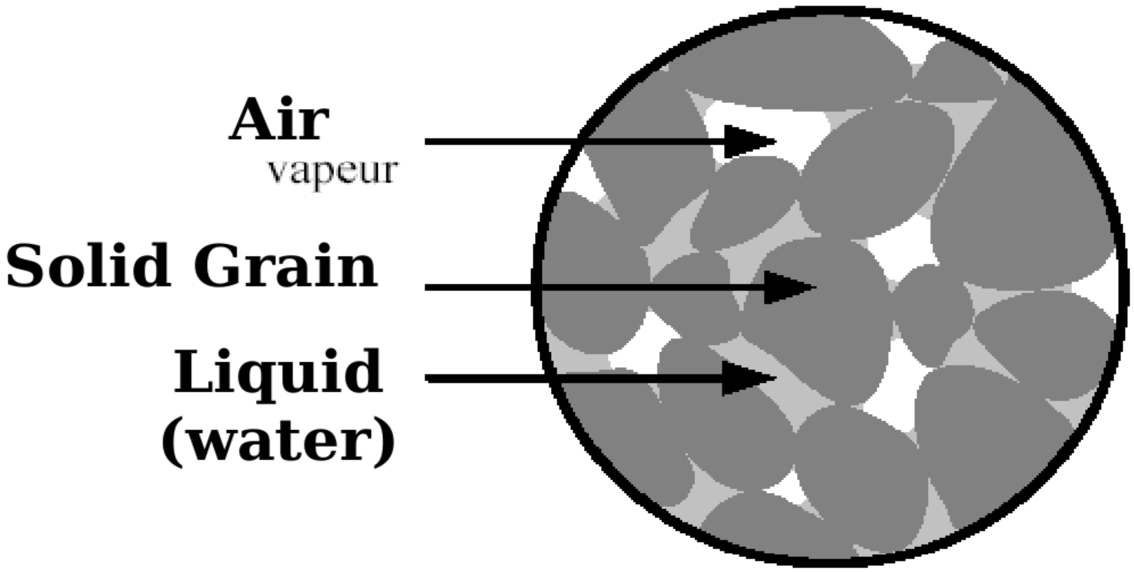
Discrete Element Modeling
Part 3. Two Phase Flow

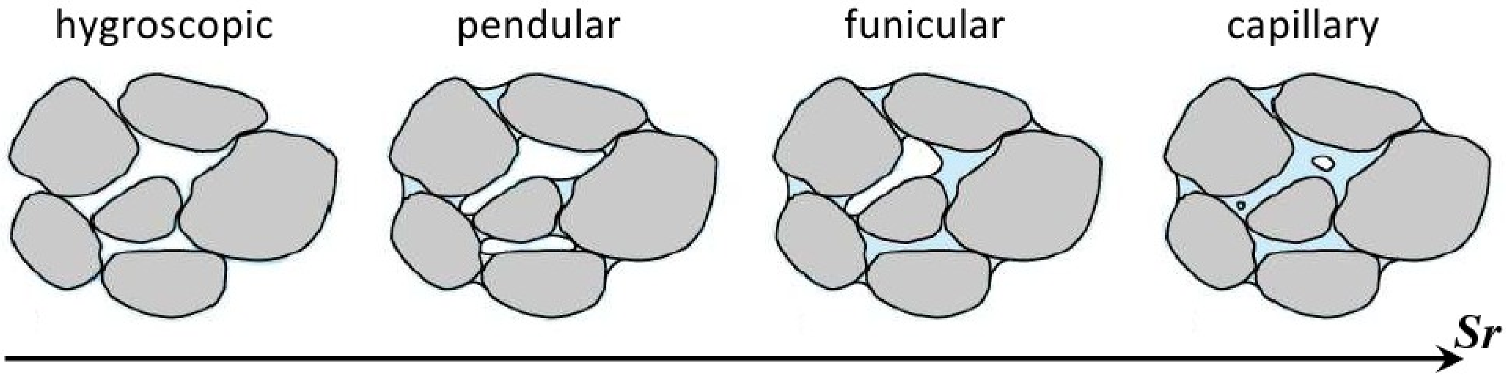
Bruno Chareyre

Part 3. Two Phase Flow

- macro-continuum scale
- micro-continuum scale
- pore scale

Capillarity





Macro-scale modeling

Unknowns:

air pressure p_n,

water pressure p_w,

water content S_r ("sat. degree")

Equations:

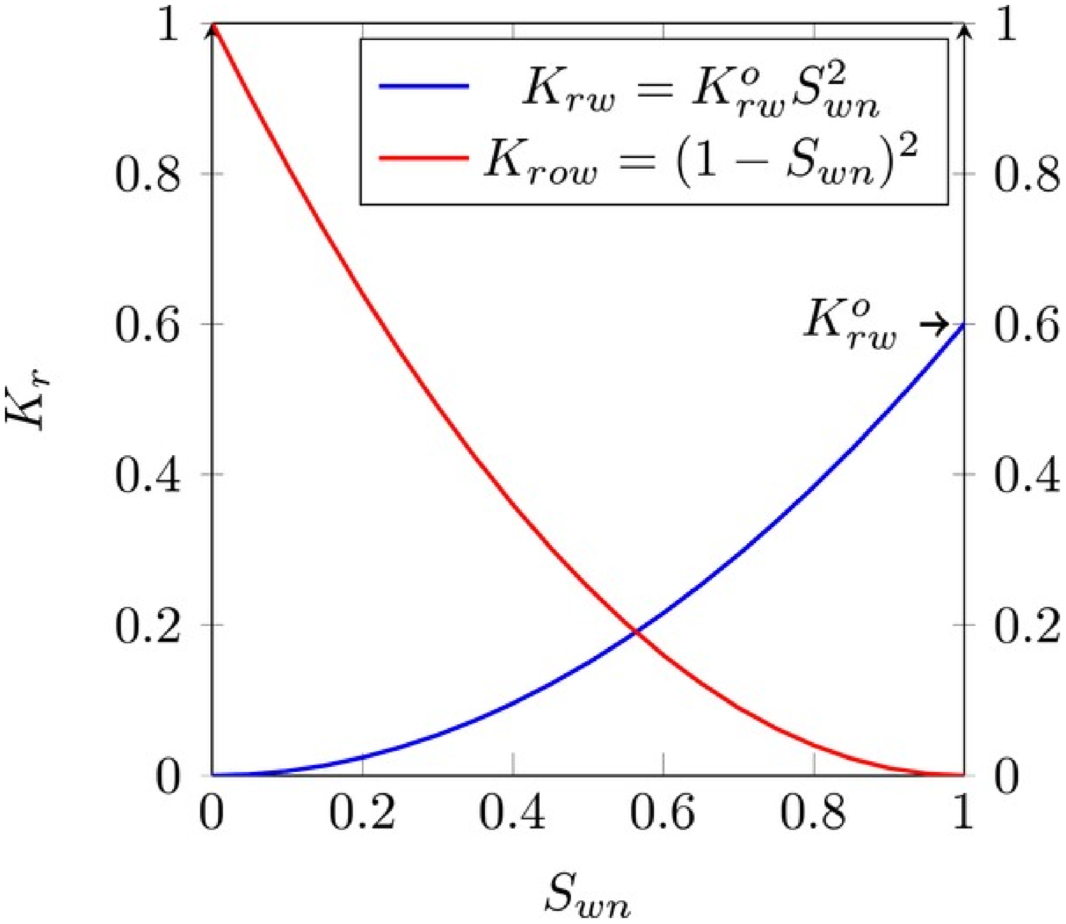
$\mathrm{div}(v_w - v_s) + \mathrm{d}S_r/\mathrm{d}t = 0$ (mass balance)

$p_c = p_n - p_w = p_c(S_r)$ (water retention)

$\mathrm{K} = \mathrm{K}(S_r)$ (Darcy with partial perm.)

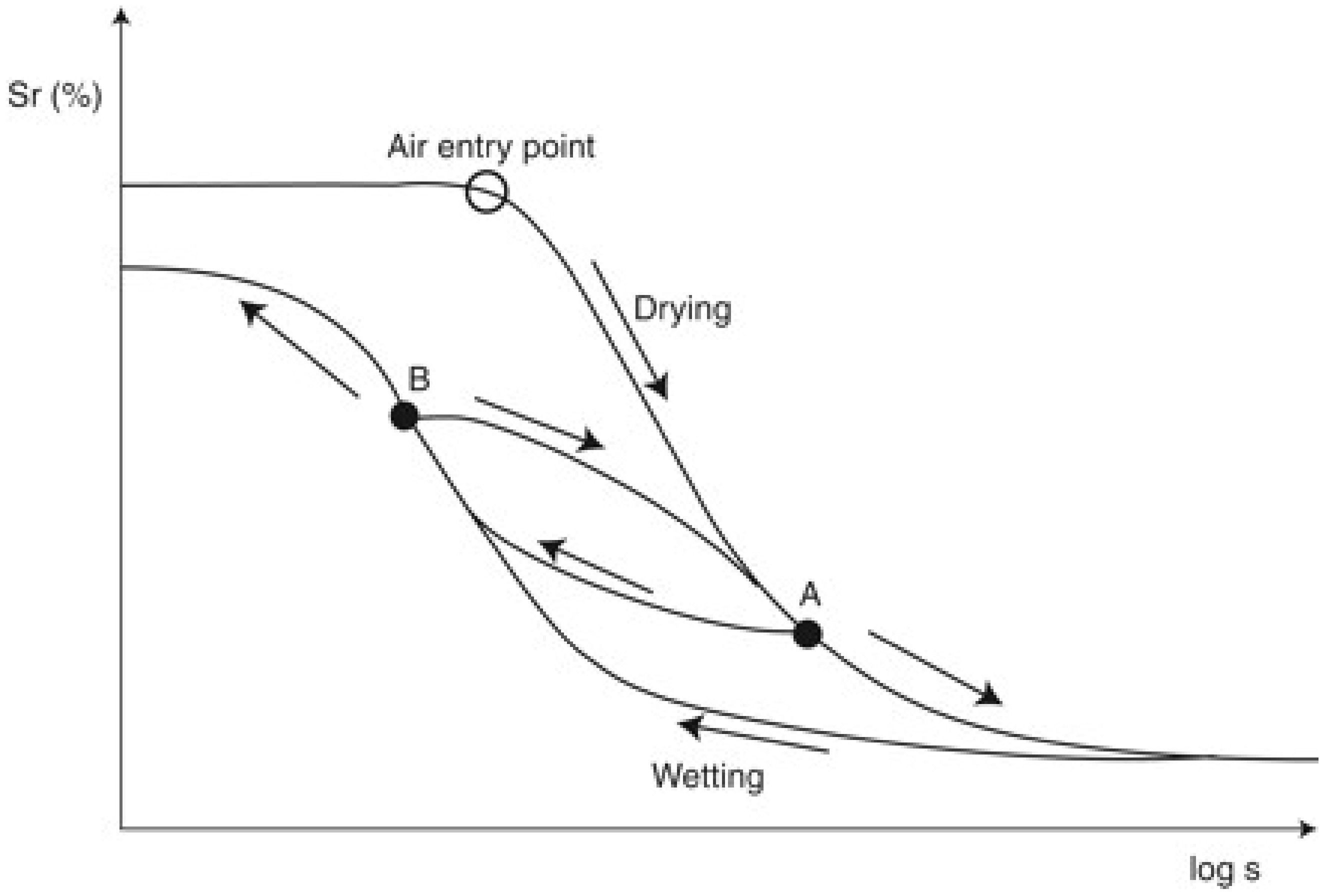
$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - S_r p_c \mathbf{I}$ (Bishop's effective stress)

Macro-scale modeling



Relative permeability, Brooks & Corey (1964)

Macro-scale modeling



Relative permeability, Brooks & Corey (1964)

