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Pore Morphology Method for Modeling Liquid Intrusion in Porous Media

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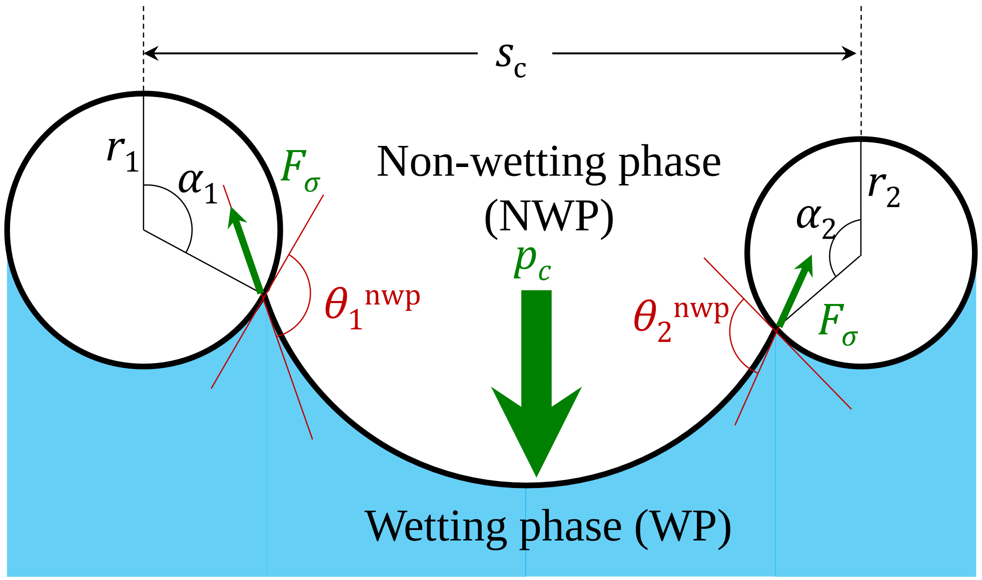
Presentation Outline

- Motivation
- Algorithm of Pore Morphology Method (PMM)
- PMM in 2-D & 3-D
- Limitation of PMM
- Conclusions

Pore Morphology Method – Motivation

Microscale simulation Method	Pros	Cons
Pore Network Model (PNM)	Simple, Computationally fast	Cannot handle complicated pore structures
Volume-of-Fluid (VOF)	Physics based, fairly accurate, handle complicated geometries	Computationally very slow
Lattice-Boltzmann Method (LBM)	Physics based, fairly accurate, handle complicated geometries	Computationally very slow
Energy Minimization Method (EMM)	Physics based, very accurate, relatively fast	Fails for disordered anisotropic geometries



In this context, PMM simulations offers an alternate way to conduct fluid intrusion simulations

