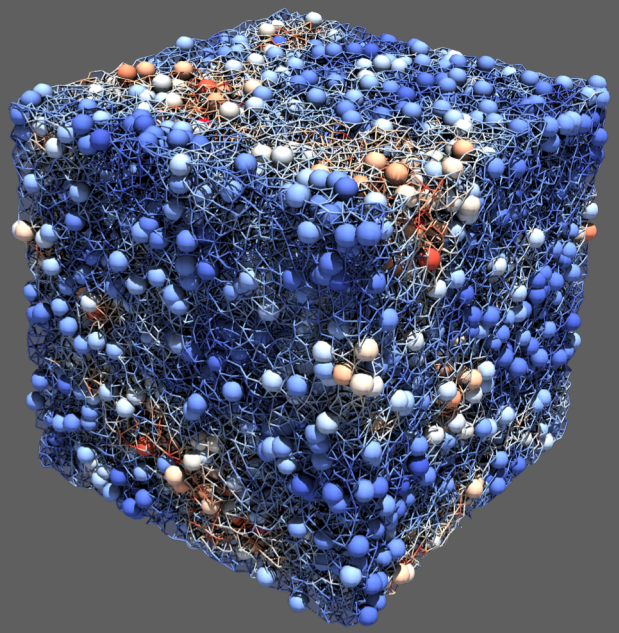
Application of a Pore Network Pore-Scale Simulation for Analysis of Single and Two-phase Flow in Porous Materials



Daniel Niblett (PhD Student)
The University of Manchester

Advanced Modeling & Simulation (AMS) Seminar Series
NASA Ames Research Center, October 23, 2018

Bio



Current

ICURe Entrepreneurial Lead – Flow and transport through Porous Materials

PhD student – Chemical Engineering 2017 - 2020

Optimisation of flow and transport in fuel cell gas diffusion layers using numerical simulations

Past

(MEng) Chemical Engineering with Industrial Experience 2013 - 2017

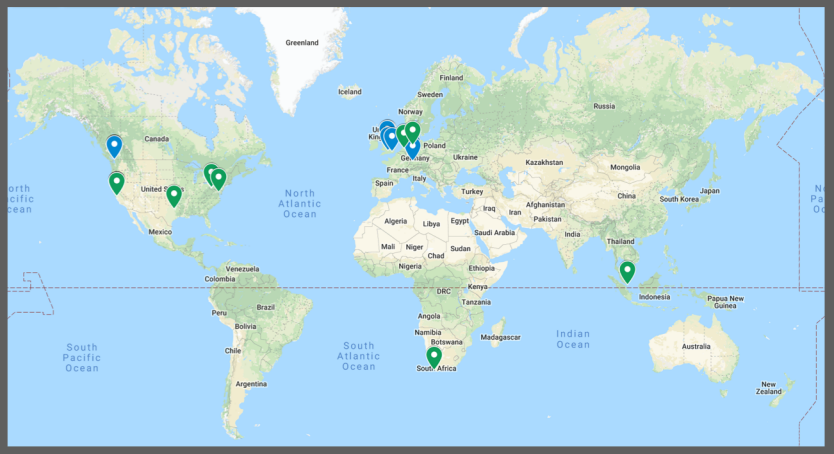
AstraZeneca - Process Engineer 2015 - 2016

Niblett, Daniel, et al. "Development and evaluation of a dimensionless mechanistic pan coating model for the prediction of coated tablet appearance." International journal of pharmaceutics 528.1-2 (2017): 180-201.

ICURe Programme

Innovation to Commercialisation of University Research (ICURe)

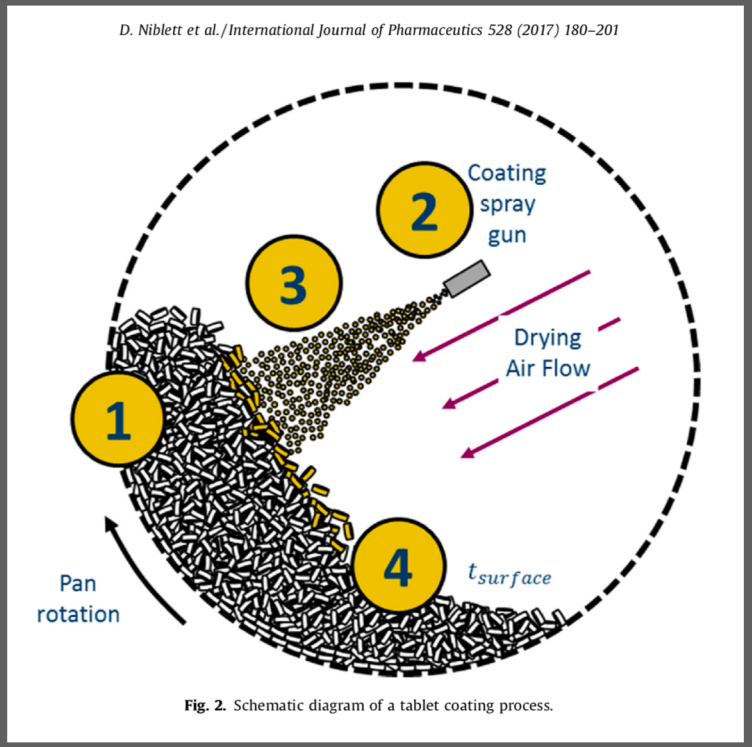
- Visit Expo and Industries worldwide (Oil&Gas, Pharmacuetical, Energy, Environmental …)
- Understand and learn about the pore scale challenges with flow and transport in porous media

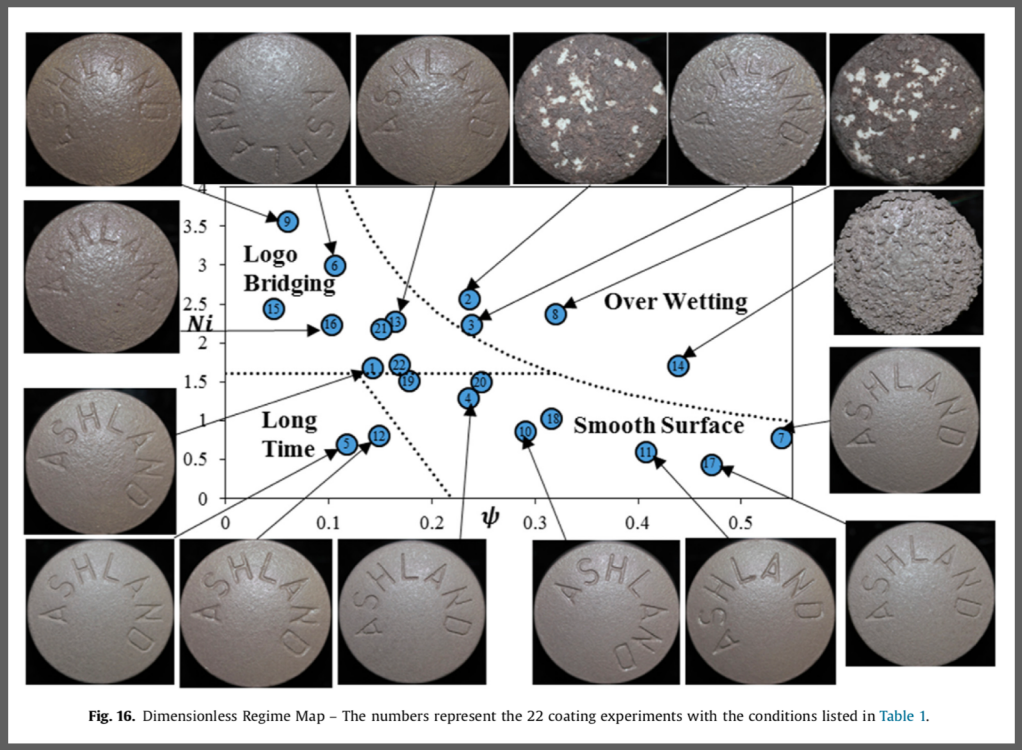


MANCHESTER 1824
The University of Manchester

ICURe

Mechanistic Models





Prediction from mechanistic understanding and modelling of local processes

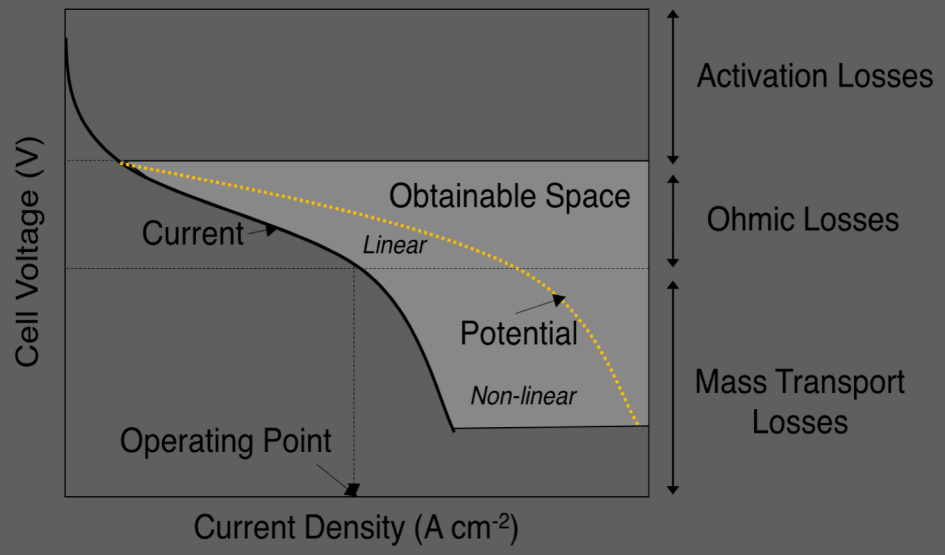
PhD Project

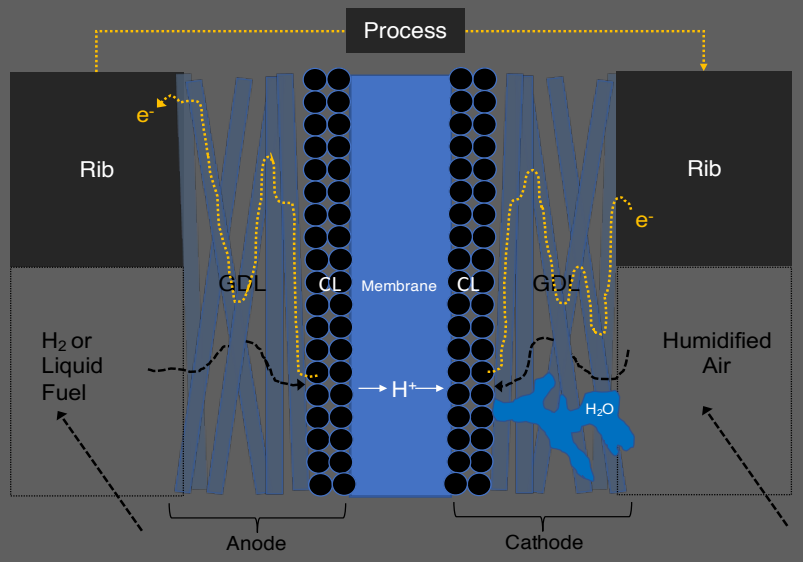
Optimisation of transport and flow through fuel cell gas diffusion layers using direct numerical simulations.

