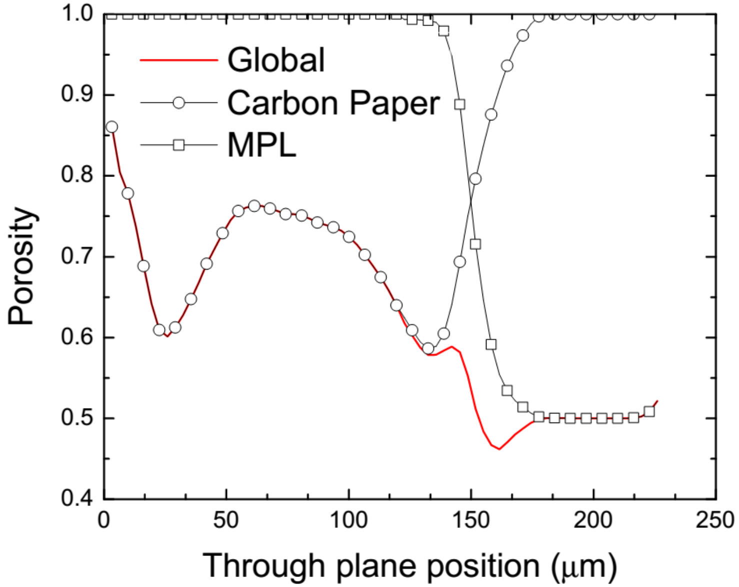


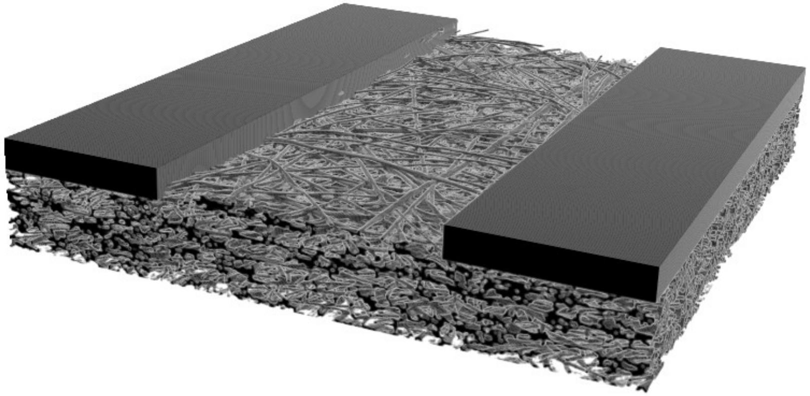
Ternary image




Black: void
Grey: fibers
Light grey: MPL

GDL porosity distribution



GDL 3D geometry

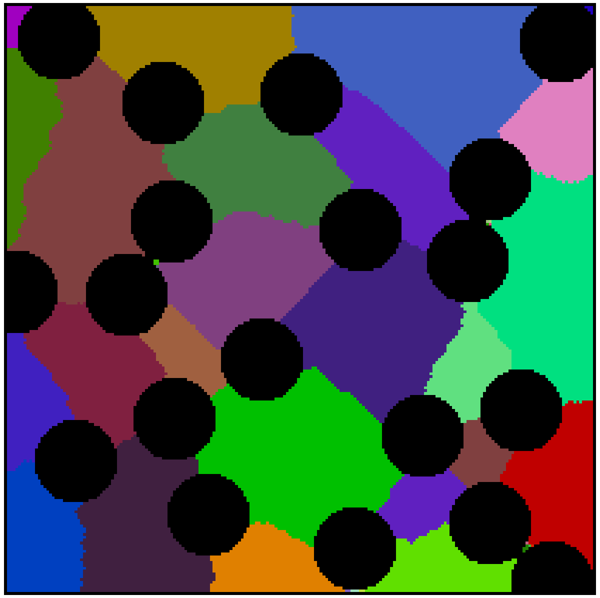
# Extraction of the equivalent pore network