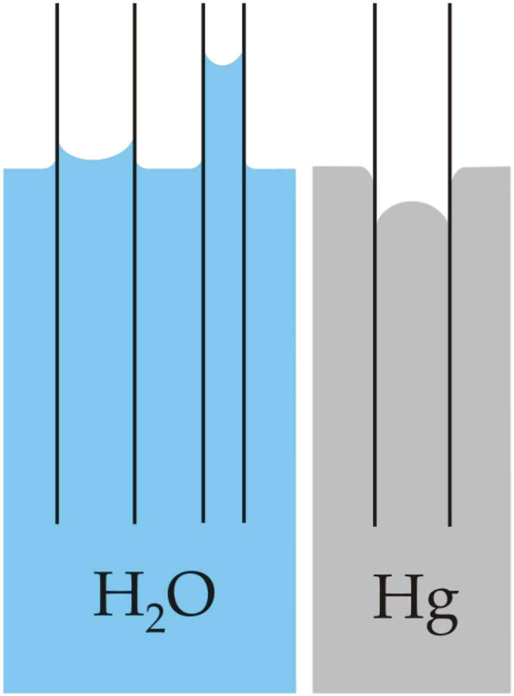
Micro-scale modeling

Unknowns:

- air pressure p_n,
- water pressure p_w,
- geometry of phases and interfaces

Jurin's law

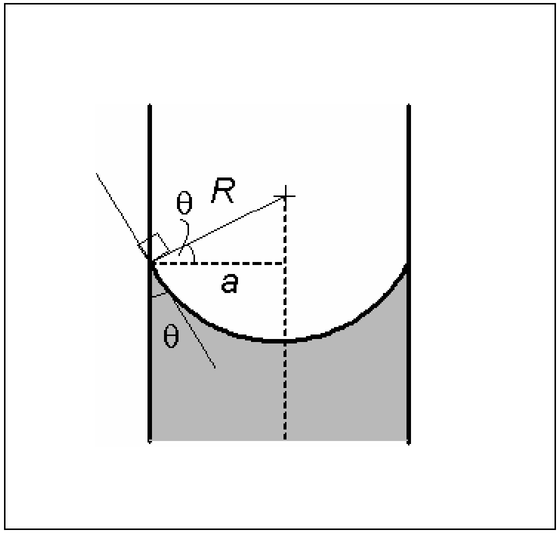
$$h = \frac{2\gamma\cos\theta}{r\rho g}$$



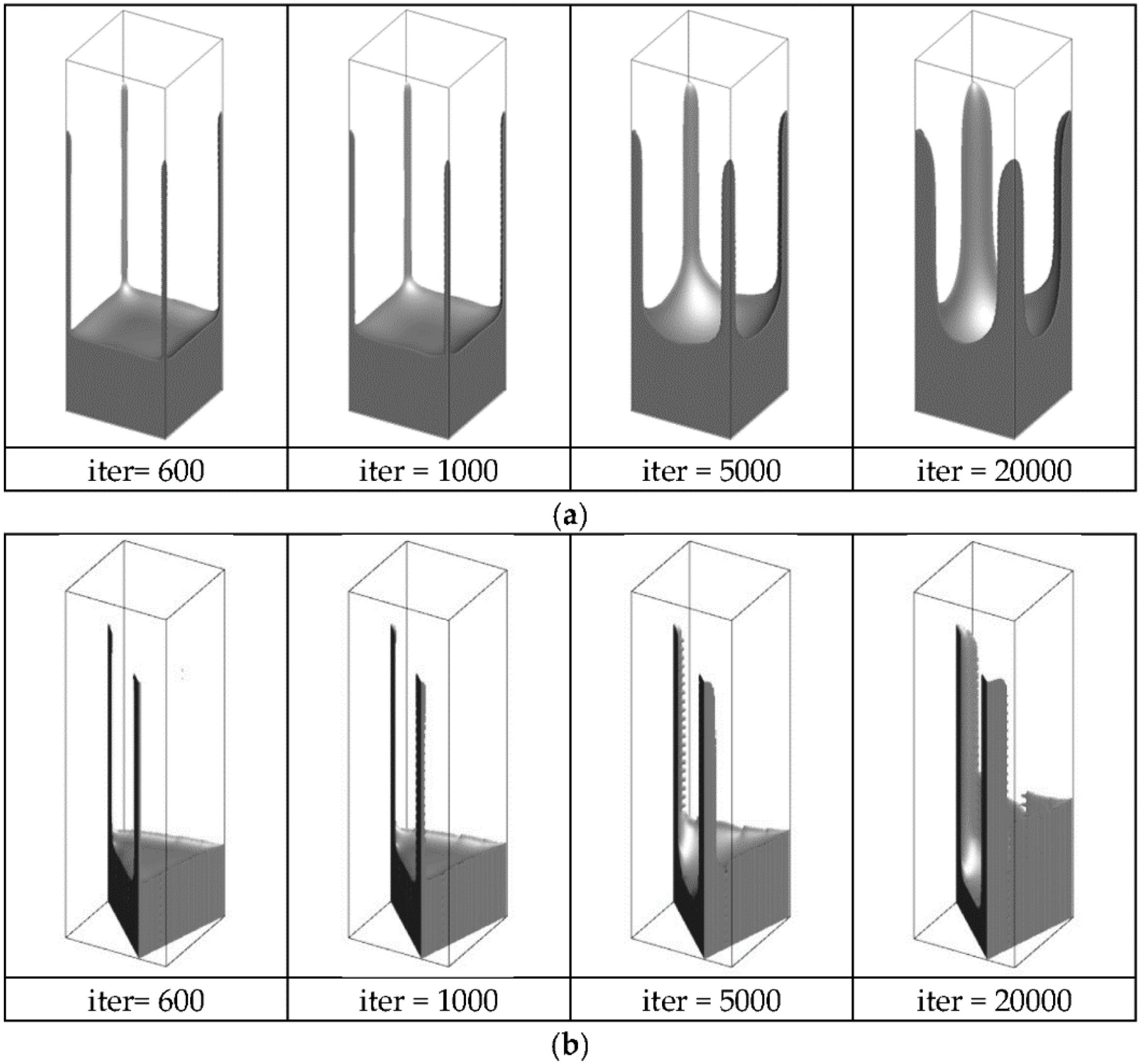
Equations:

Young-Laplace

$$\begin{aligned}\Delta p &= -\gamma\nabla\cdot\hat{n}\\ &= 2\gamma H\\ &= \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\end{aligned}$$

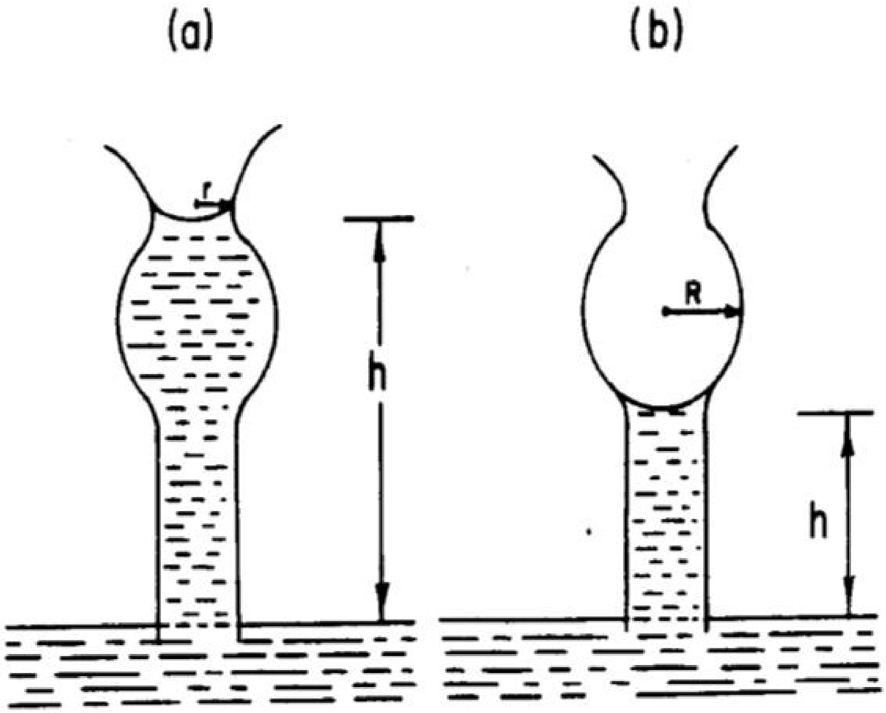


Micro-scale modeling



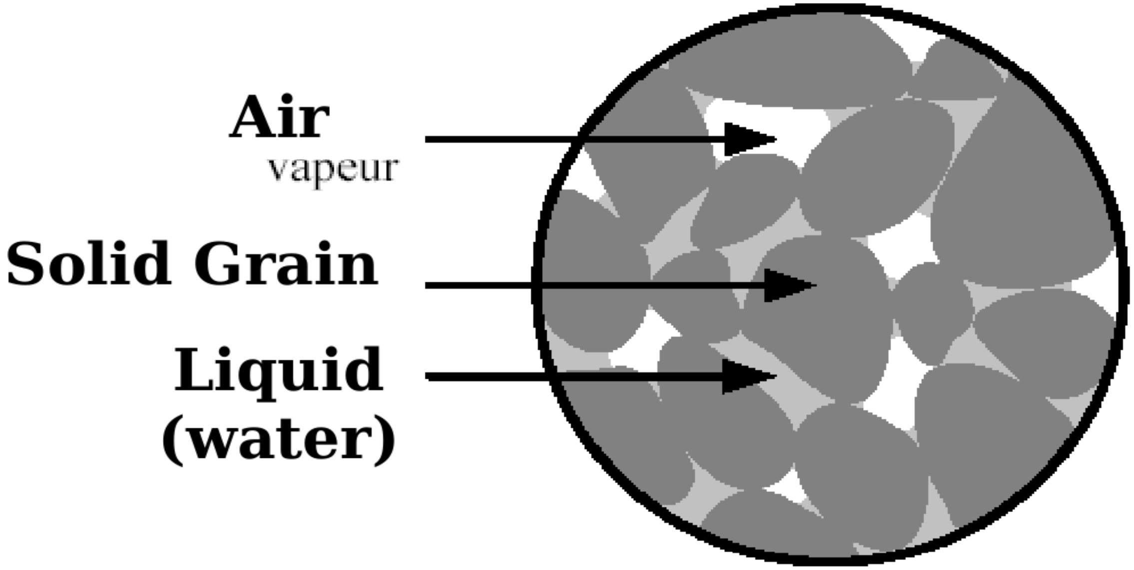
Micro-scale modeling

Hysteresis



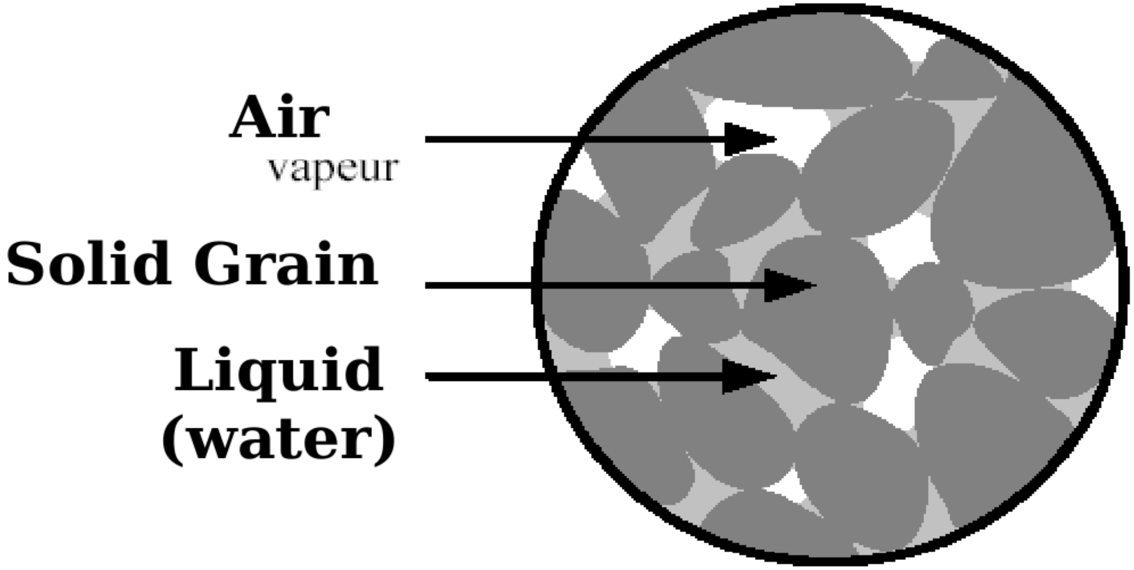
"Ink-bottle" effect determines equilibrium height of water in a variable-width pore: (a) in capillary drainage (desorption) and (b) in capillary rise (sorption).