So Far

- Patent Idea – Looking to acquire patent before publication
- Investigation into the pore scale two-phase flow of water and air in fibrous gas diffusion layer (GDL)
- Relationship between fibrous microstructural design and effective transport properties
- Understanding the interfaces between gas channels, Microporous layer, GDL

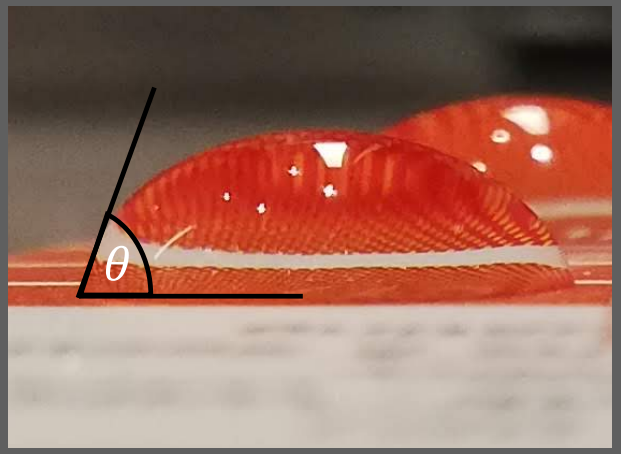
Fuel Cell Introduction





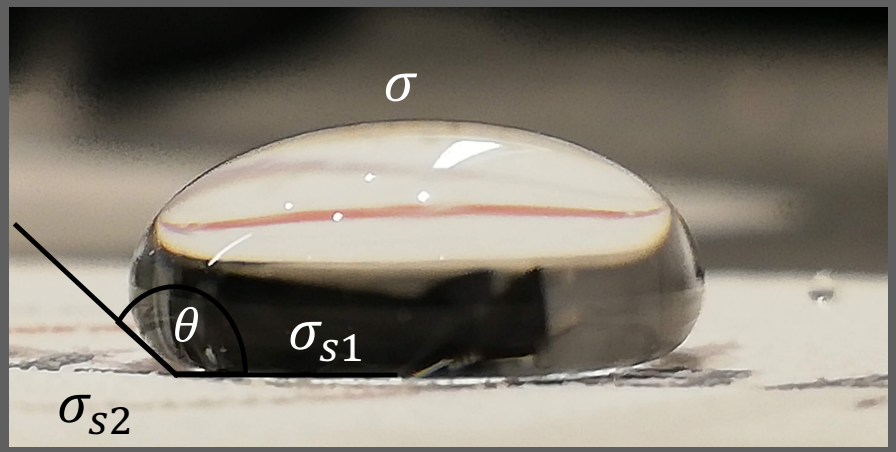
Wettability

"wetting fluid"

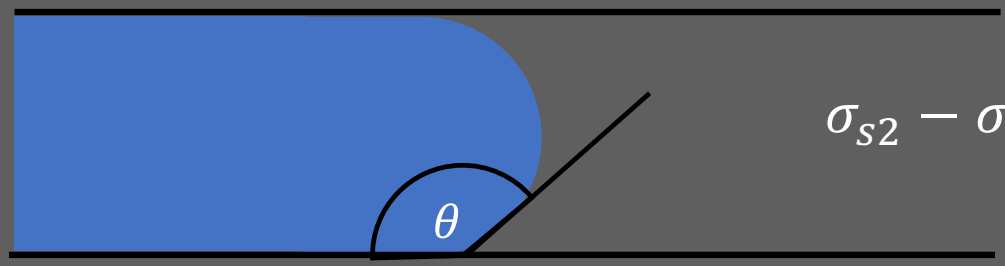


Hydrophilic $\theta < 90°$

"non-wetting fluid"

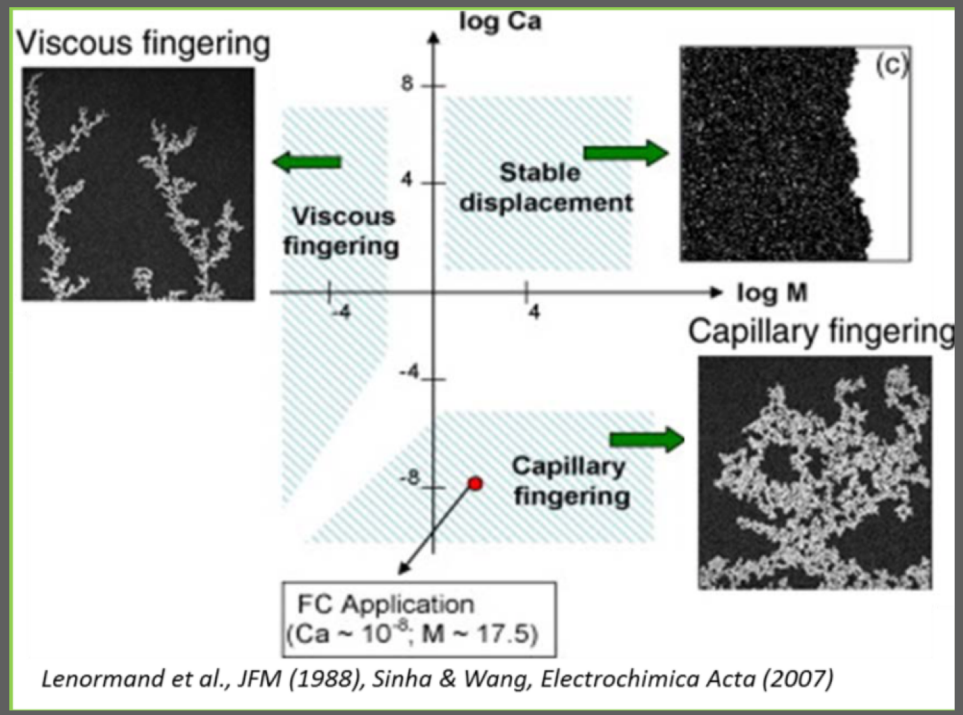


Hydrophobic $\theta > 90°$



$$\sigma_{s2} - \sigma_{s1} = \sigma^{nw} \cos\theta$$

Dynamic Properties



Lenormand et al., JFM (1988), Sinha & Wang, Electrochimica Acta (2007)

Capillary Number

$$\mathrm{Ca} = \frac{u\mu_I}{\sigma}$$

u Fluid velocity
μ_I Invading Fluid viscosity
σ Surface Tension

Viscosity Ratio

$$\mathrm{M} = \frac{\mu_I}{\mu_D}$$

μ_D Defending fluid viscosity

Where saturation is important, pore scale mechanisms cannot be ignored

Original Simulation Method

Volume of Fluid Method (VOF) – OpenFOAM

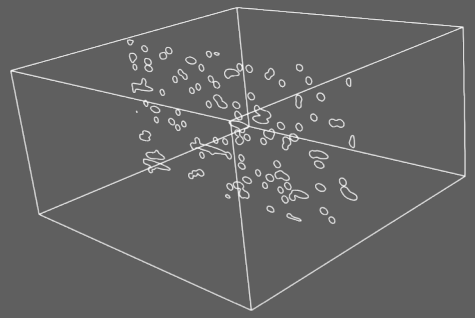
Interface Method – IsoAdvector – For sharp Interface

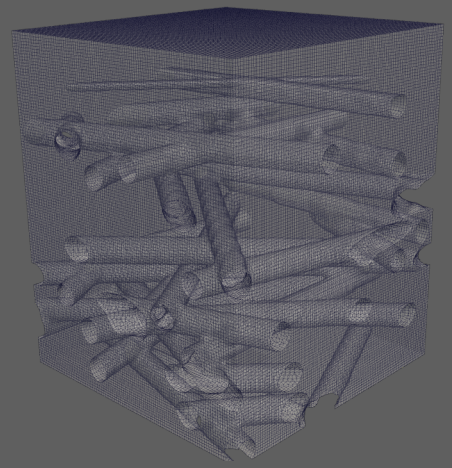
Problems:

- High resolution mesh needed between pore throats **10 cell width**
- Scales of system (mm to µm) results in small time step **10^{-8} s**
- Difficult to realise REV in 3D due to the mesh size **10^{-9} cells**
- Two-phase flow interface problems at low capillary numbers
  - Spurious currents
  - Smearing of interface – interface diffusion