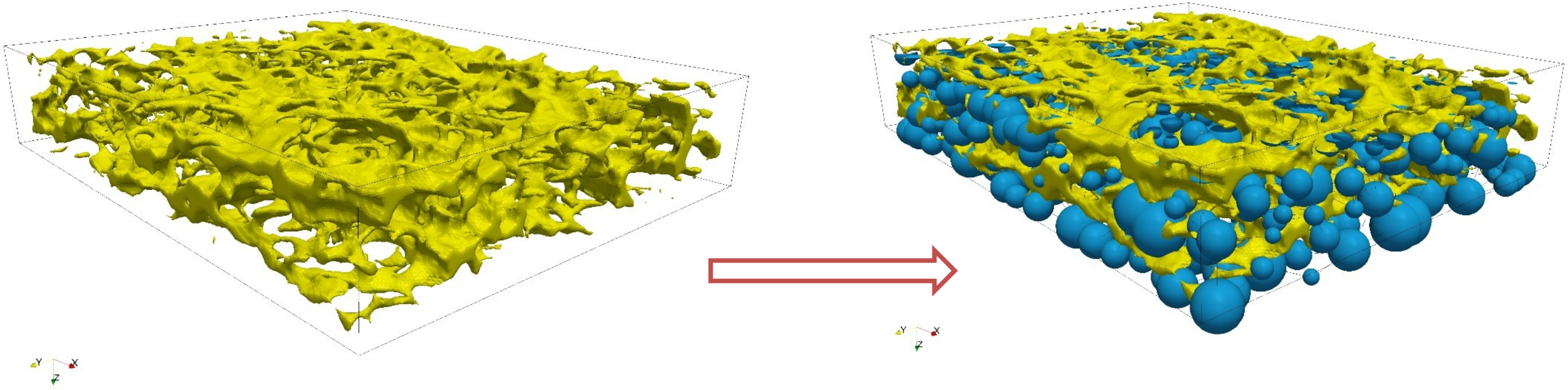
In house C++ code extracts the pores

- Volume, surface, hydraulic diameter, positions

And the throat

- Diameter, length, connectivity



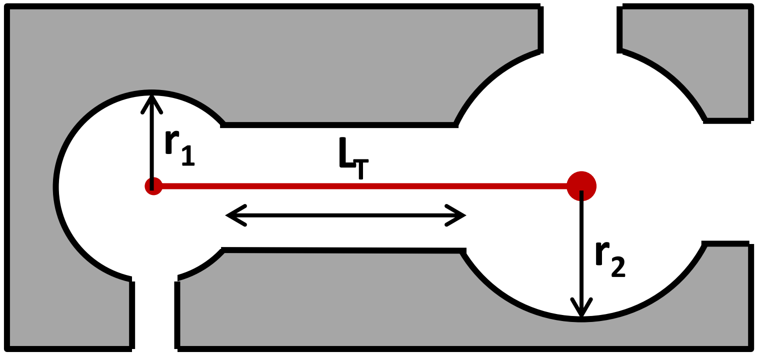


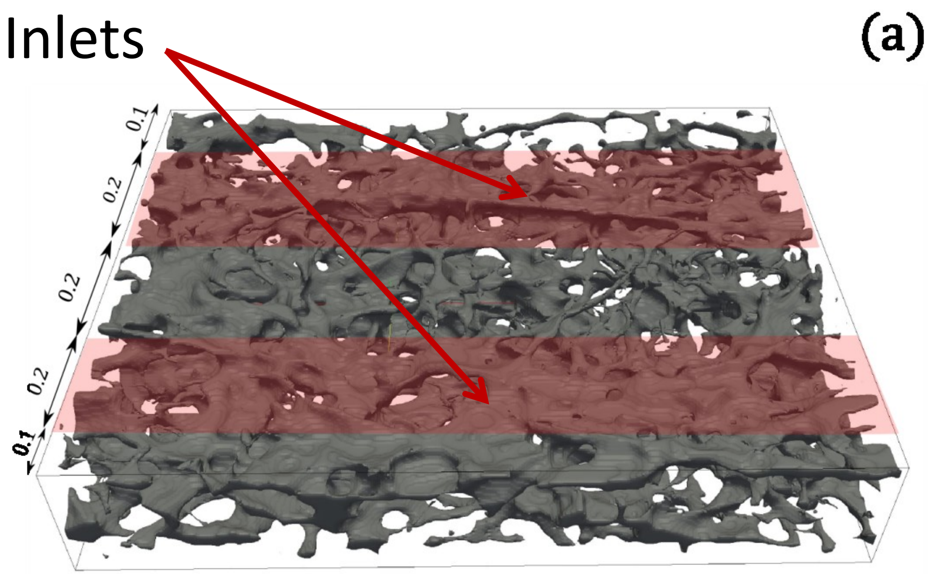
# Effective diffusivity characterization via OpenPNM