Micro-scale modeling

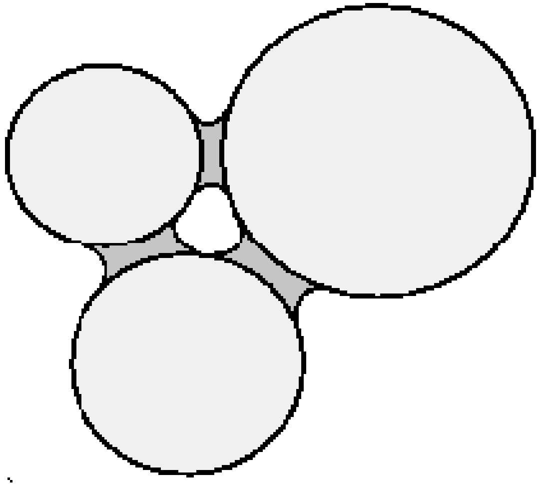


Fluid flow in such system goes through various processes:
- 1-phase flow in saturated subdomains
- film flow at the surface of the solid phase or “corner” flow
- movement of interfaces (e.g. moving bubbles or change of S_r)
- vapor transfer

Micro-scale modeling



At **low water content** levels interfacial phenomena lead to **intergranular** water **menisci**

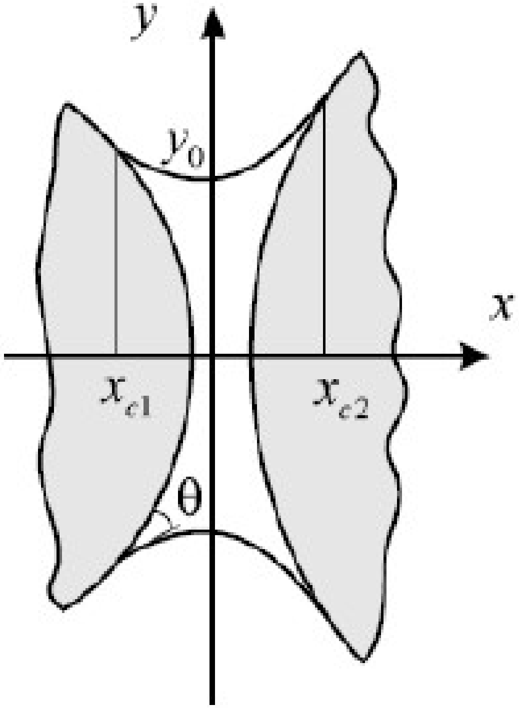


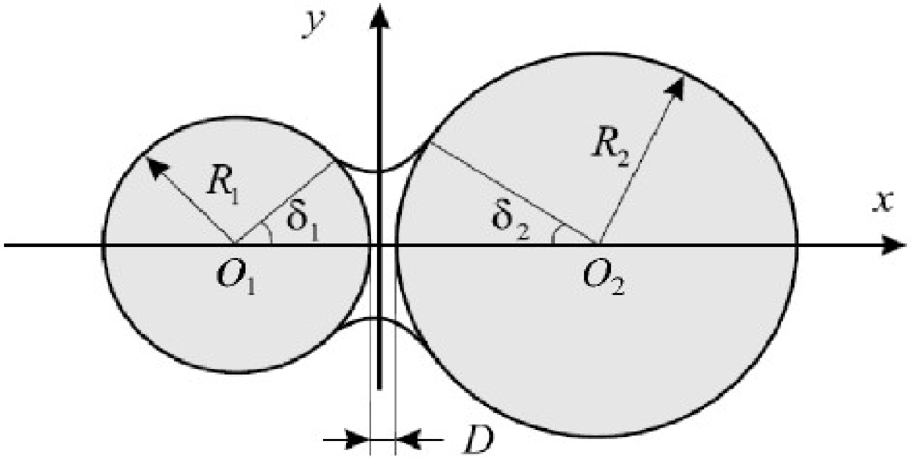
Micro-scale modeling: pendular bridge

Young-Laplace equation:

$$p_c = \gamma_{wn} C$$

$$C^* = \frac{-1}{y^*\sqrt{1+y'^{*2}}} + \frac{y''^*}{(1+y'^{*2})^{\frac{3}{2}}}$$

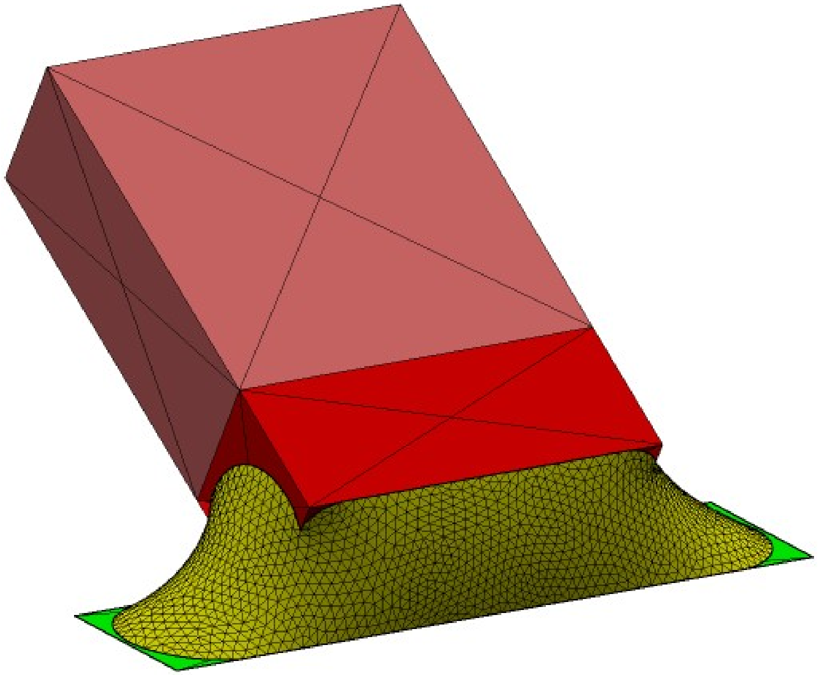




$$\begin{cases} F_{cap} = 2\pi\sigma y_0 + \pi\Delta u y_0^2 \\ V_{cap} = \pi\int y^2(x).dx \end{cases}$$