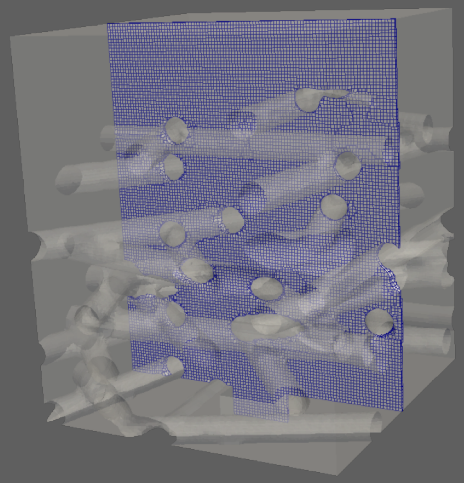
Domain and Simulation



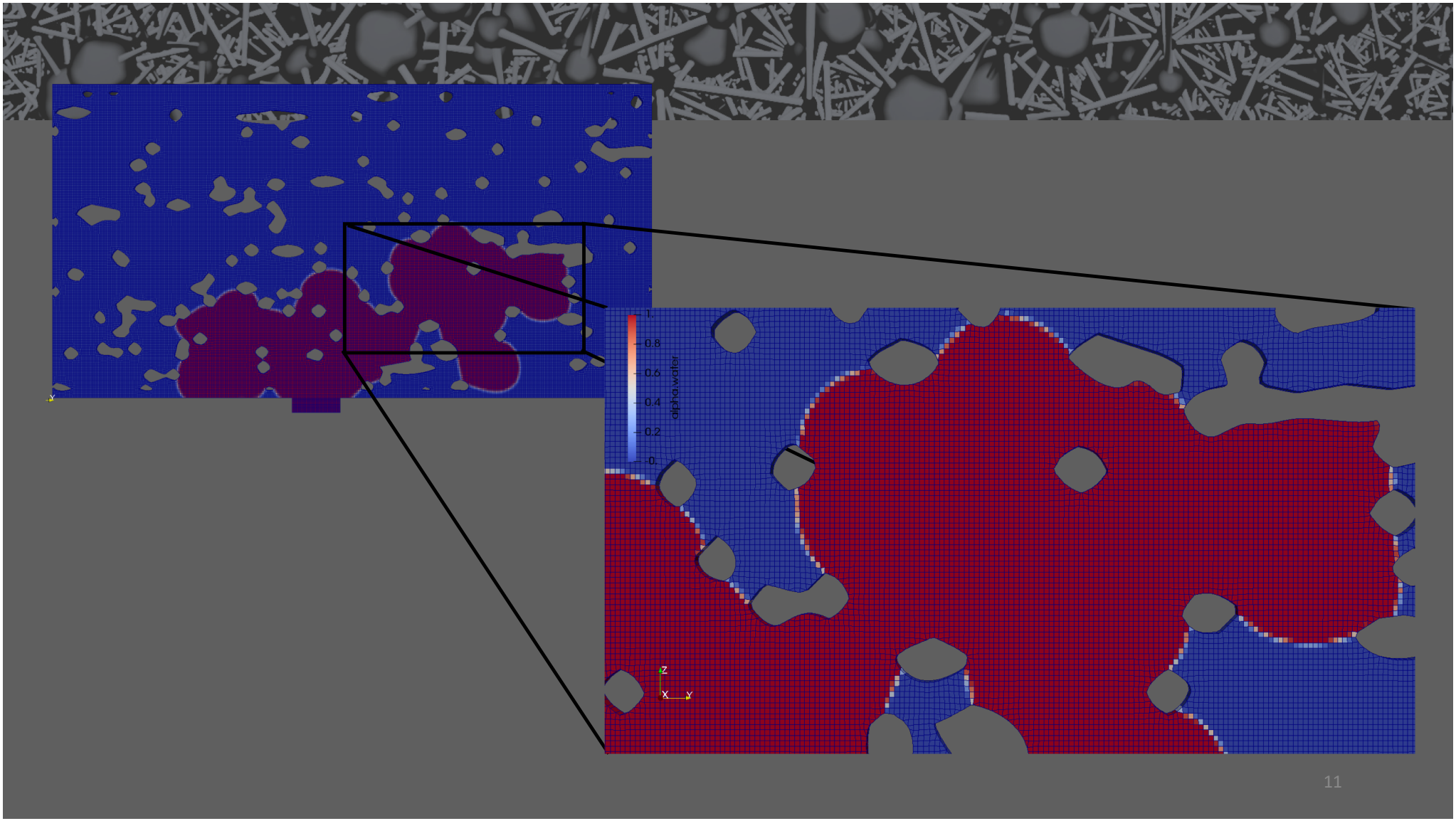




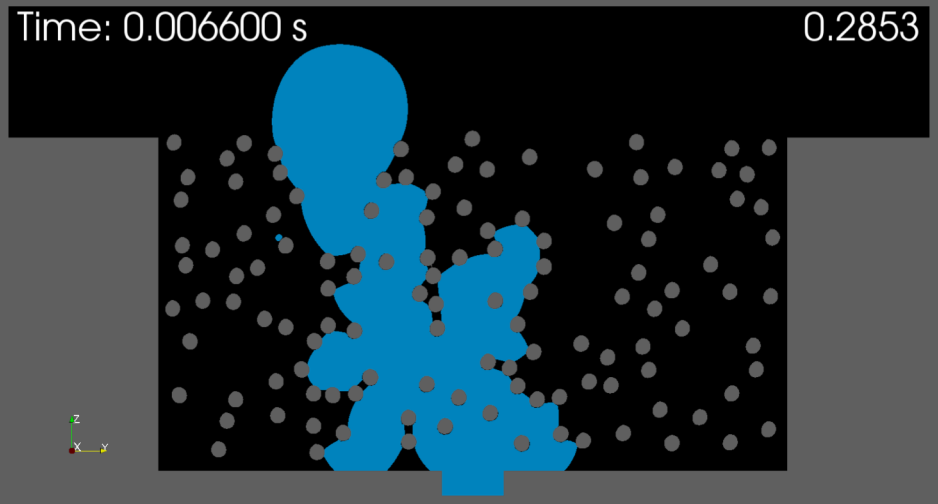
2D
Time Saving (1 week)



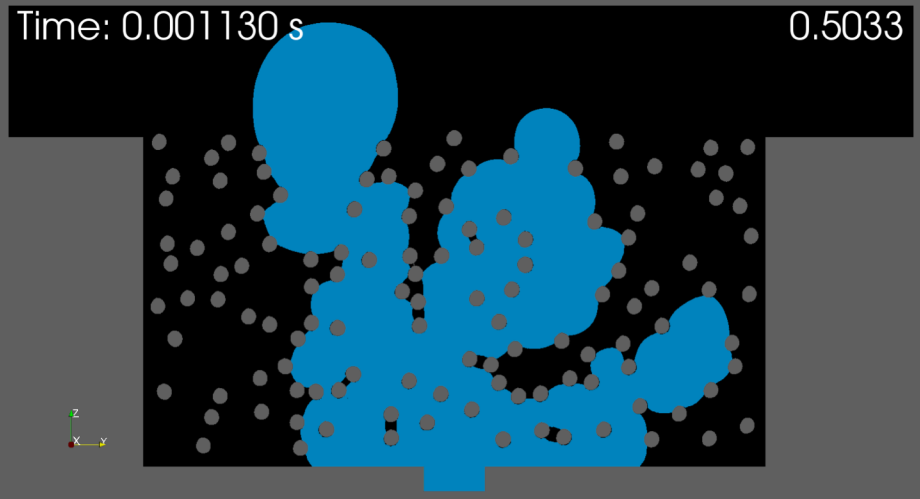
3D
More accurate
representation (1 month)