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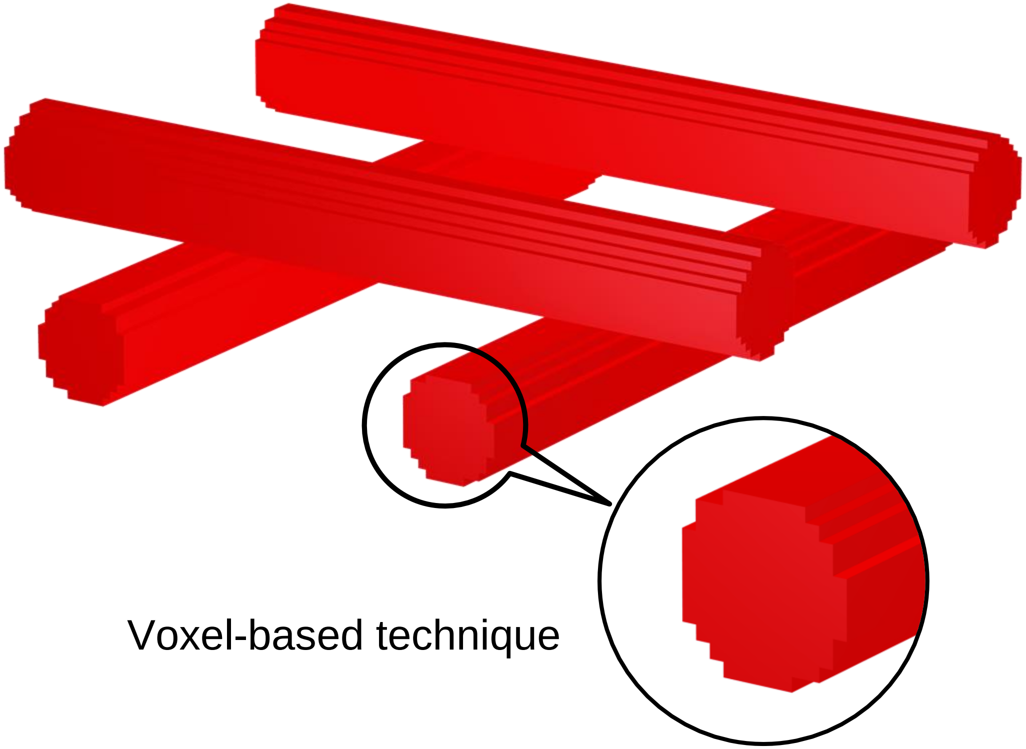
Pore Morphology Method (PMM)



Voxel-based technique

0	0	0	0	0	0	0	0	0
0	0	0	0	2	0	0	0	0
0	0	0	2	1	2	0	0	0
0	0	2	1	1	1	2	0	0
0	2	1	1	1	1	1	2	0
0	0	2	1	1	1	2	0	0
0	0	0	2	1	2	0	0	0
0	0	0	0	2	0	0	0	0
0	0	0	0	0	0	0	0	0

Example in a 2-D domain

0 = Non-wetting phase (NWP)
1 = Solid
2 = Wetting Phase (WP)