Micro-scale modeling: numerical methods

Minimzation techniques

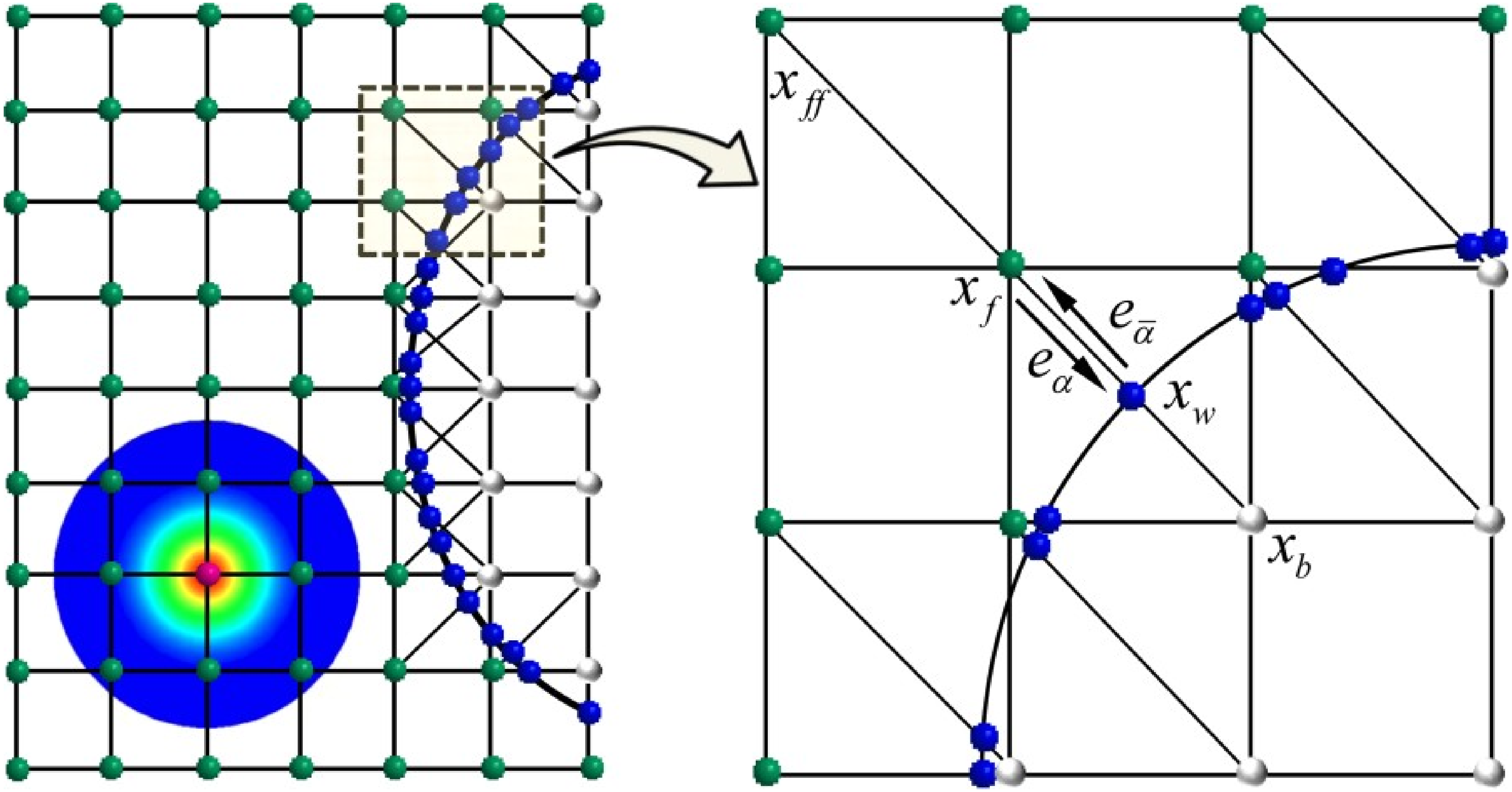


Surface Evolver

http://facstaff.susqu.edu/brakke/evolver/evolver.html

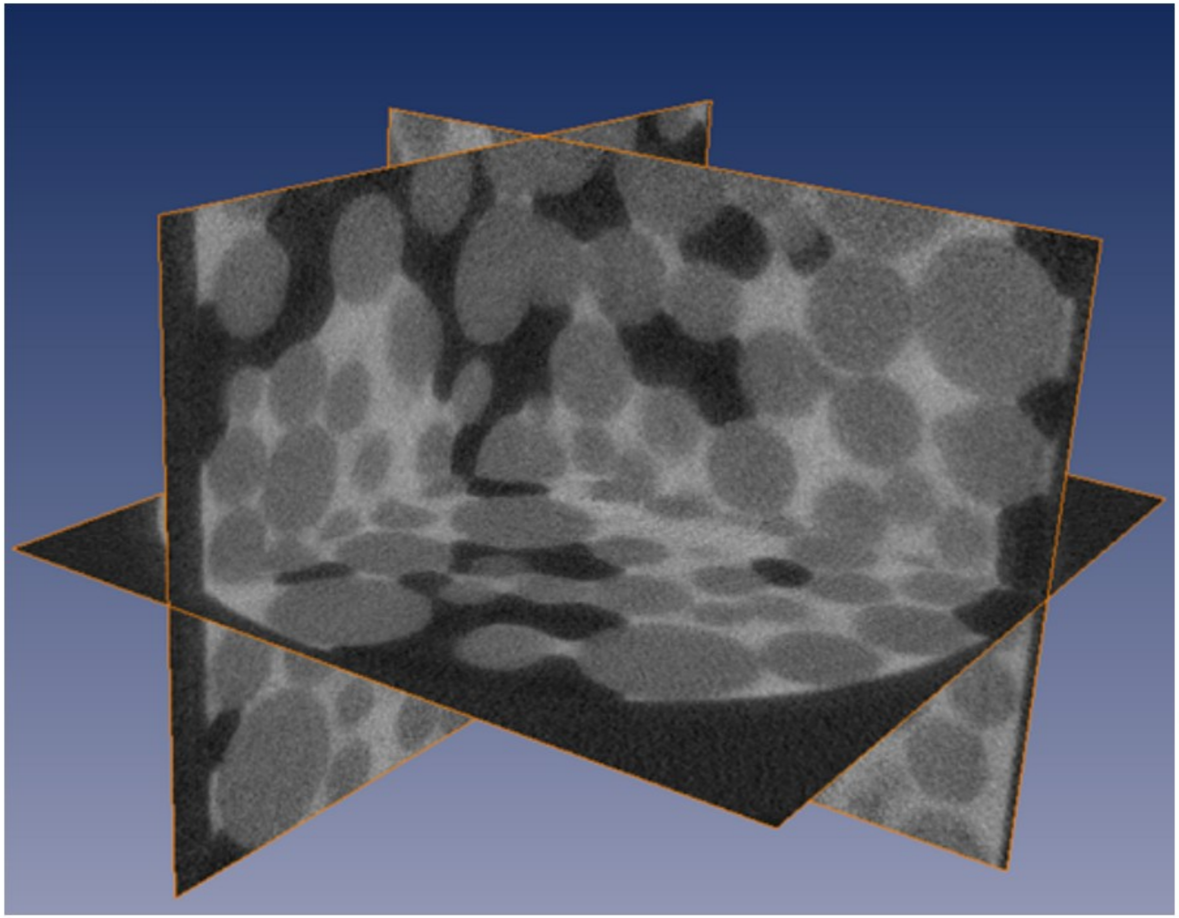
Micro-scale modeling: numerical methods

Lattice-Boltzman method, Shan & Chen 2-phase field (and live examples)



Pore-scale modeling

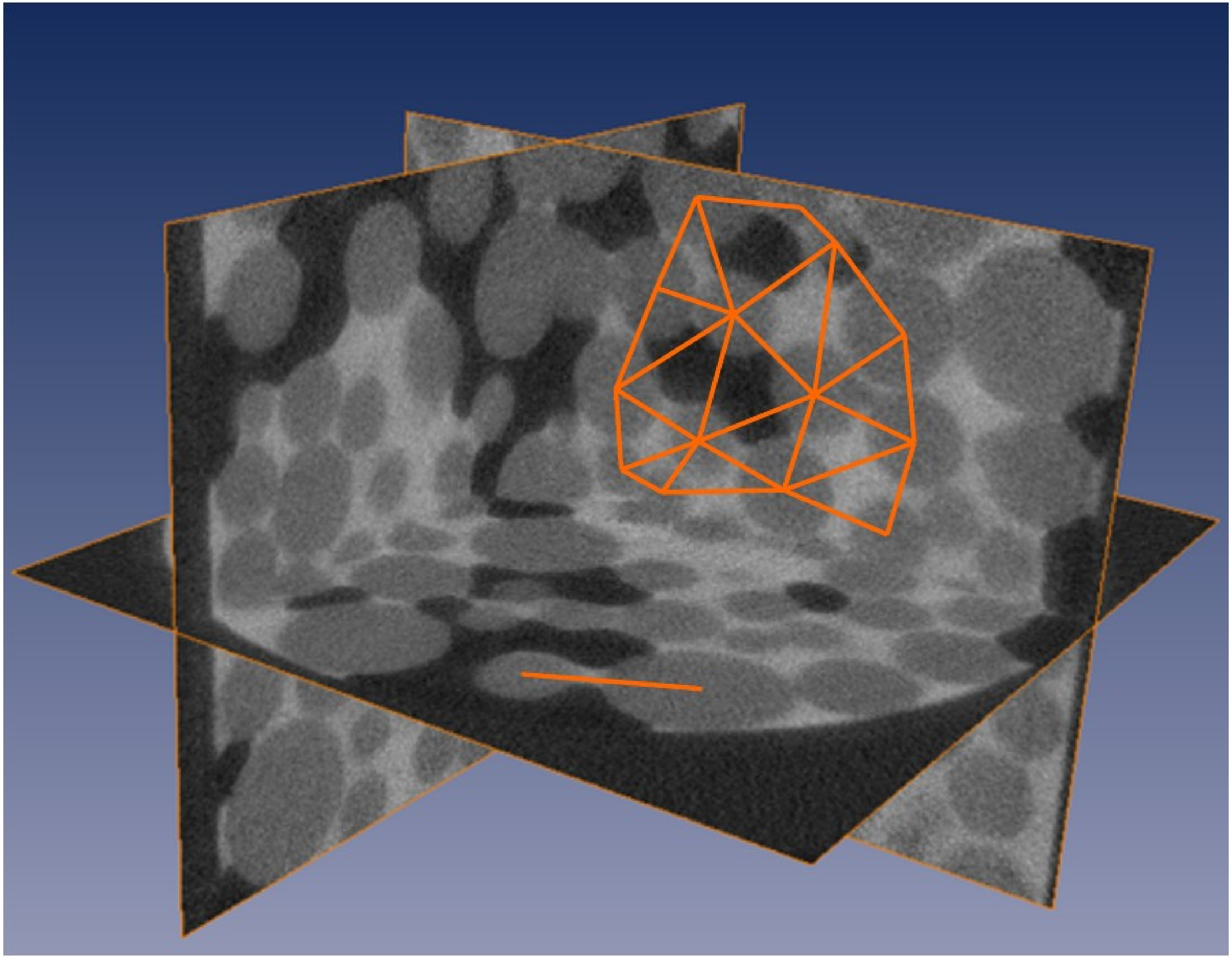
Distribution of immiscible phases in *quasistatic* primary drainage (Culligan et al. [1])



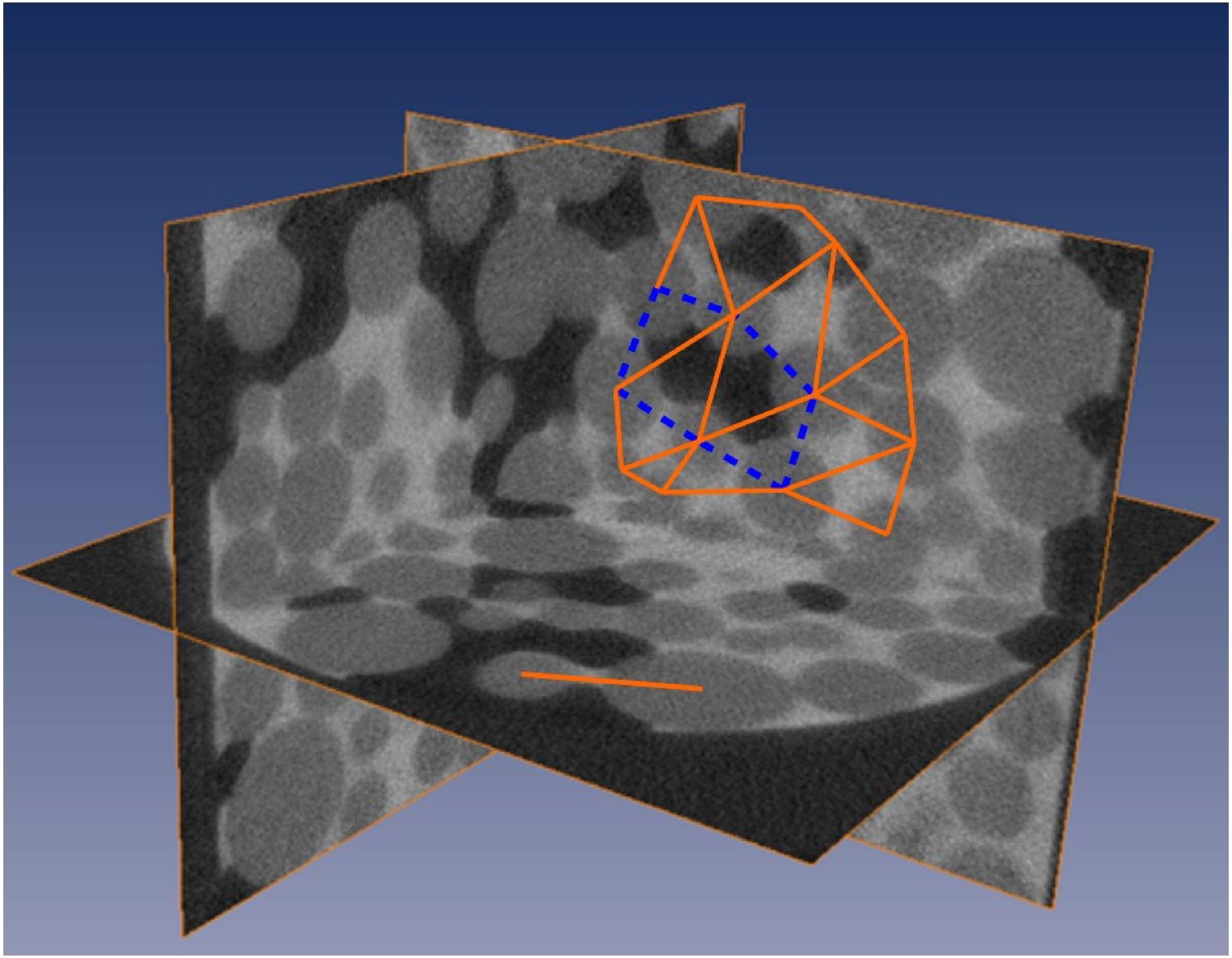
---

[1] Culligan, Wildenschild, Christensen et al., *Water Resources Res.* (2004)