1
0.8
0.6
0.4
0.2
0
alpha.water
Z
X
Y

Capillary Number Effect



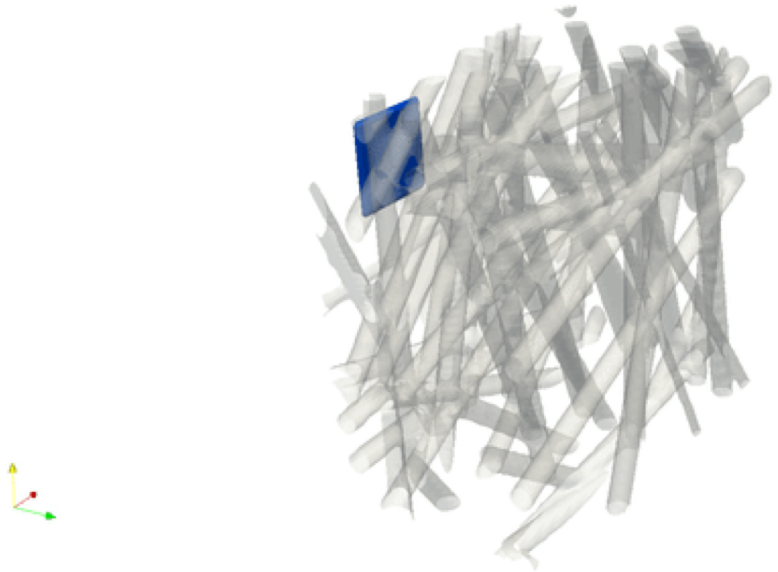
$Ca = 1.4 \times 10^{-3}$



$Ca = 1.4 \times 10^{-2}$

More pores invaded, GDL blocked for reactant access to catalyst layer

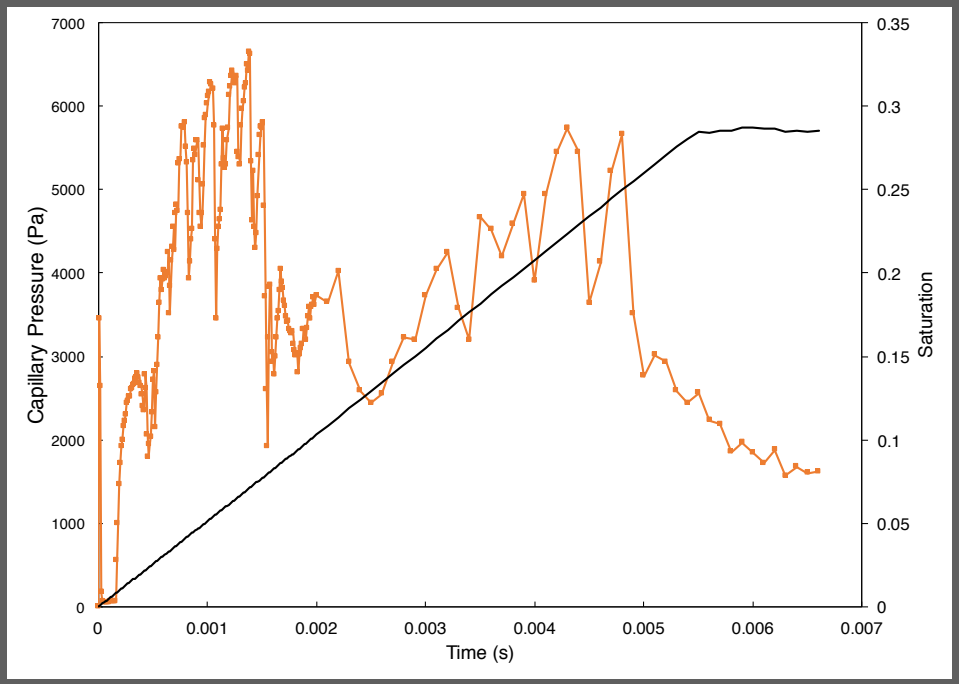
Two-phase Flow Animations



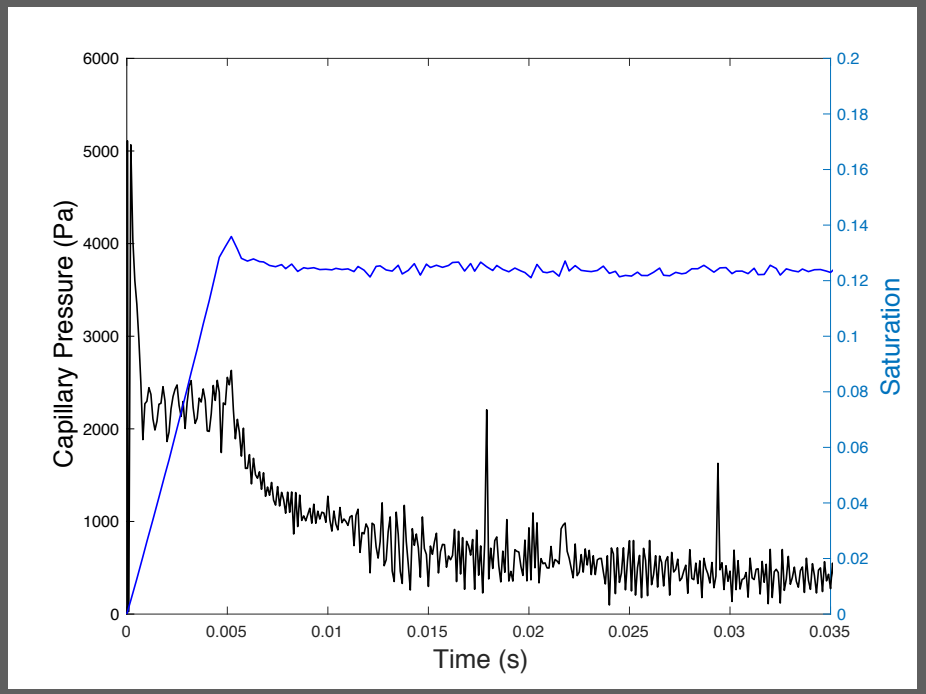


Patent Idea - Performance Increase

Can the GDL be improved?

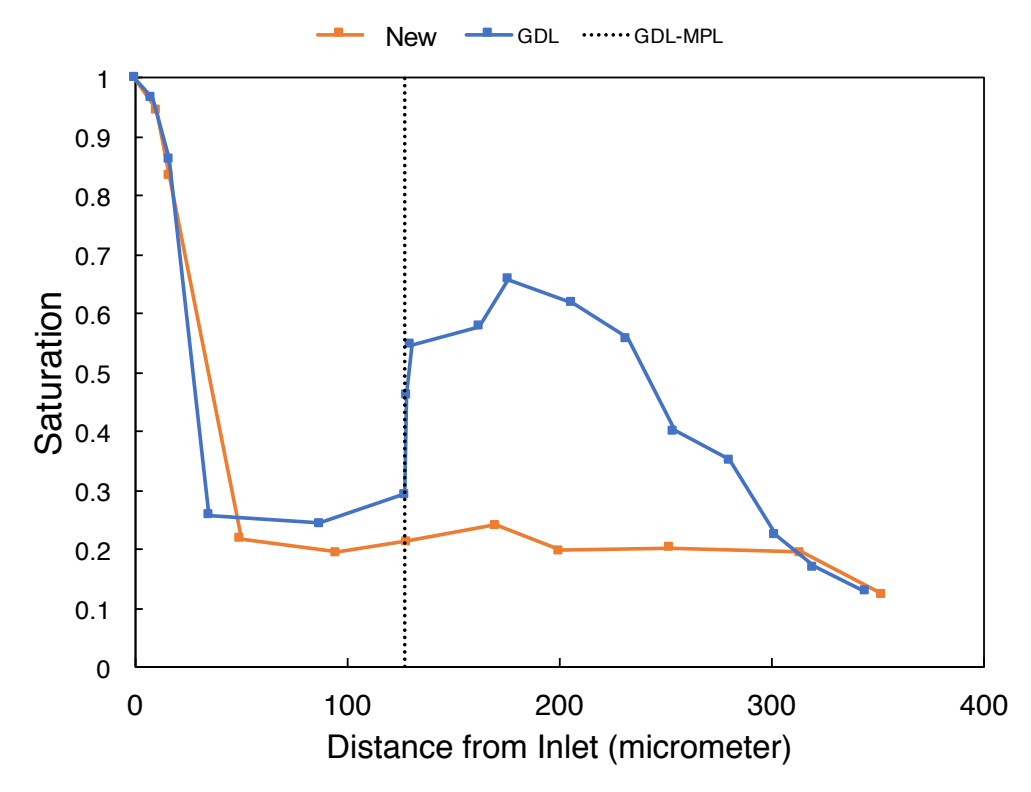


Standard



New Method

Simulations with Artificial MPL



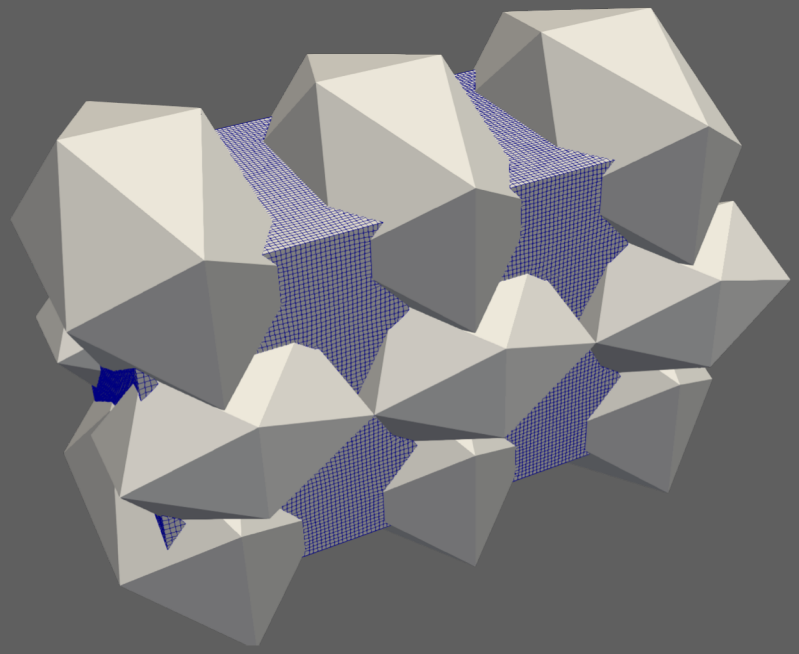
Simulation Results

- Water management at high current density
- MPL crack importance for water transport.
- New method could possibly improve water management

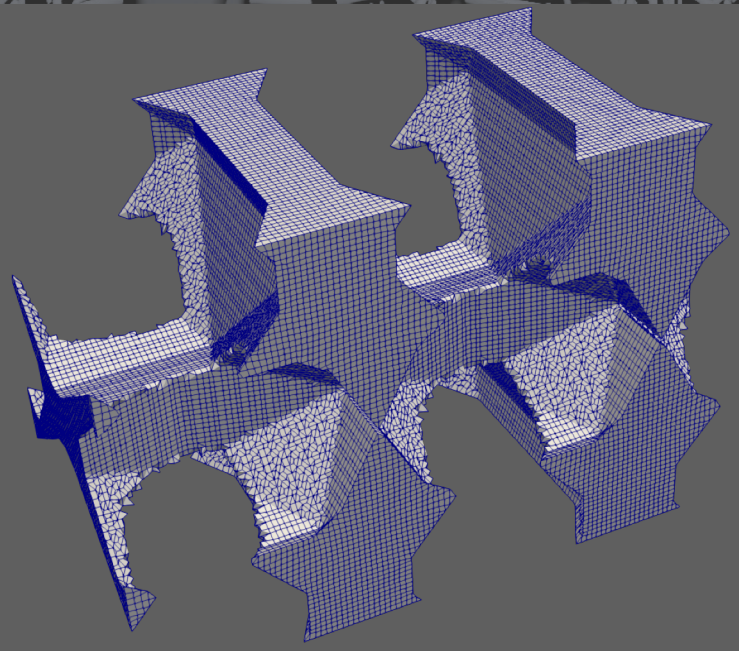

PORTRE
Pore-scale Transport Reaction Energy

Advantages and applications of pore-scale modelling

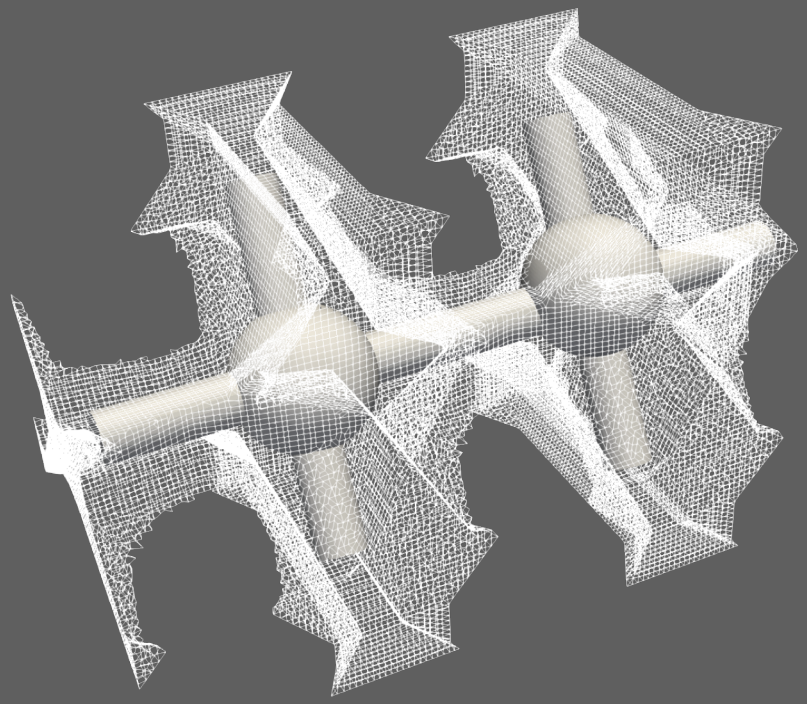
- Continuum-scale models are based on empirical and ***even incorrect*** assumptions.
- To couple phenomena it requires physically-based understanding of processes.
- Advances in computational makes the detailed pore-scale simulations more feasible.
- Evaluating the validity of new theories is not always feasible using experimental approaches.