Morphological Operations

0	0	0	0	0
0	1	1	1	0
0	1	1	1	0
0	1	1	1	0
0	0	0	0	0

Binary Image

1	1	1
1	1	1
1	1	1

Structuring Element

Dilation

1	0	0	0	0
0	1	1	1	0
0	1	1	1	0
0	1	1	1	0
0	0	0	0	0

Process of Dilation

1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

Dilated Image

Erosion

0	0	0	0	0
0	0	1	1	0
0	1	1	1	0
0	1	1	1	0
0	0	0	0	0

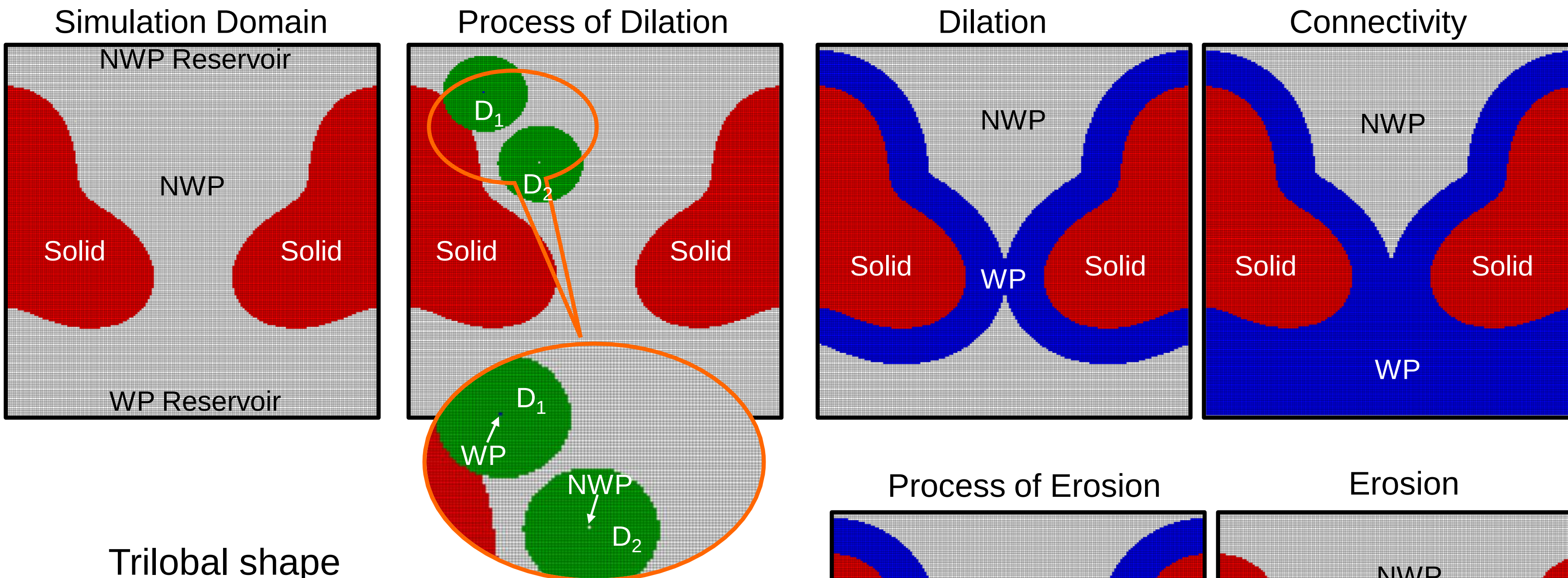
Process of Erosion

0	0	0	0	0
0	0	0	0	0
0	0	1	0	0
0	0	0	0	0
0	0	0	0	0

Eroded Image

Dilation – enlarges image
Erosion – shrinks image

Our PMM Algorithm Using MATLAB

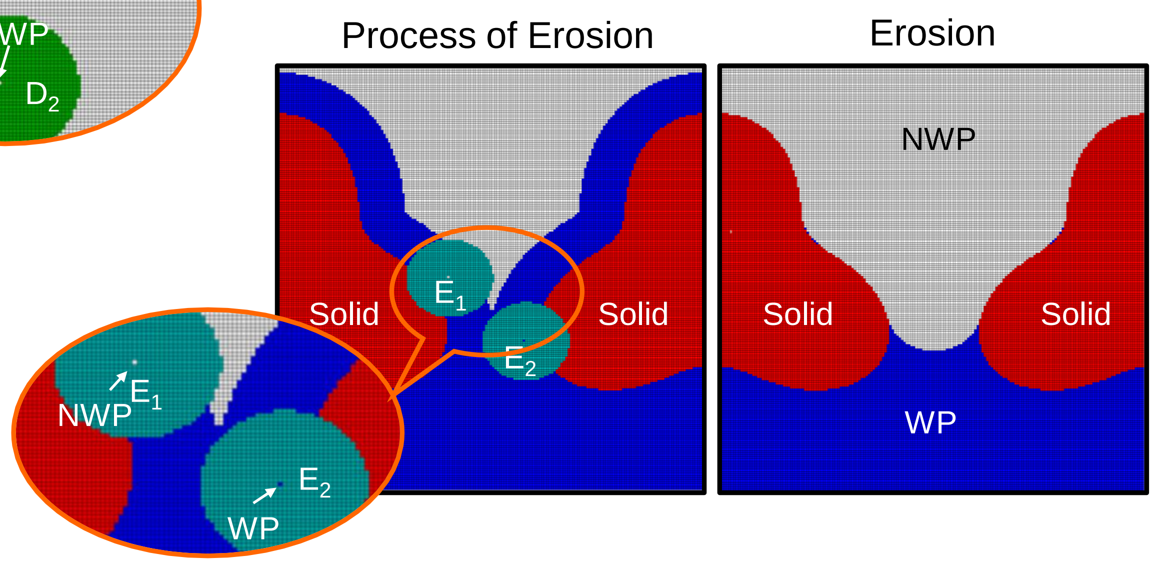


Trilobal shape

$$r = 3[1 - A_m \sin(3\gamma)] \cos\gamma$$

Young-Laplace equation for erosion radius

$$p = \frac{\sigma}{r}(2D) \qquad p = \frac{2\sigma}{r}(3D)$$



Non-Zero Contact Angle

Fixed contact angle model:

$$p = \frac{m\sigma}{r} \cos\theta^{w}$$

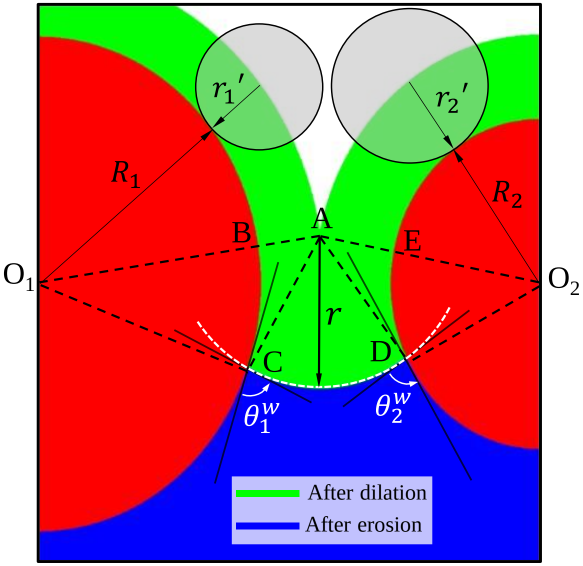
Schulz model:

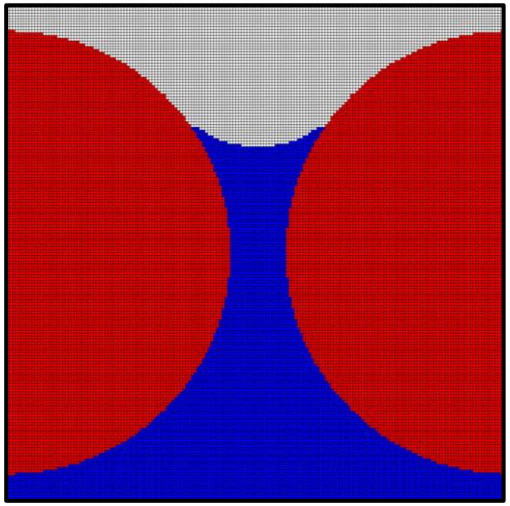
$$r_i' = r\,|\cos\theta_i^{w}|$$

Locally variable contact angle model:

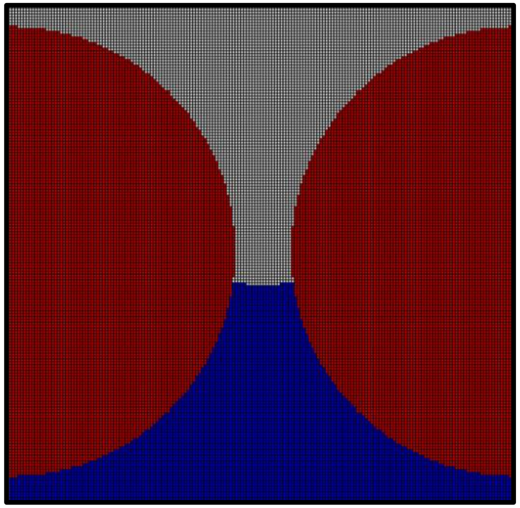
$$r_i' = \sqrt{R_i^2 + r^2 + 2R_i r \cos\theta_i^{w}} - R_i$$

- r_i' → Dilation radius
- R_i → Fiber radius
- r^2 → Erosion radius calculated from Young-Laplace equation
- θ_i^{w} → Contact angle