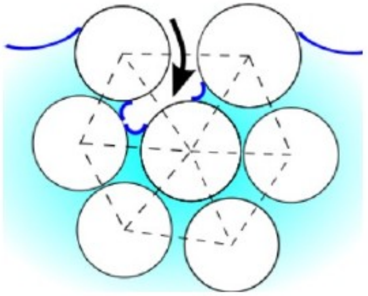
Pore-scale modeling



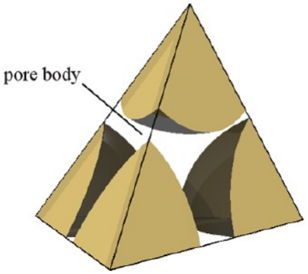
Pore-scale modeling

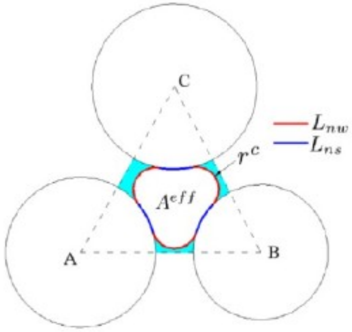


Pore-scale modeling

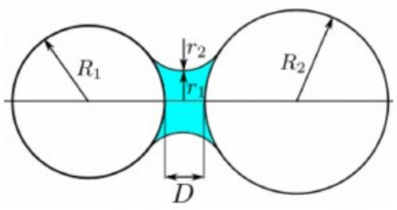


Pores: binary transition between saturated and dry states





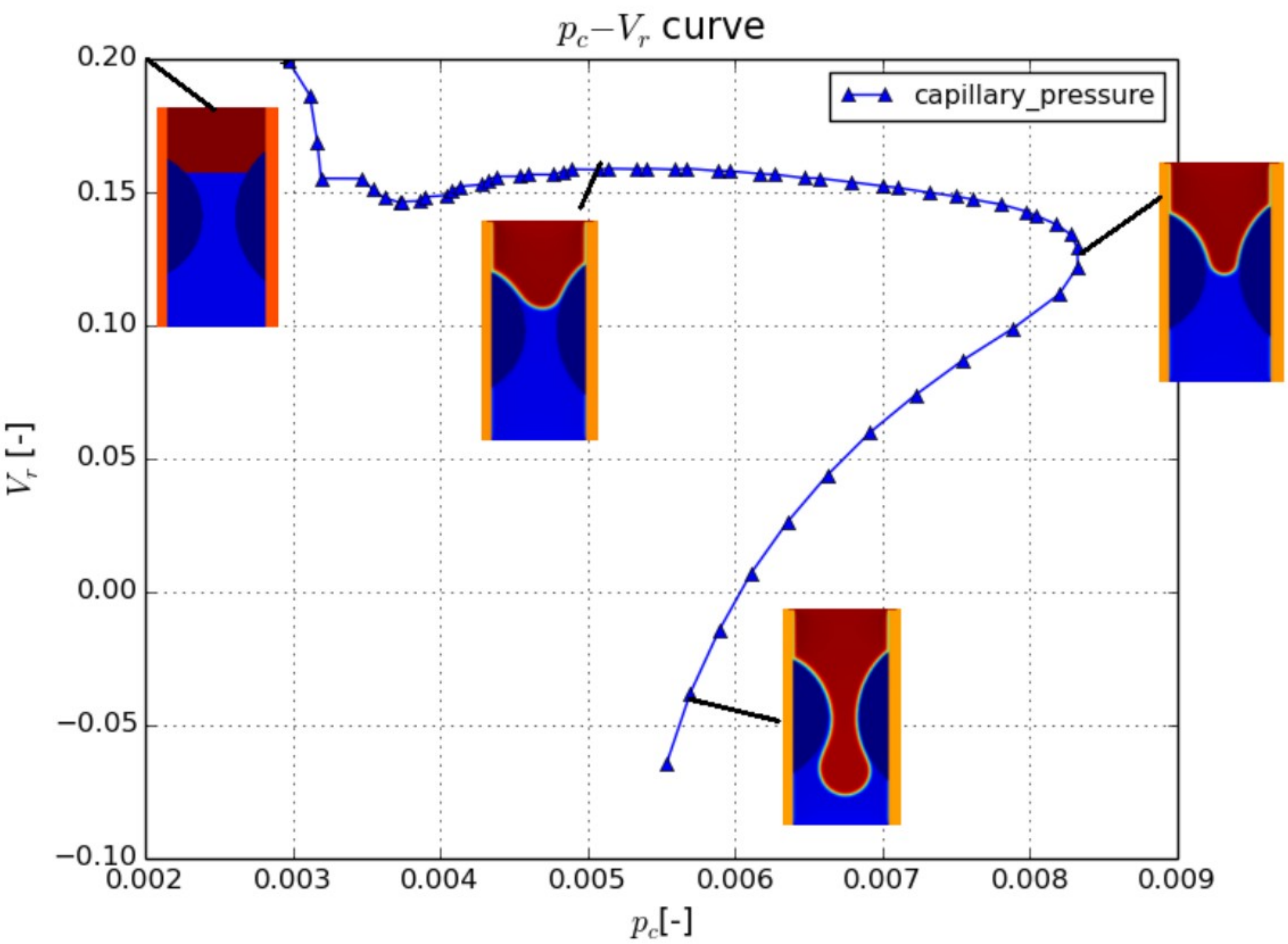
Throats: local rule $p_c < p_c^e$ + parametrization of p_c^e wrt. local geometry (MSP method)
(p_c^e: local entry capillary pressure)



Pendular bridge

Pore-scale modeling

The 3-sphere problem

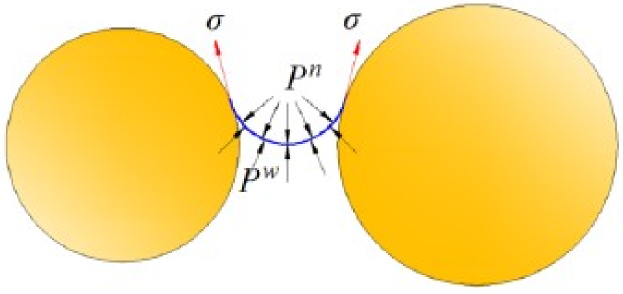


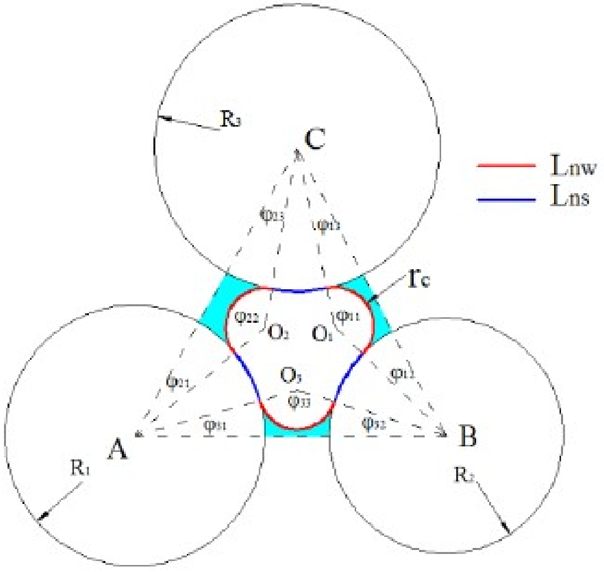
Pore-scale modeling

The 3-sphere problem

The approach for calculating P_e^c is based on MS-P method suggested by Ma et al. (1996); Mayer and Stowe (1965); Princen (1969) and Joekar-Niasar et al. (2010), which follows from the balance of forces for pore throat section.

$$\sum F(r_c) = F^c(r_c) + T^l(r_c) = 0$$

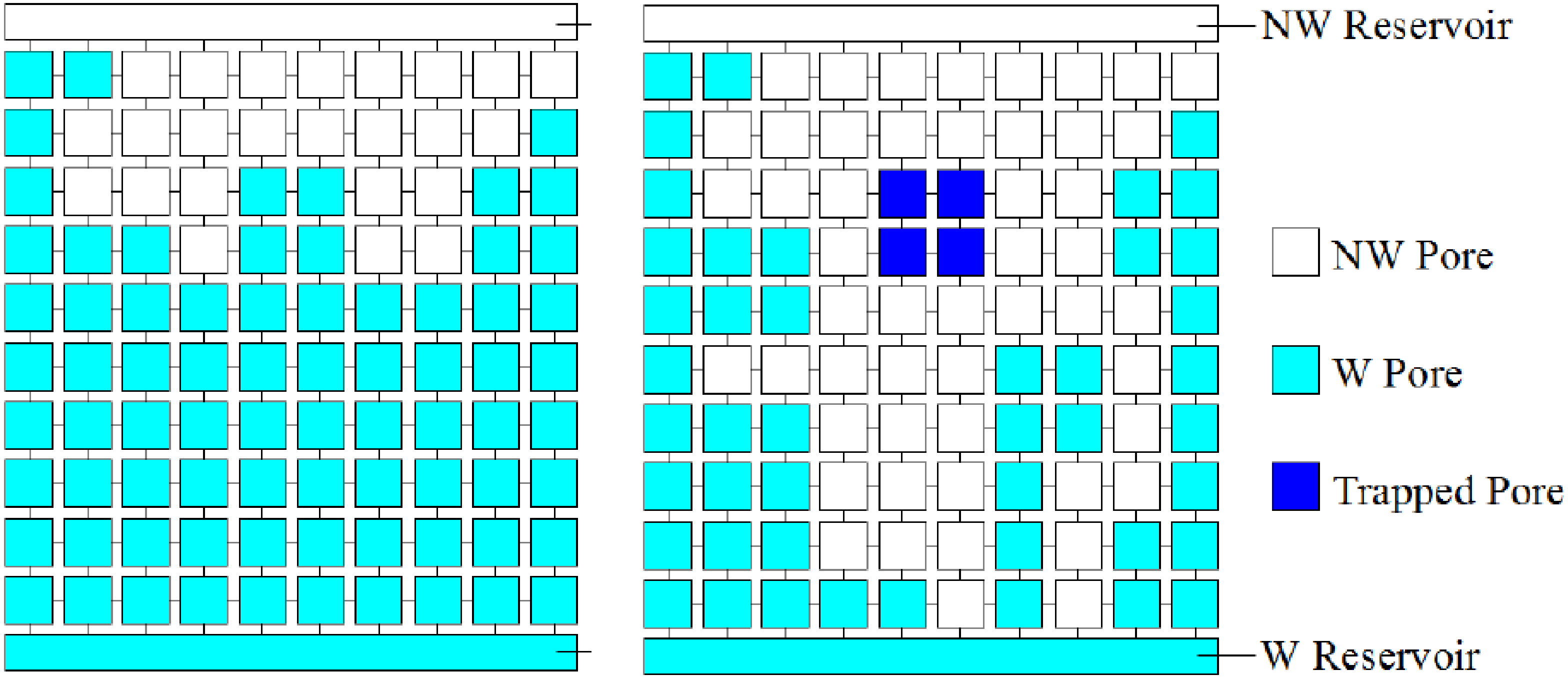




Pore-scale modeling

Network evolution and disconnected phases

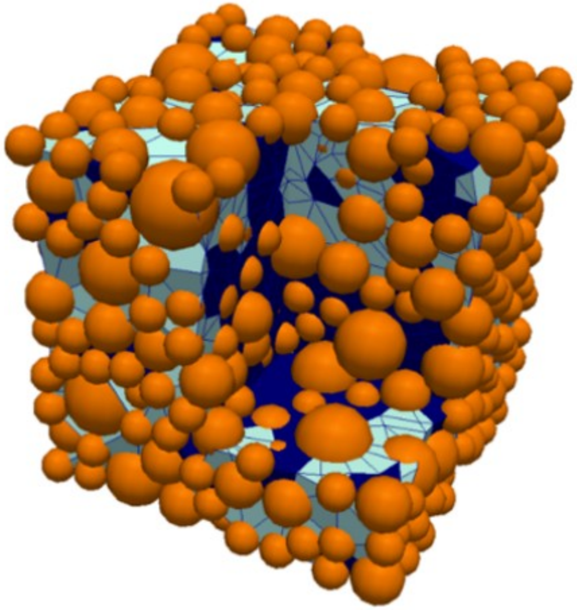
An idealized view of primary drainage

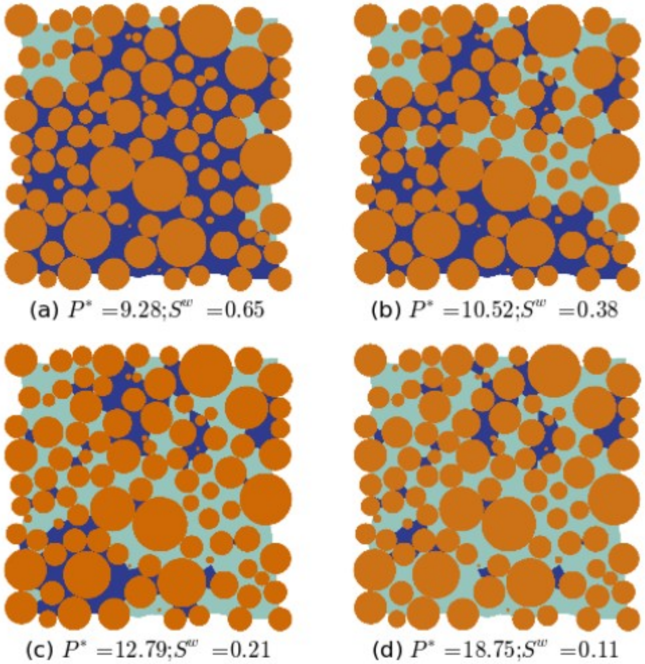


Pore-scale modeling

Network evolution and disconnected phases

The network model has been implemented in C++, and it is freely available as an optional package of the open-source software **Yade** (Smilauer et al. (2010)).
The C++ library CGAL (Boissonnat et al. (2002)) is used for the triangulation procedure.