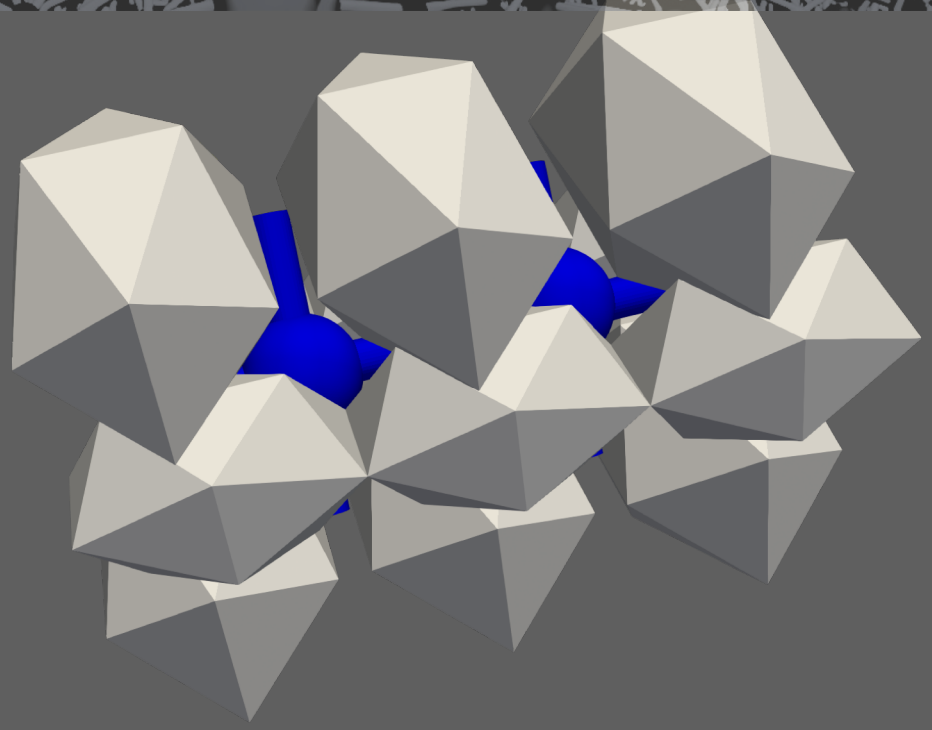
9 Pore Units



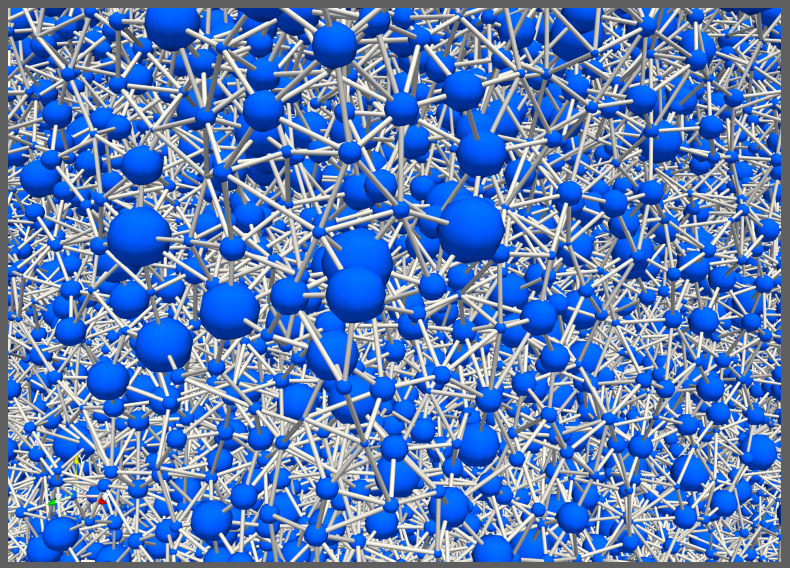
200,000 cells

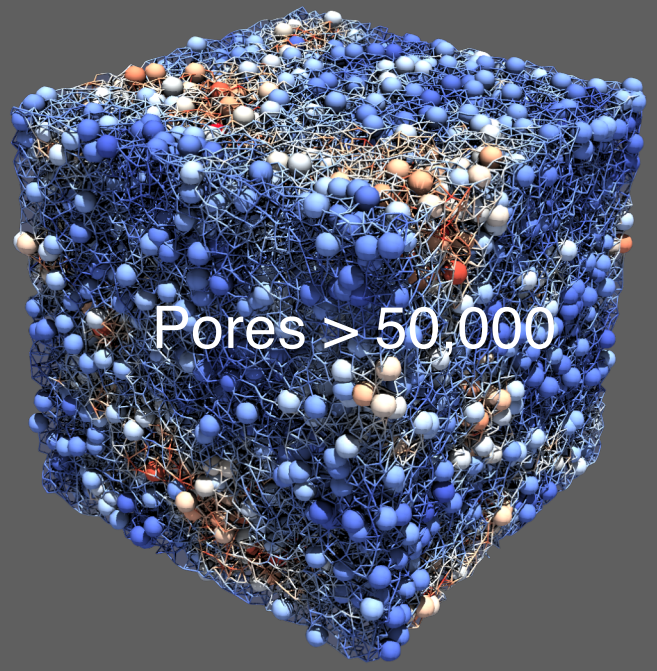


9 Pore Units



2 pore body
7 pore throat





Larger Domain Scales Achievable

FVM equivalent 1 billion cells

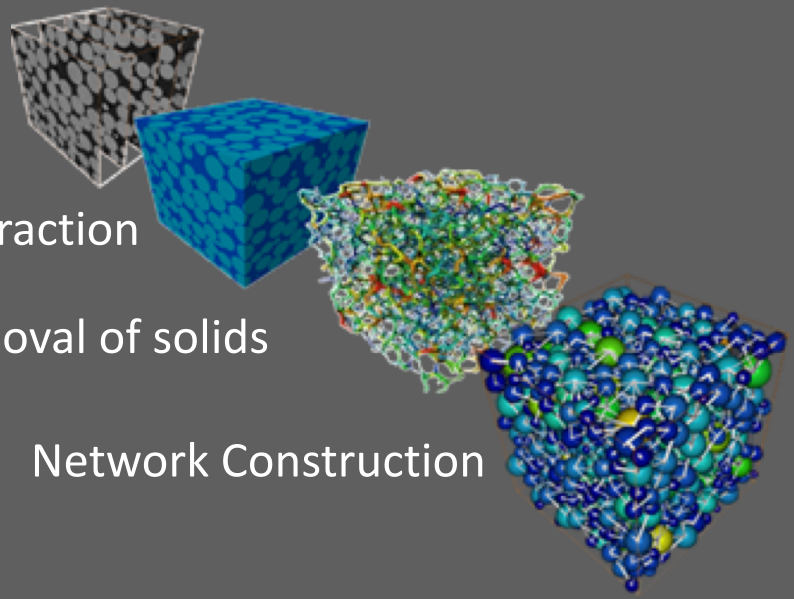
Network Extraction

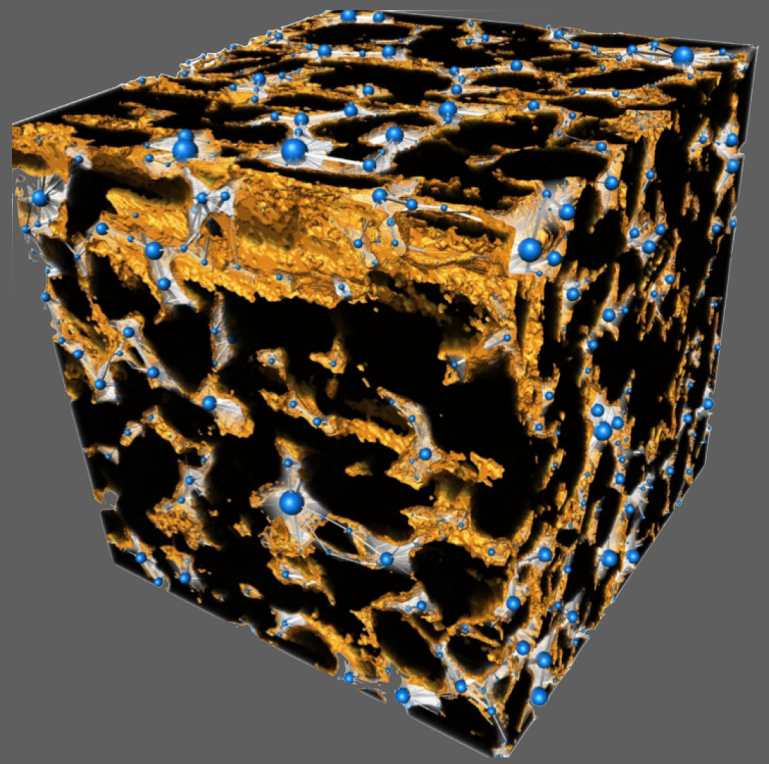
Micro-CT scan

Volume extraction

Removal of solids

Network Construction





Methodology

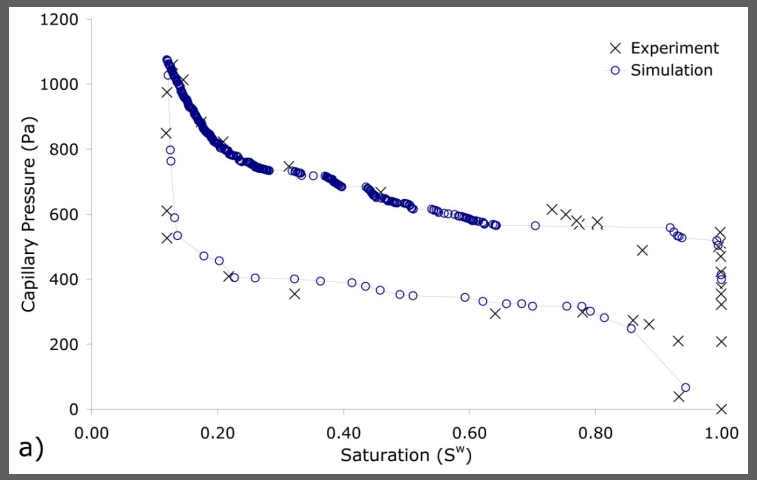
Low Reynolds number – stokes flow, Poiseuille flow

$$Re = \frac{\rho D u}{\mu} < 1$$

Interfacial Tension forces become important

$$P_c = P^n - P^w = f(S_w, \kappa_i)$$

Capillary Pressure (P_c) a function of saturation and specific interfacial area.



Network Continuity

Regular network mass conservation rules:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = j$$

j Sink/Source Term (Reactions, phase change …)

Incompressible flow

$$\frac{\partial \rho}{\partial t} = 0$$

Mass continuity simplifies to volume continuity across network and in pore units

$$\nabla \cdot u = 0$$

Network Continuity

The change in the saturation in time, and therefore volume of the pore i must be equal to the sum of all the flows into and out of pore i:

$$V_i \frac{\partial S_i^\alpha}{\partial t} + \sum_{j=1}^{N_i} Q_{ij}^\alpha = 0$$

Pore throat flow calculated using the pressure of phase between i and j hydraulic conductivity.