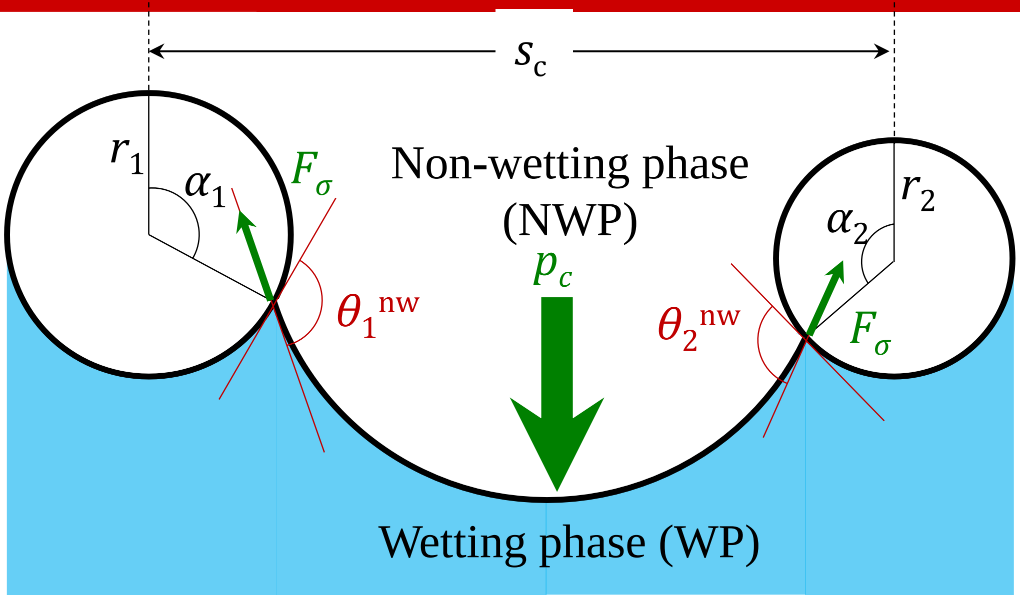


0° CA



80° CA

Force Balance in 2D



Analytical expression for capillary pressure

$$p = -\sigma \frac{\sin(\alpha_1 + \theta_1^{nwp}) + \sin(\alpha_2 + \theta_2^{nwp})}{s_c - r_1 \sin\alpha_1 - r_2 \sin\alpha_2}$$