(a) $P^* = 9.28; S^w = 0.65$

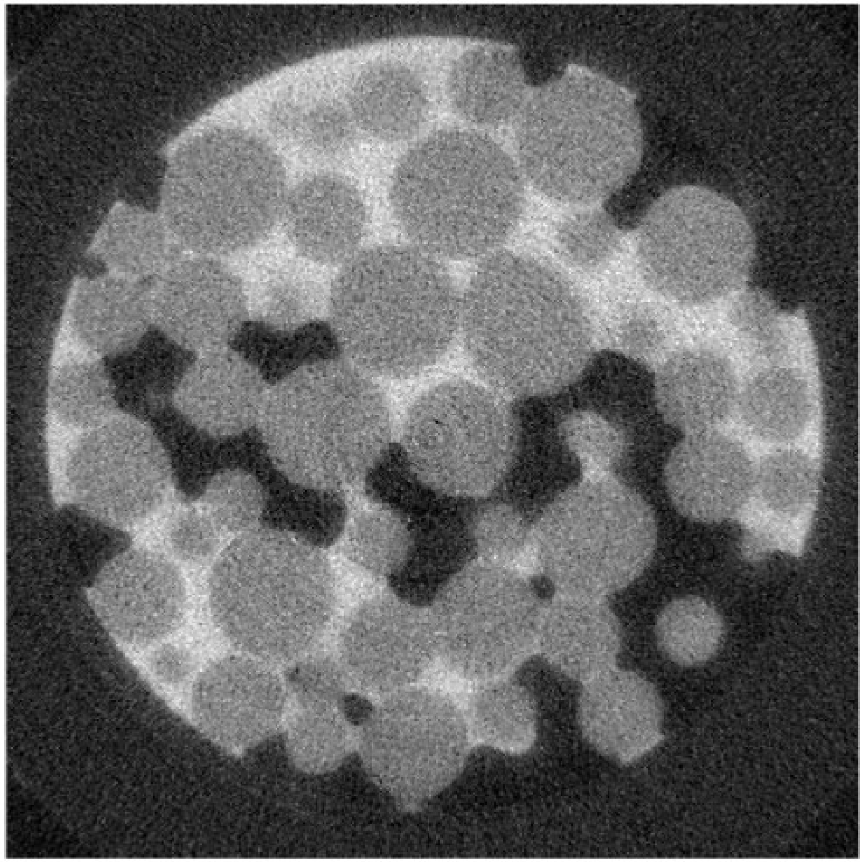
(b) $P^* = 10.52; S^w = 0.38$

(c) $P^* = 12.79; S^w = 0.21$

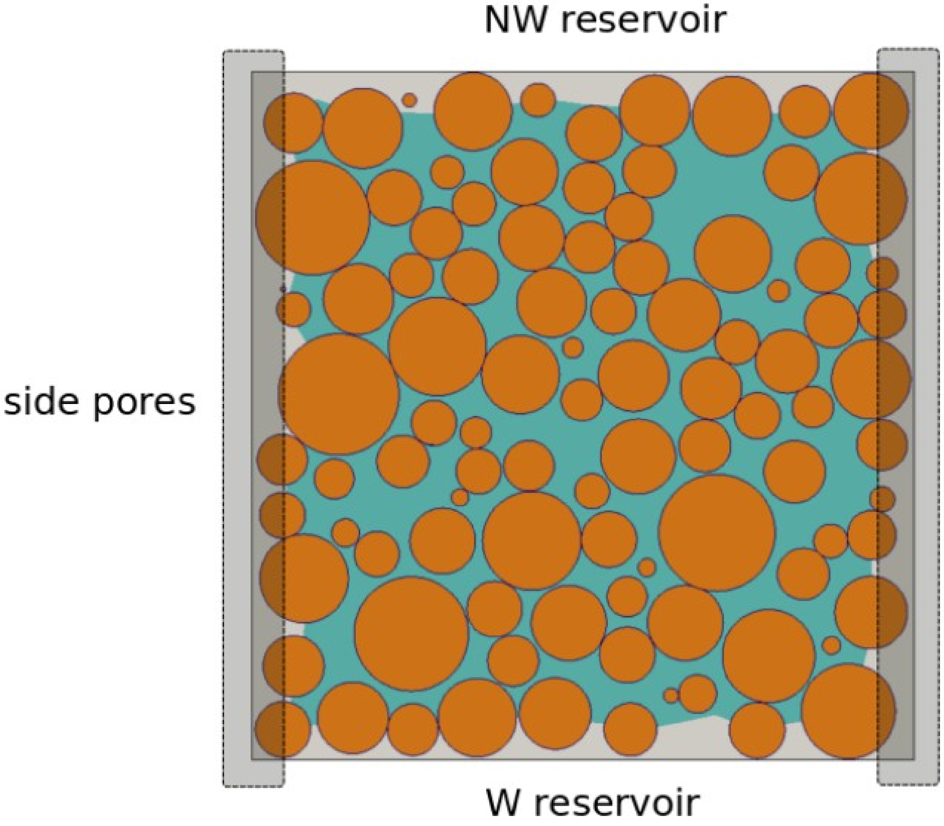
(d) $P^* = 18.75; S^w = 0.11$

Pore-scale modeling

Model verification

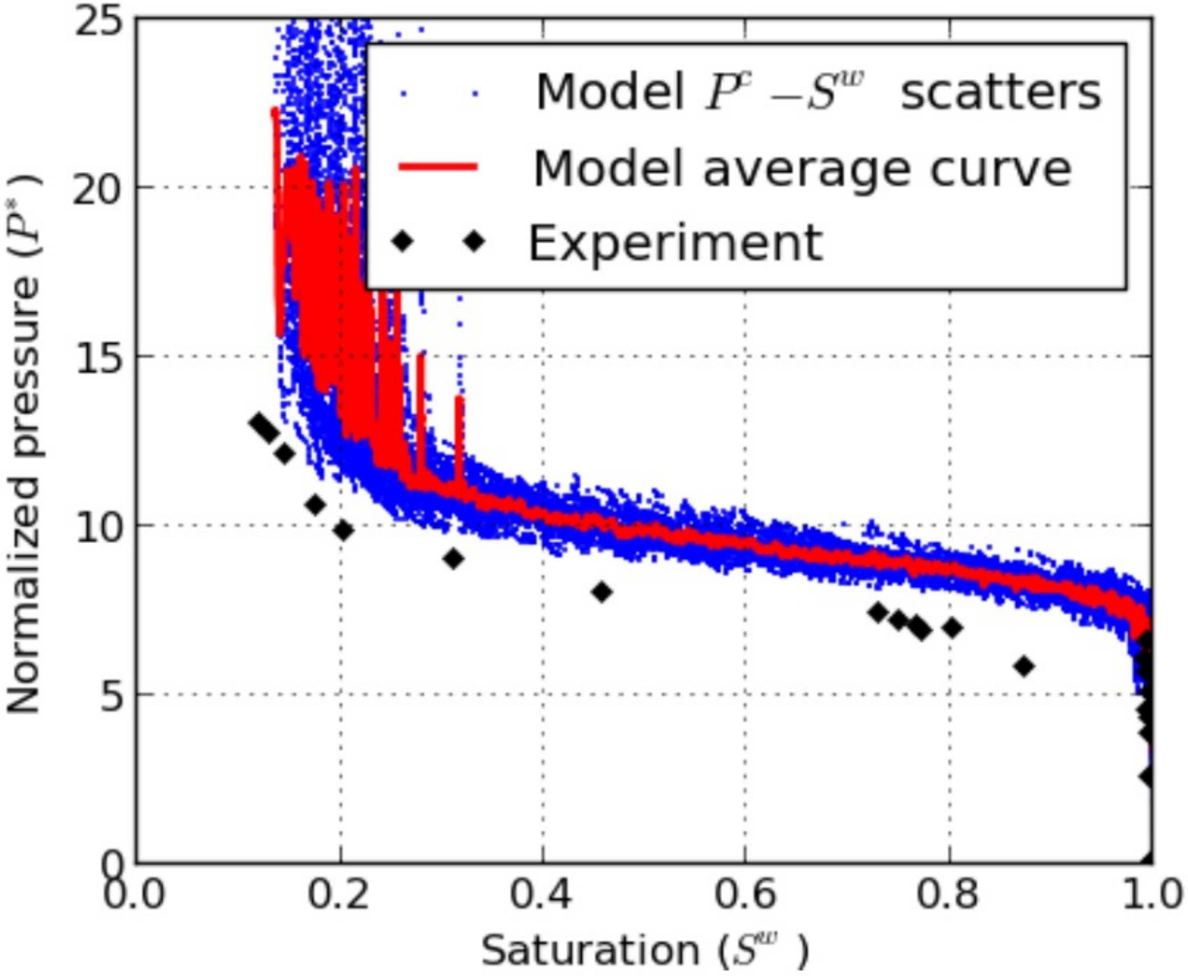


Culligan K. et al., 2004



Pore-scale modeling

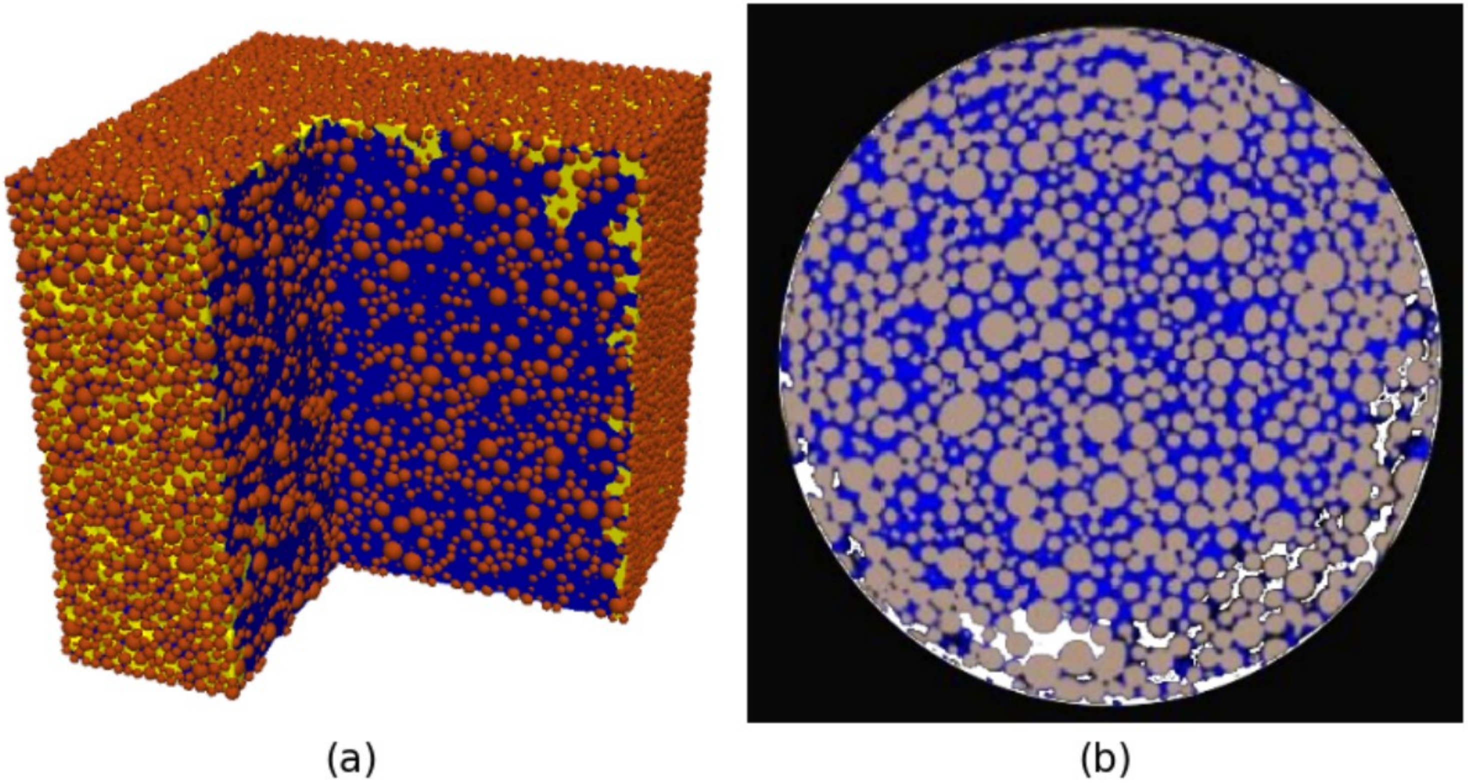
Model verification



Pore-scale modeling

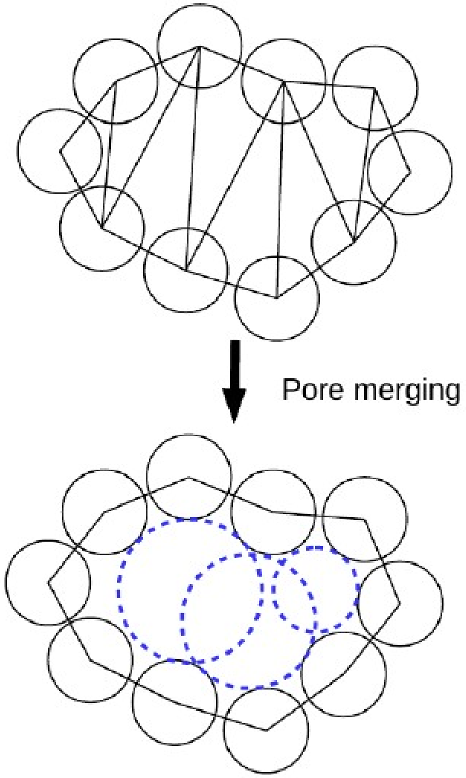
Model verification

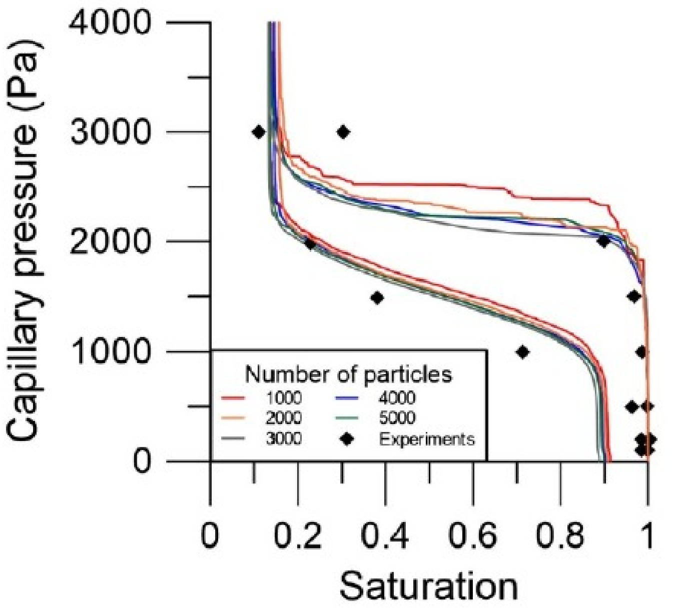
Permeable side boundary condition (open side). Experimental scan image by Khaddour G. et al. (2012).