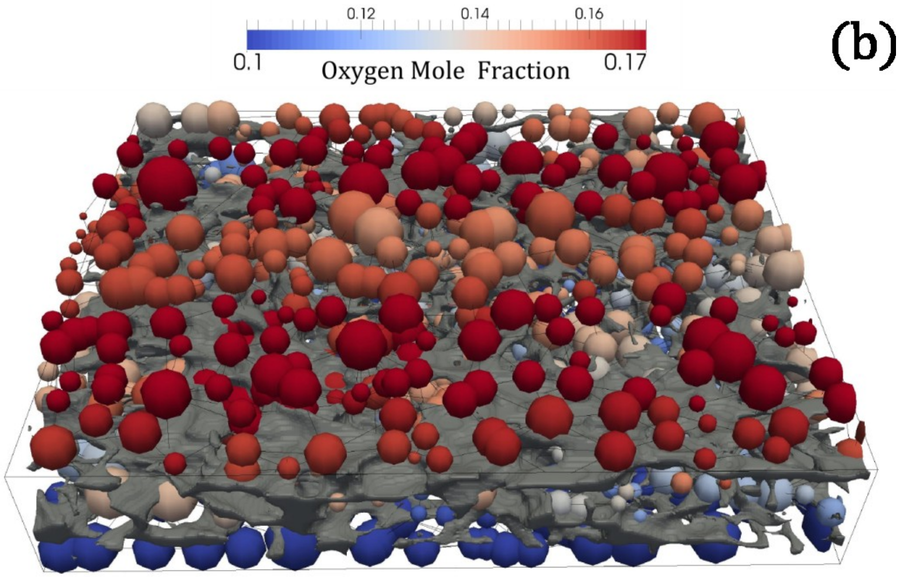
Fick's law:

Conductance at the pore scale:

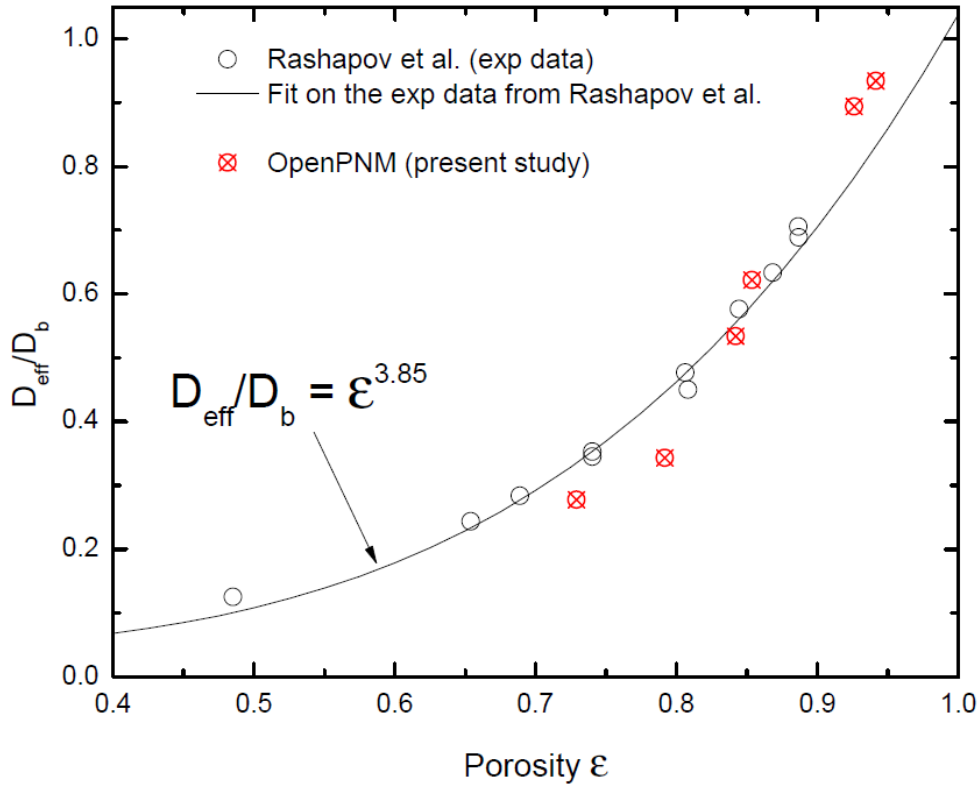
Pore 1 Pore 2 Throat



# Effective diffusivity characterization via OpenPNM



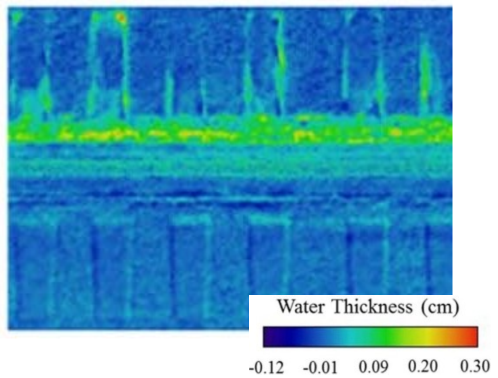

R. Rashapov et al., A method for measuring in-plane effective diffusivity in thin porous media, Int. J. Heat Mass Transf. 85 (2015) 367–374.

Calculation of the effective diffusivity was validated on experimental data

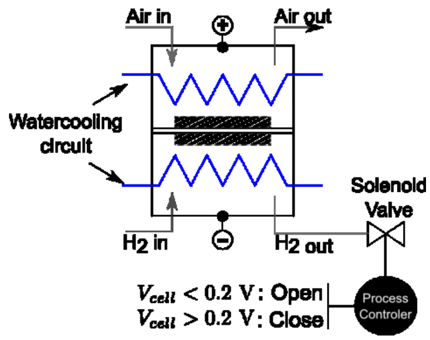
➔ This methodology is an alternative to the experimental measurement

# Summary of the experimental approache

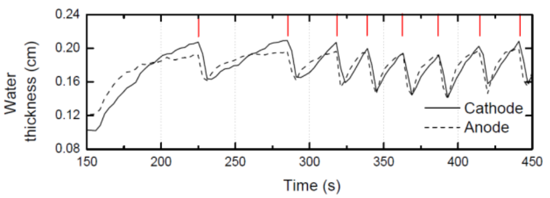
1. The liquid water was measured in an operating fuel cell using X-ray synchrotron radiography




2. For the first time, the liquid water in both anode and cathode GDL was visualised in an operating PEMFC in DEA



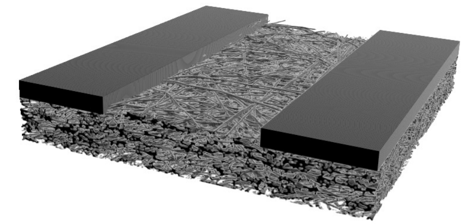

3. Fuel cell voltage degradations were linked to both anode and cathode GDL flooding, and strong correlations between anode and cathode liquid water content were observed



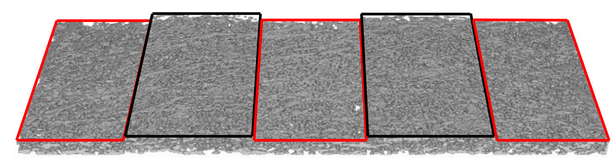
# Summary of the pore network modelling

1. New Open source pore network modelling package is available

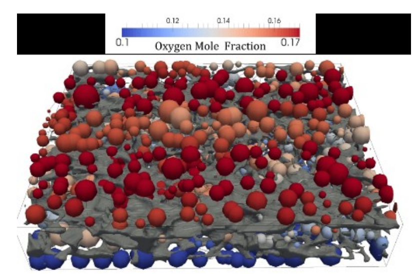
**http://openpnm.org/     Version 1.0 released 4 months ago**



2. Pore network modelling based on micro-computed tomography is an accurate tool
    - Porous media characterization
    - Simulation of mass transport



3. Various aspects of the porous media can be studied
    - Transport Properties characterisation
    - Impact of the operating condition (compression rate)
    - Multiphase transport



# Thank You.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