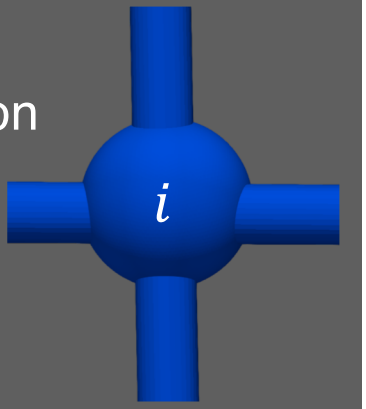
$$Q_{ij}^\alpha = K_{ij}^\alpha (P_i^\alpha - P_j^\alpha)$$

Hydraulic conductivity is affected by viscosity and interface configuration

$$K_{ij}^\alpha = f(k, \mu, \Delta_{ij})$$

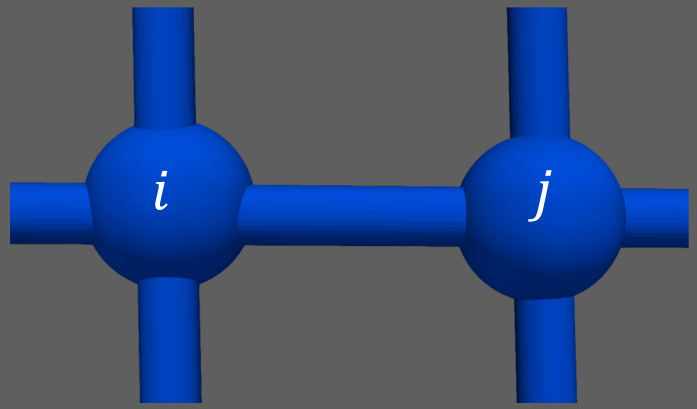
The sum of the non–wetting and wetting fluids must be unity.

$$S_n + S_w = 1$$



Fluid Flow

In each throat, the flow rate is calculated using Poiseuille equation:



$$q_{ij} = \frac{\pi}{8\mu} r_{ij}^{4} \frac{P_i - P_j}{l_{ij}}$$

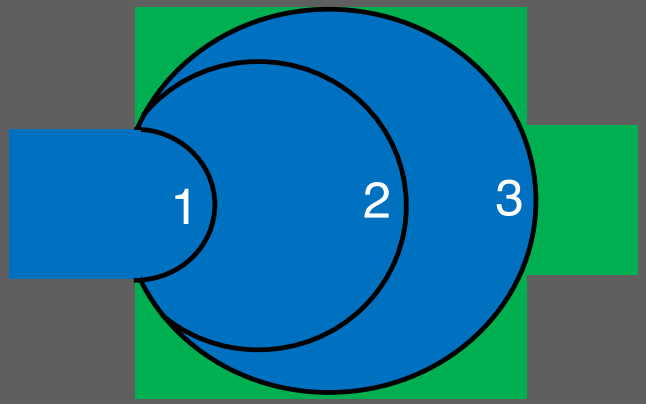
K_{ij}^{α}

Geometry (cross section, length) and fluid properties (viscosity, contact angle)

Local rules

Local rules within pore body:

- Drainage – Invasion of non-wetting phase
- Imbibition – Invasion of wetting phase
- Shape effect on filling mechanisms



$$P_i^C = 2\sigma^n \kappa_i$$

κ_i Interface curvature inside pore body

κ_i found by either analytical or computational methods for various pore shapes and wettability

$$\kappa_i = f(S_w, \theta, \Delta_i)$$

PNM Methodology

Entry Capillary Pressure $$P_c = \frac{2\sigma \cos\theta}{r}$$

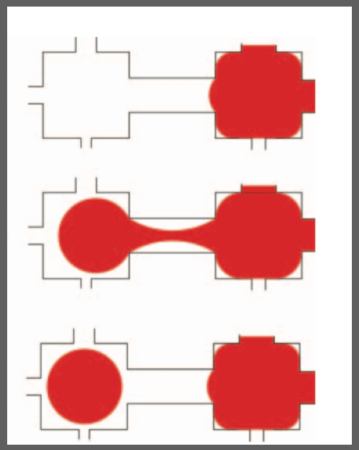
- If P_c is larger than the entry capillary pressure, the non-wetting fluid will invade the pore.
- In Quasi-static PNM, Capillary pressure can be set and all the pores possible will be filled.
- During imbibition (invasion of the wetting fluid), the only resistance to flow is from the pore body filling.

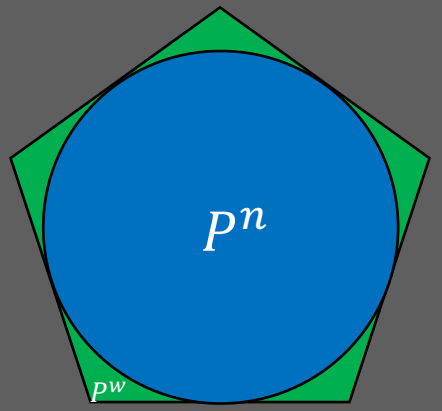
Relative Permeability

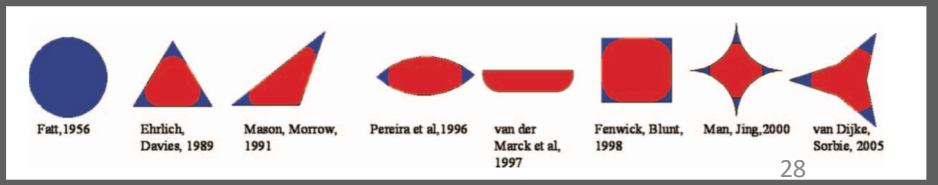
In two-phase flow, both fluids can occupy pore throats and bodies

Hydraulic conductivity of both non-wetting and wetting phases allows for simulation of real mechanisms:

- Counter-current and co-current flow
- Trapping and snap off
- Interface dynamics and ganglia movement







Quasi-static and Dynamic



$$p_i^n - p_i^w = f(\kappa_i) = f(s_i^w)$$

$$s_i^w + s_i^n = 1$$

appended to the local rules:

$$K_{ij}^{\alpha} = K_{ij}^{\alpha}(\kappa_{ij}, \mu_{ij}^{\alpha})$$

$$p_{e_{ij}}^c = f(r_{ij})$$

$$p_{s_{ij}}^c = f(r_{ij})$$



$$V_i \frac{\Delta s_i^{\alpha}}{\Delta t} = -\sum_{j=1}^{N_i} Q_{ij}^{\alpha}, \alpha = w, n$$

$$Q_{ij}^{\alpha} = K_{ij}^{\alpha}(p_i^{\alpha} - p_j^{\alpha})$$

$$p_i^n - p_i^w = f(\kappa_i) = f(s_i^w)$$

$$s_i^w + s_i^n = 1$$

appended to the local rules:

$$K_{ij}^{\alpha} = K_{ij}^{\alpha}(\kappa_{ij}, \mu_{ij}^{\alpha})$$

$$p_{e_{ij}}^c = f(r_{ij})$$

$$p_{s_{ij}}^c = f(r_{ij})$$

Multi-physics Modules

- Solute Transport

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (vc) + R$$

- Electro-kinetic flow
- Reactive transport
- Mixed Wettability
- Phase change
- Dynamic alteration to the PNM
- Mechanisms for synthetic porous materials

Transport and Speed Validation

1 to 24 h (32 p)

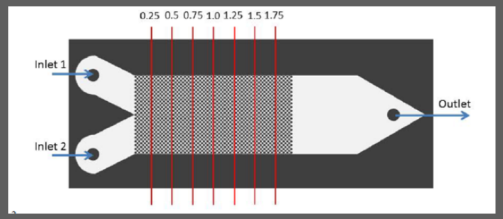
1 to 45 h (32 p)

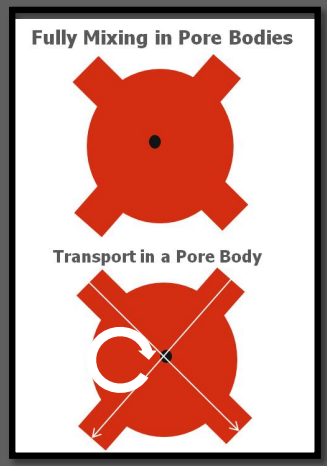
2 min (1 p)
1 min (1 p)

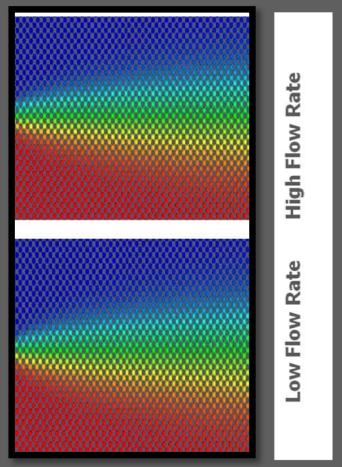
1 to 7 day
(46 to 96 p)

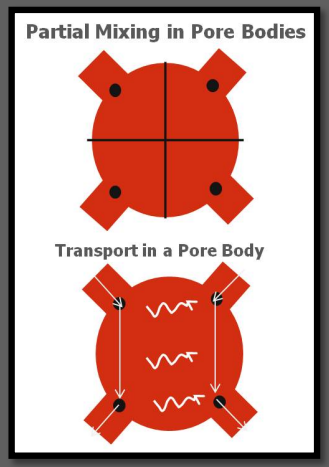
4 to 7 hours

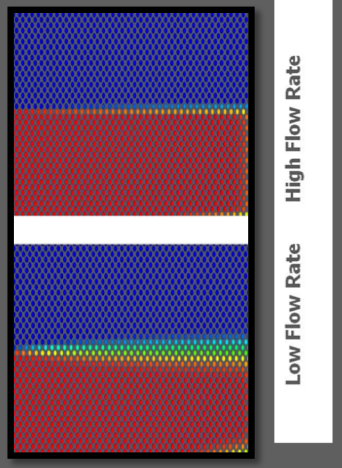
Name	Institution	Numerical Method for Fluid Flow
SNL-LB	Sandia National Laboratory	lattice Boltzmann
UI/LANL-LB	University of Illinois and Los Alamos National Laboratory	lattice Boltzmann
SGS-PN	Shell	pore network
UT-PN	University of Texas	pore network
PNNL-CFD	Pacific Northwest National Laboratory	computational fluid dynamics - finite volume
PNNL-C	Pacific Northwest National Laboratory	(continuum) integrated finite difference