Pore-scale modeling

The imbibition process is mainly controlled by the pore size instead of the throat size. A pore-merging algorithm has been developped [1]





---

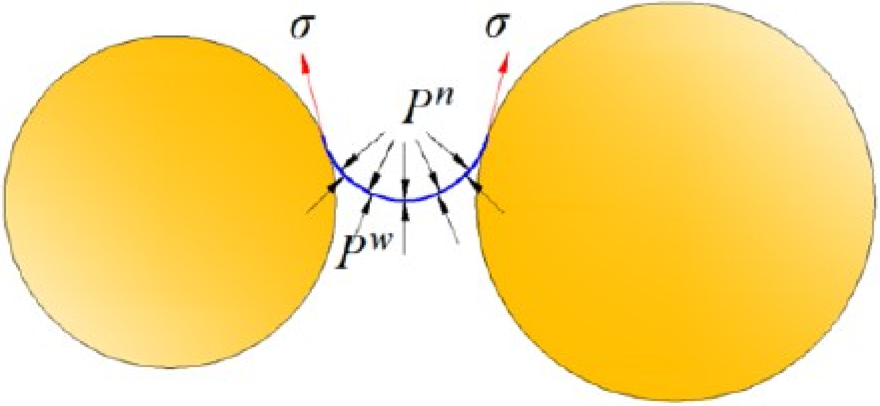
[1] Sweijen, Nikooee, Hassanizadeh, Chareyre, *Transp. Porous Med.* 2016

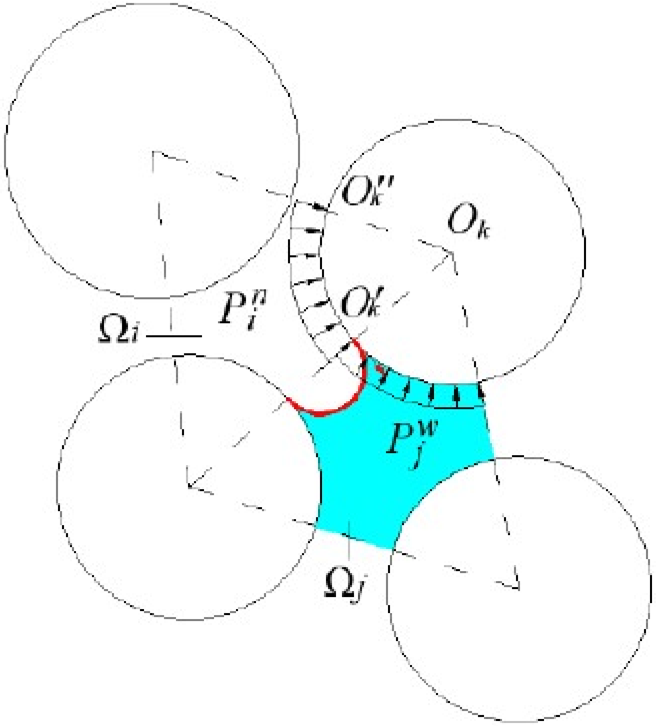
Pore-scale modeling

Capillary force and deformation

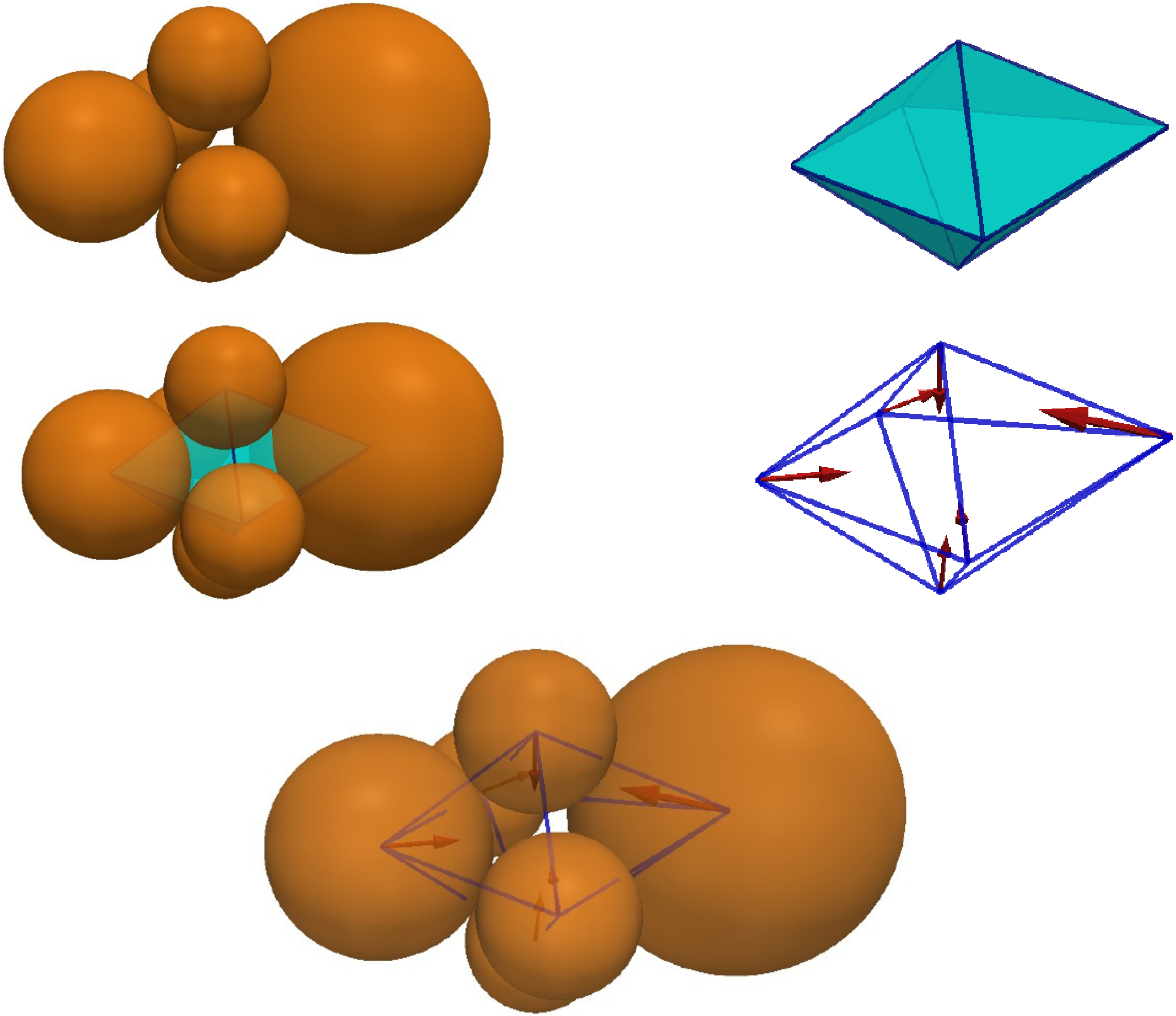
The total force F^k generated on particle k includes the effects of W-phase P^w, NW-phase P^n and NW-W interface tension σ^{nw}.