Here,

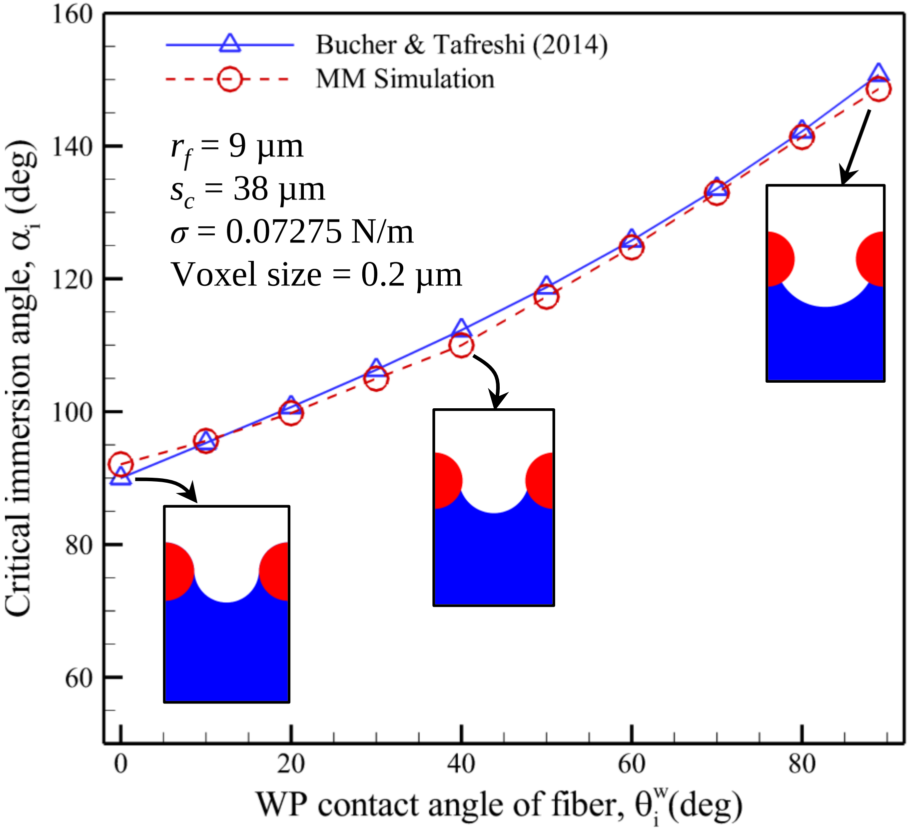
α_1 & α_2 *are* immersion angle

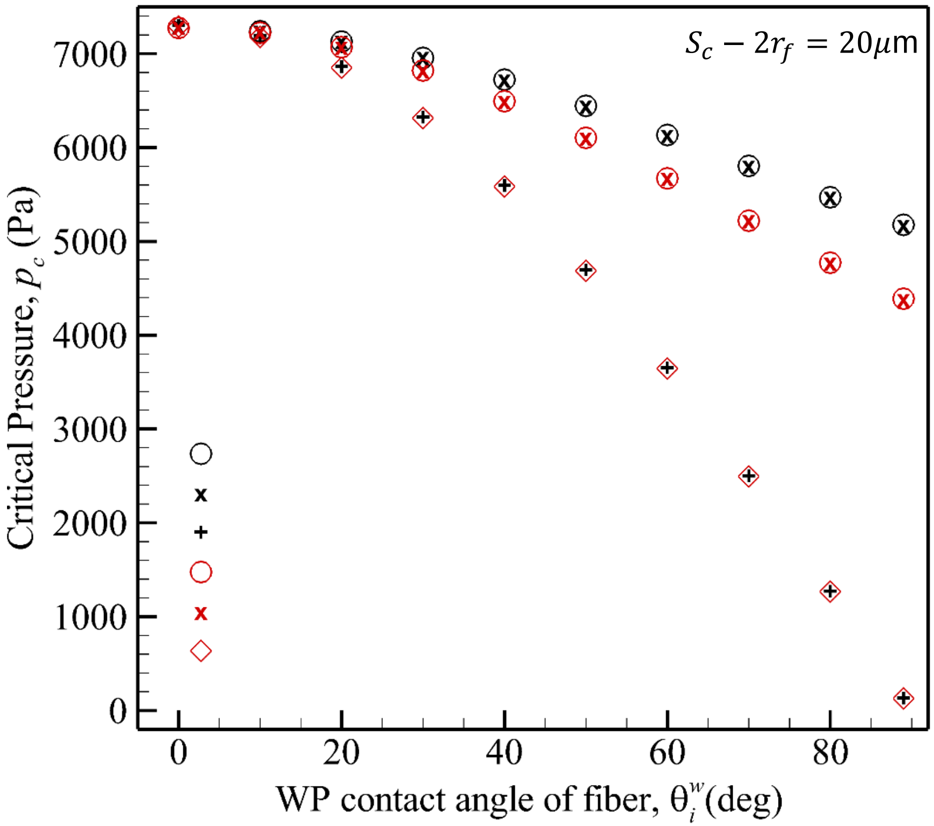
r_1 & r_2 are the circles radii

θ_1^{nwp} & θ_2^{nwp} are YLCA between the NWP and fiber

σ is surface tension & s_c is distance between center of fibers

Critical Pressure and Immersion Angle





With increase of WP contact angle, critical immersion angle increases and critical pressure decreases

T.M. Bucher, H.V. Tafreshi, Colloids and Surfaces A 461, 323 (2014)