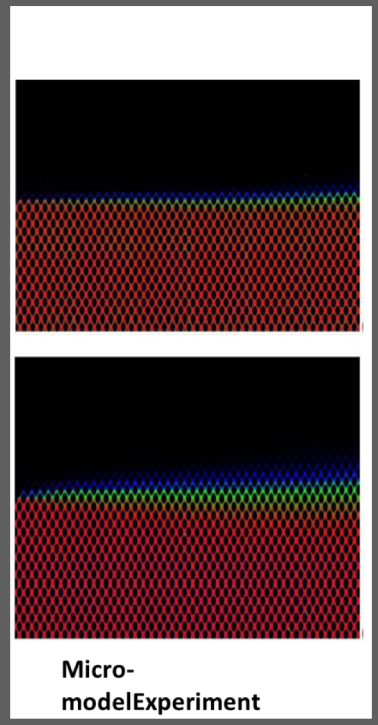








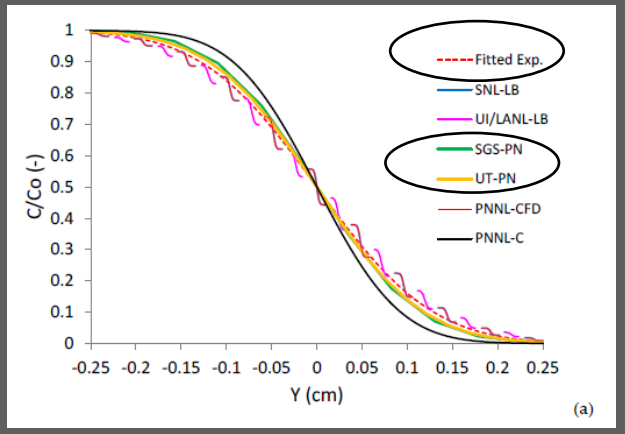




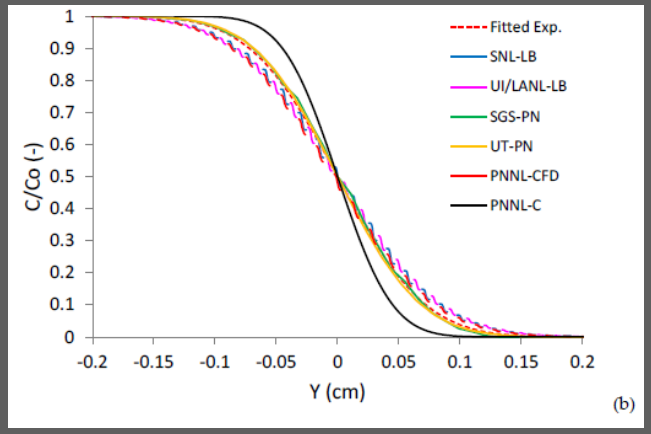
Ref: Oostrom et al, Comp Geo, 2014, 1-23

Experimental Validation

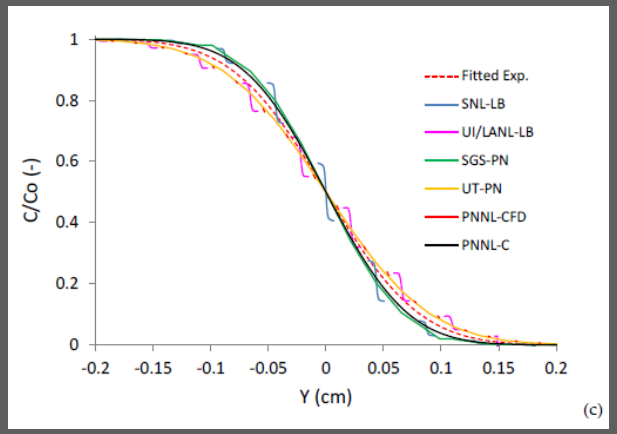
Experiment I; effect of injection rate



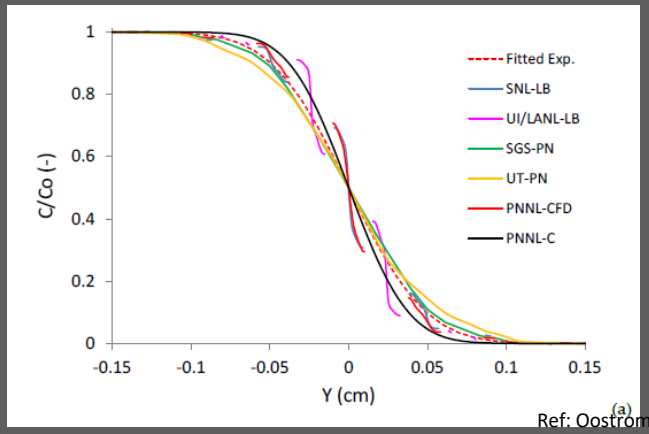
Experiment II; effect of pore size



Experiment III; effect of aspect ratio

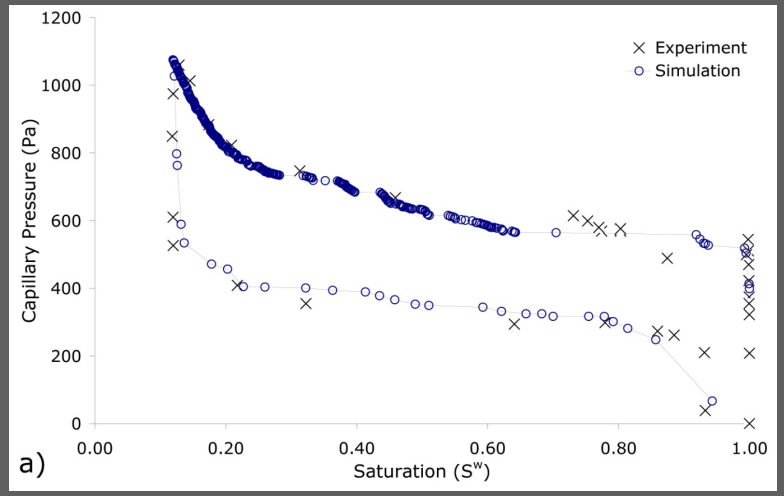


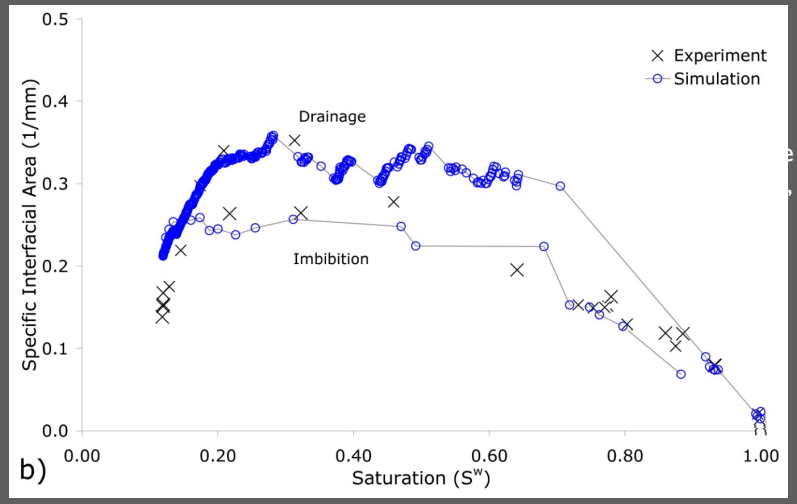
Experiment IV; effect of heterogeneity



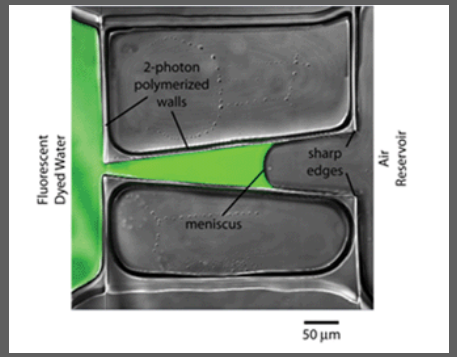
Ref: Oostrom et al, Comp Geo, 2014, 1-23

Two-phase pore-network models: simulations vs. experiments



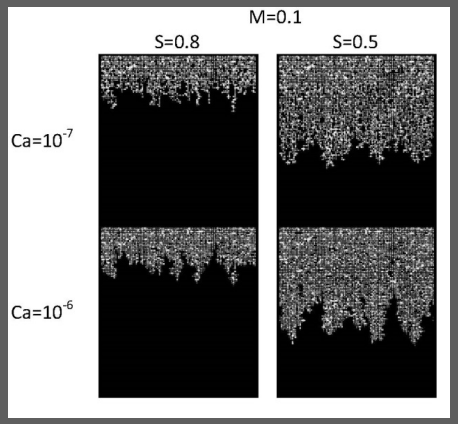


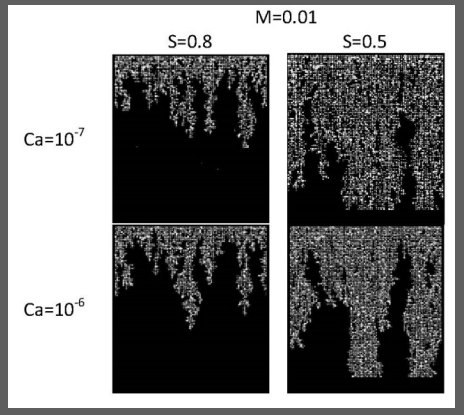
Generally, the imbibition saturation curve has not been able to be accurately modelled