$$F^k = F^{n,k} + F^{w,k} + F^{\sigma,k}$$

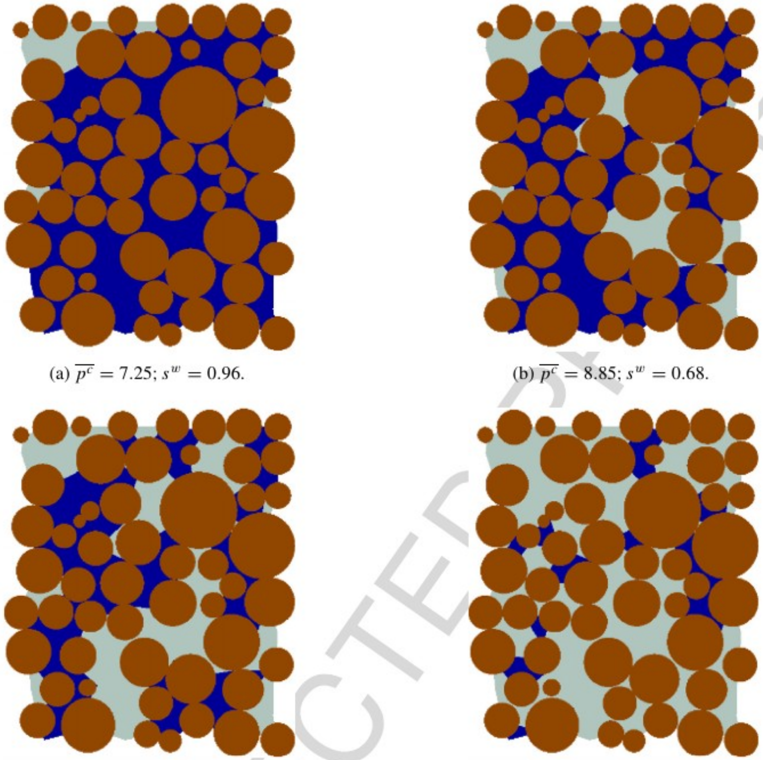




Pore-scale modeling



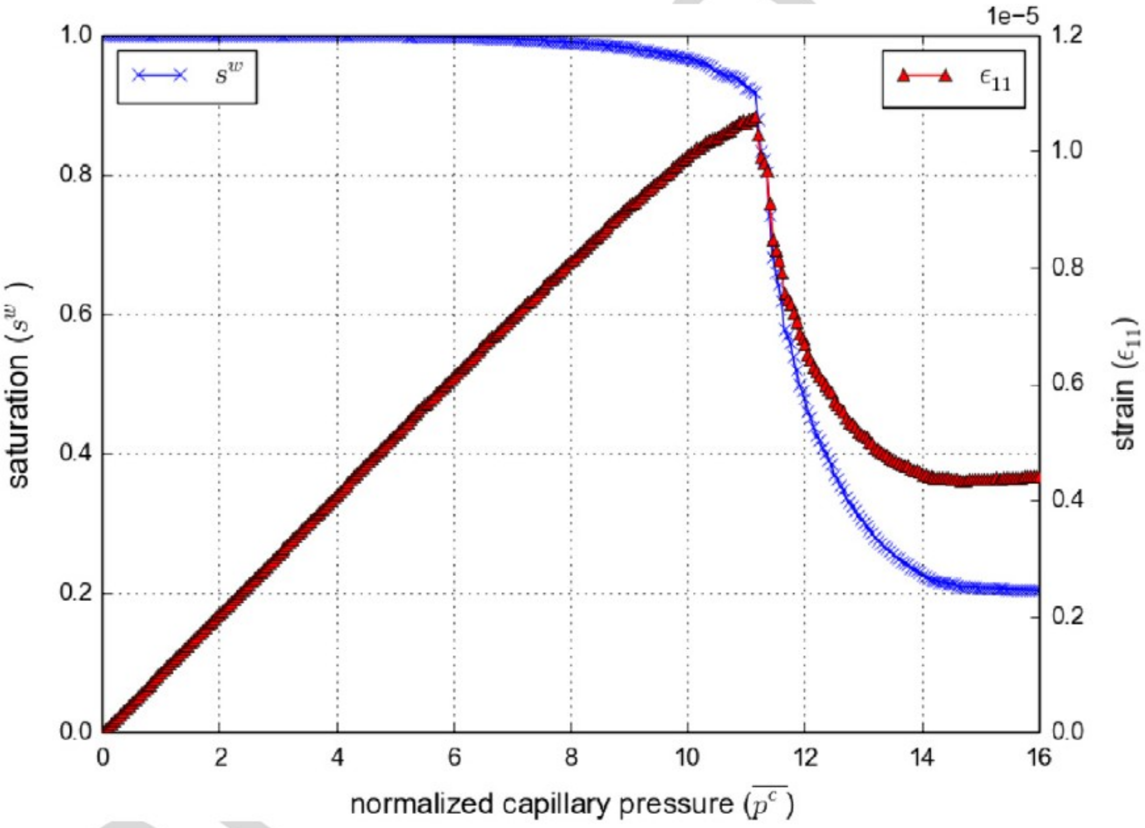
Pore-scale modeling


(a) $\overline{p^c} = 7.25; s^w = 0.96.$

(b) $\overline{p^c} = 8.85; s^w = 0.68.$

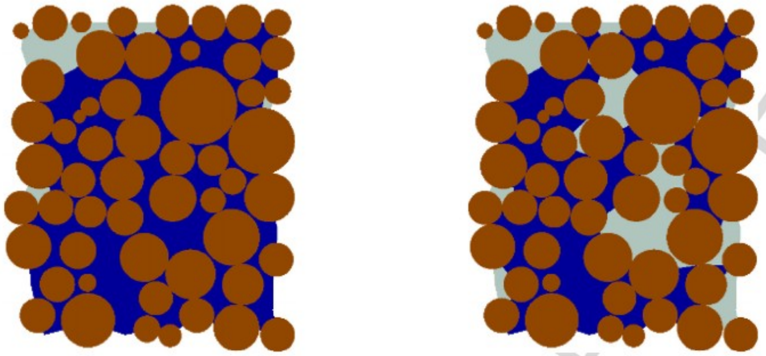
(c) $\overline{p^c} = 9.00; s^w = 0.62.$

(d) $\overline{p^c} = 13.2; s^w = 0.18.$



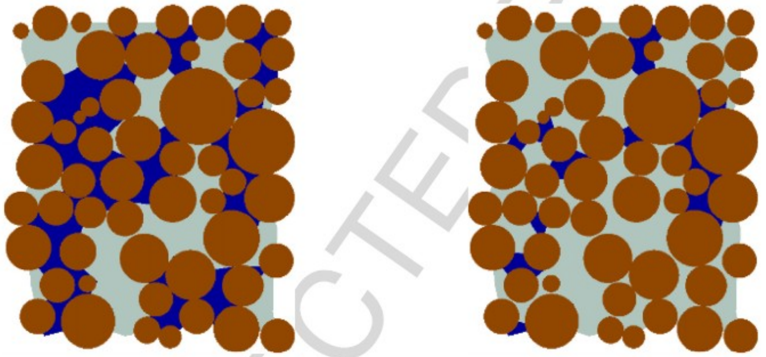
Pore-scale modeling

Conclusion:
The optimal water content for a sand castle is S_r=1 (?!!...)



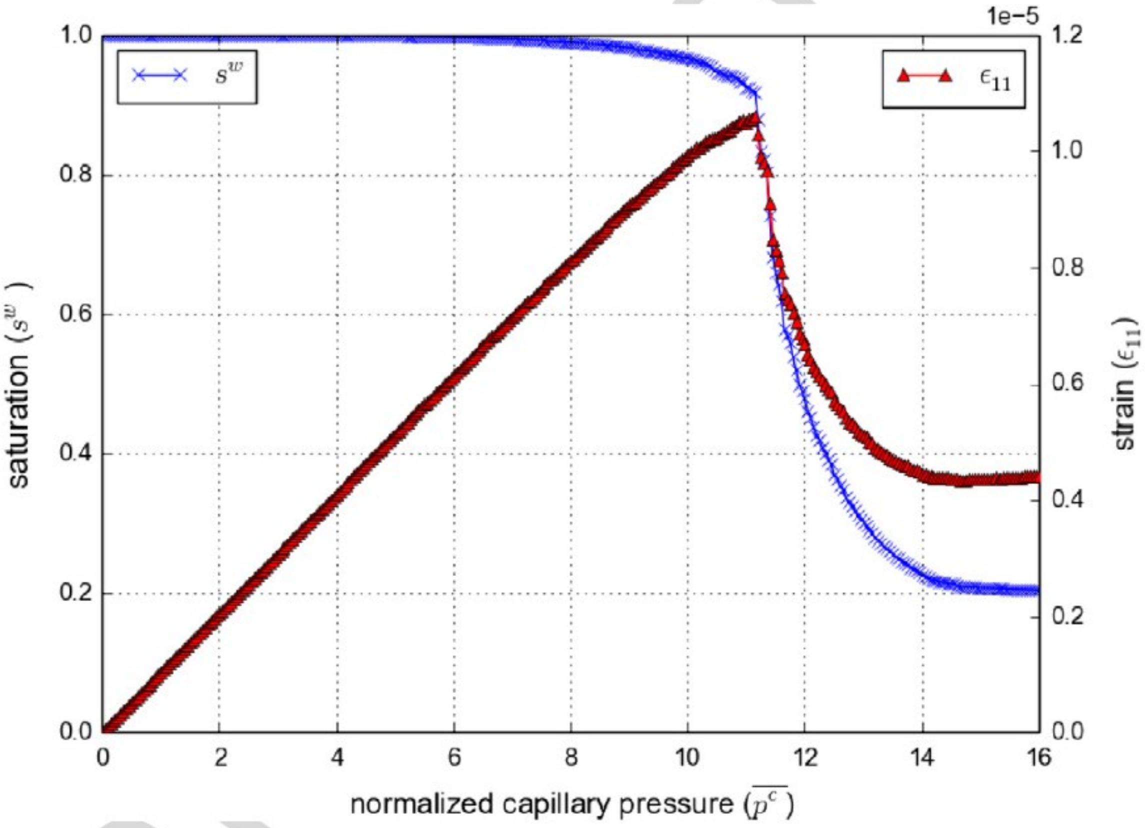
(a) $\overline{p^c} = 7.25$; $s^w = 0.96$.

(b) $\overline{p^c} = 8.85$; $s^w = 0.68$.



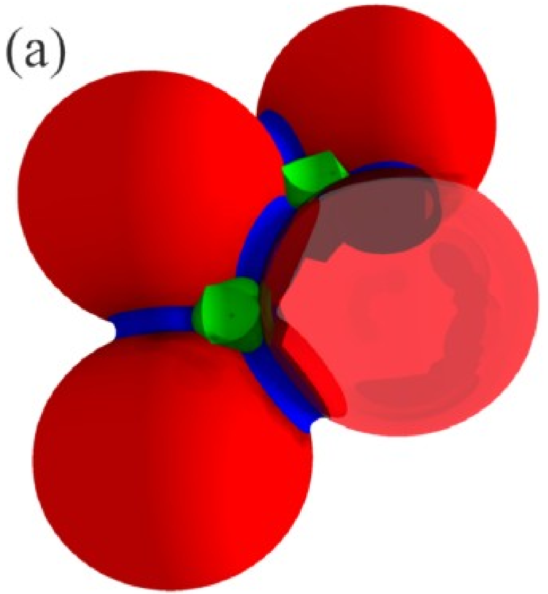
(c) $\overline{p^c} = 9.00$; $s^w = 0.62$.

(d) $\overline{p^c} = 13.2$; $s^w = 0.18$.



Further issues

- Imbibition (still), cooperative invasion at macro-throats
- Large deformations, splitting or merging trapped clusters or bridges (Melnikov et al.[1])
- Residual permeability in the drained regions (Mani et al.[2]), i.e. film flow and/or vapor transfer.
- Partial wettability.



On all aspects, a need for high resolution experiments and/or solutions by micro-continuum models.

---

[1] Melnikov, Mani, Wittel, Thielmann, Herrmann, *PRE* 2015

[2] Mani, Kadau, Herrmann, *PRL* 2012