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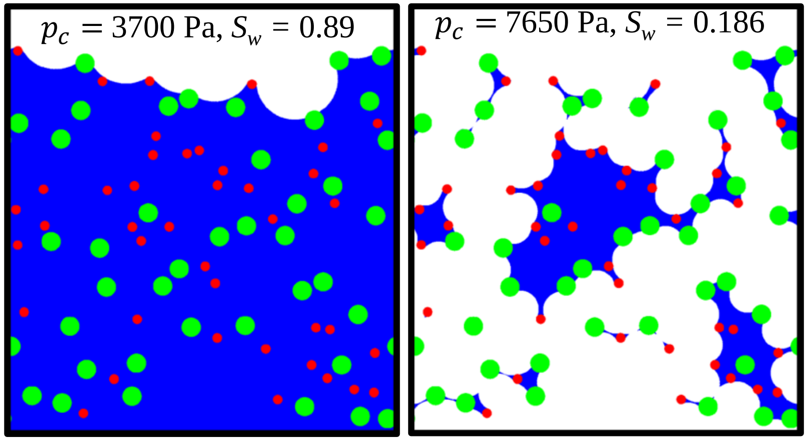
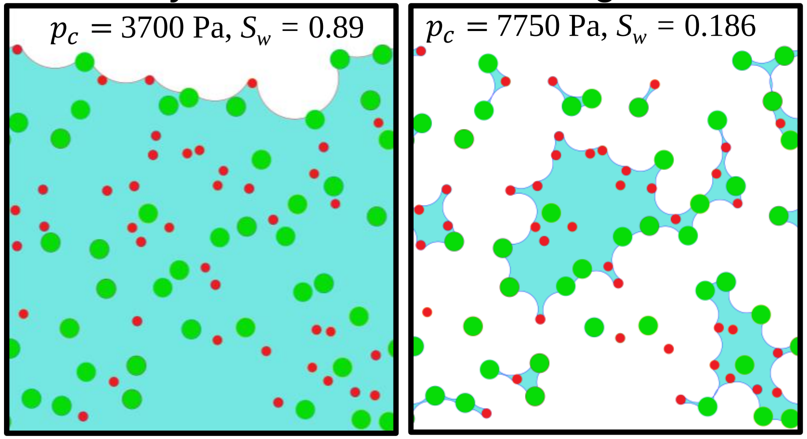
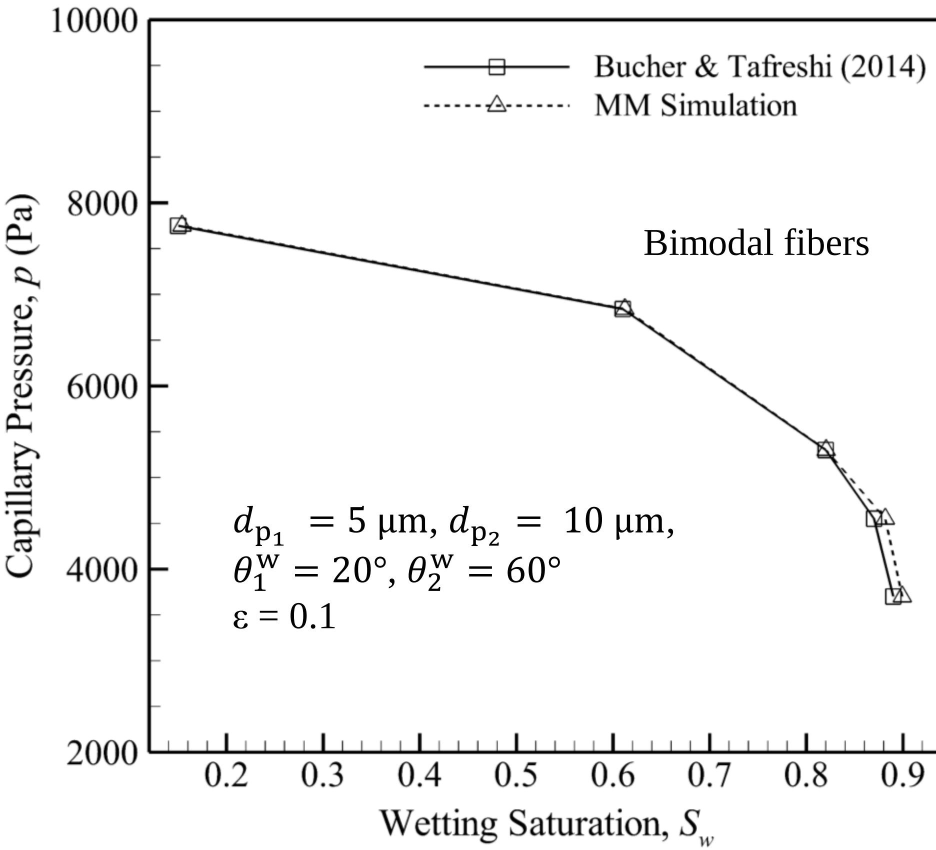
Saturation Patterns in Randomly Distributed Fibers