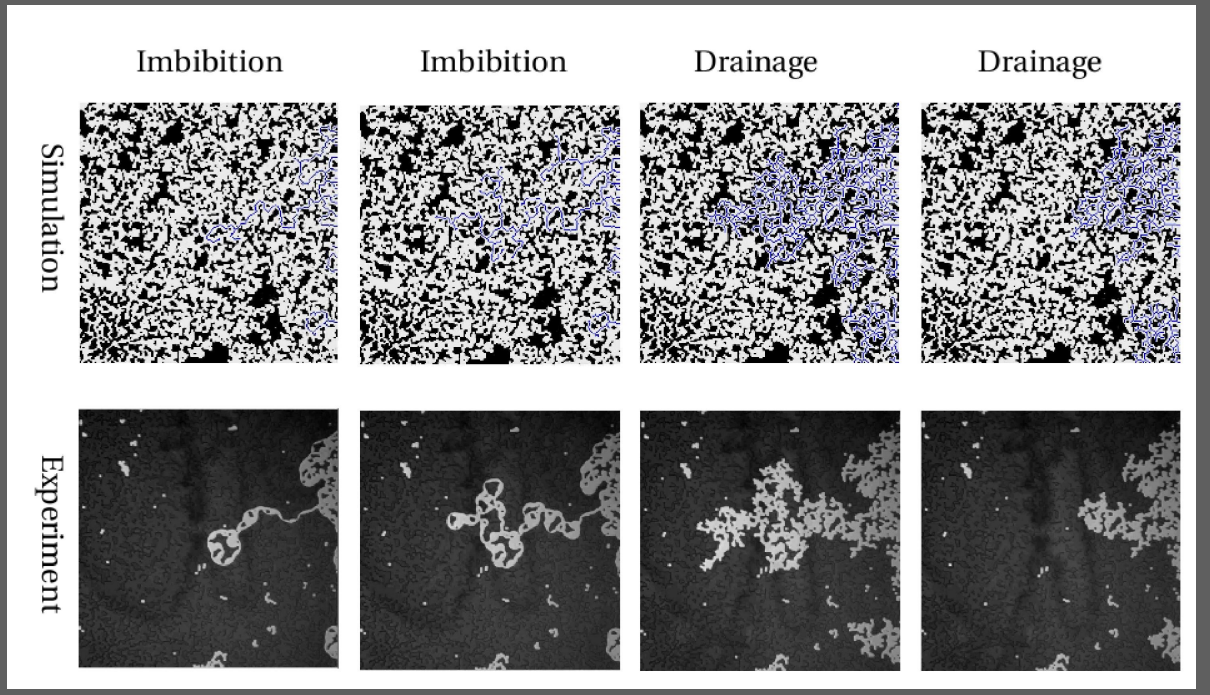


An irregular unstrucutred network with hyperbolic polygonal cross sections.
Joekar-Niasar et al, WRR, 2010

Saturation Patterns







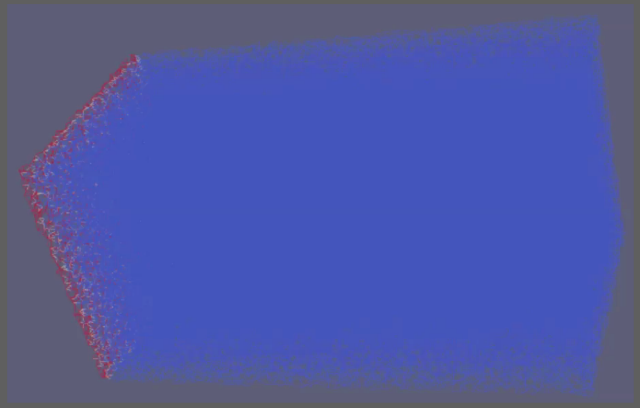
-Joekar-Niasar et al, WRR, 2009

-Joekar-Niasar, V., Hassanizadeh, S. M. (2011), International Journal of Multiphase Flow

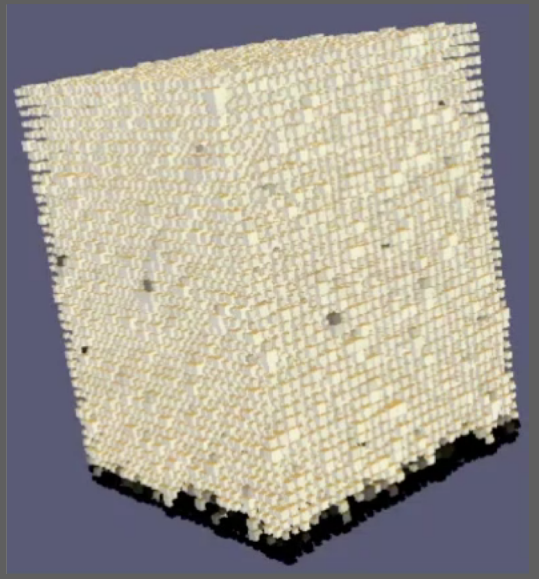
-Joekar-Niasar, V., Hassanizadeh, S.M. (2011), WRR

-Joekar-Niasar, V., Hassanizadeh, S.M. (2012), Transport in Porous Media

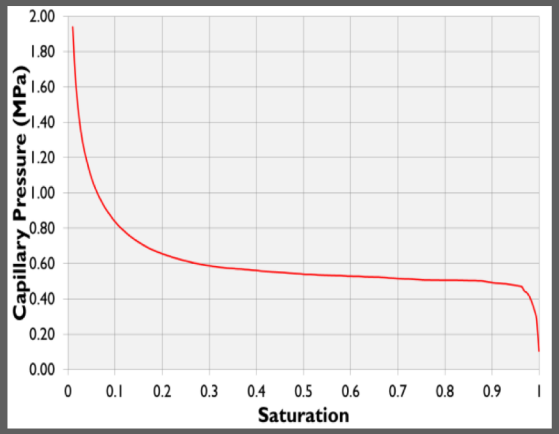
Dynamic Transport and Flow

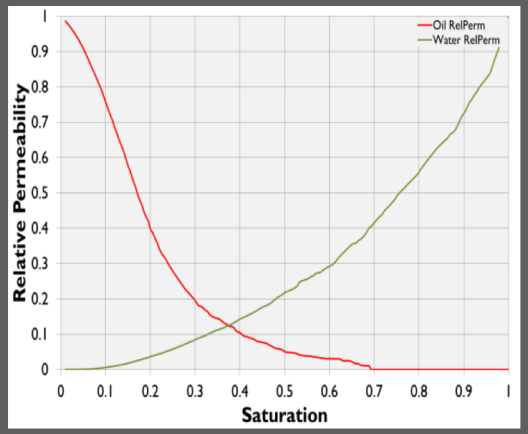


Pore-scale simulation of advection-diffusion in a sandstone rock.

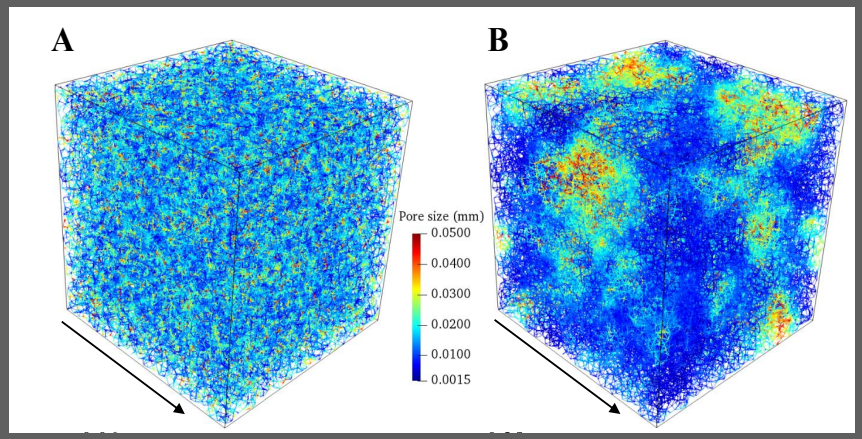


Dynamic Two-phase flow simlation of viscous fingering



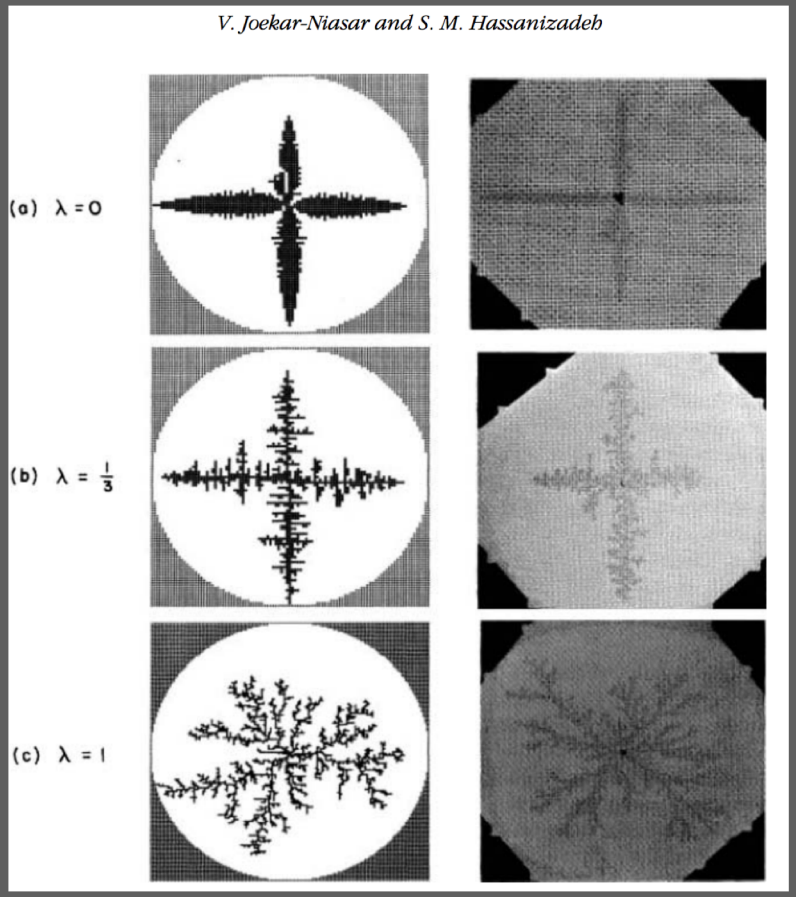


Capillary Pressure Saturation and Relative Permeability Saturation curves



Uncorrelated (A) and correlated (B) pore networks (56,000 Pores)

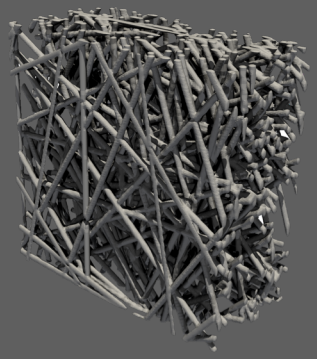
V. Joekar-Niasar and S. M. Hassanizadeh



Applications

Various Applications with flexible added physics:

- Oil & gas reservoir engineering
- Groundwater
- Pharmaceuticals
- Fuel Cell Electrodes
- Battery Electrodes
- Filtration



What other mechanisms or areas could this be applied?

Discussion

- Compared to other pore-scale modelling techniques, pore-network modelling can still provide more flexibility in tractability and decoupling of processes. There is a huge potential in further development of hybrid pore-scale models.
- Pore-scale modelling provides valuable insight into physics of porous media phenomena, such as multiphase flow, mixing, .., given than some processes have never been studied using such models.
- Multi-process pore-scale modelling is an emerging area
- Investment in “benchmarking” of various pore-scale models is on going.

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Interest

- Applications to various industries will uncover future research an commercial demands, are there any areas where this could apply?

- Any questions?

Thank you!

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