PMM simulation



Analytical Interface Tracking Method





Excellent agreement was observed between PMM simulation and Analytical Interface Tracking Method

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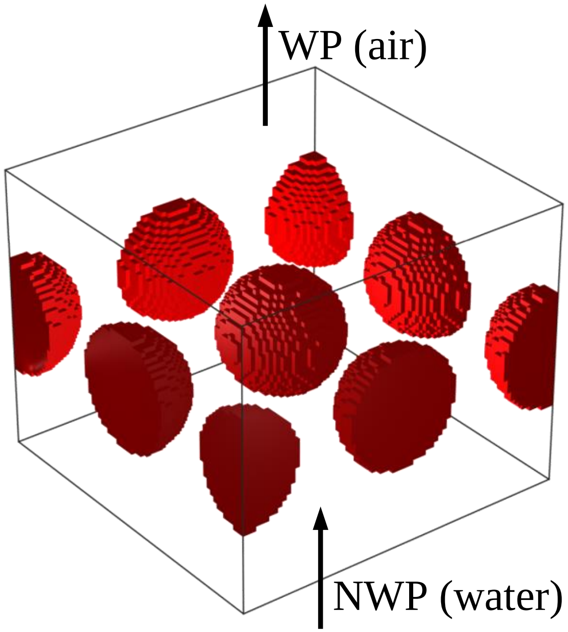
PMM in 3D Spherical Particles

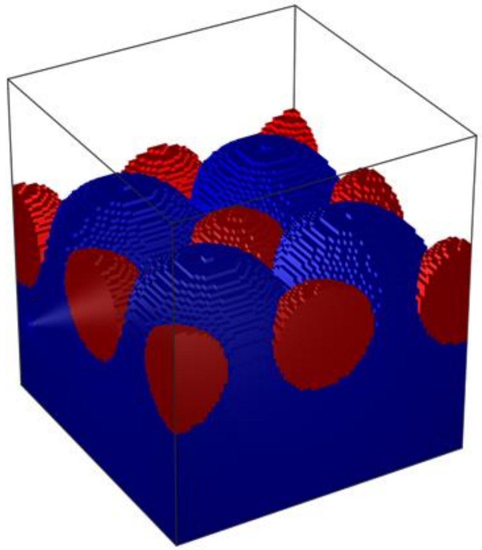
Force balance equation

$$p_c d_p \left[4\left(\frac{\pi}{6\varepsilon}\right)^{2/3} - \pi(\sin\alpha_c)^2\right] = 4\pi\sigma\sin\alpha_c\cos\left(\frac{3\pi}{2} - \alpha_c - \theta^w\right)$$

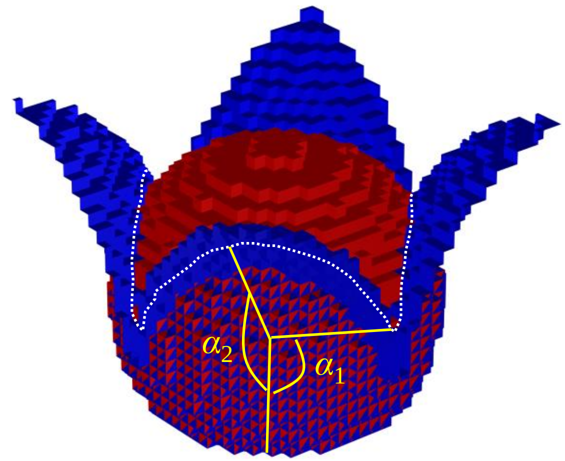
Simulation domain



Erosion



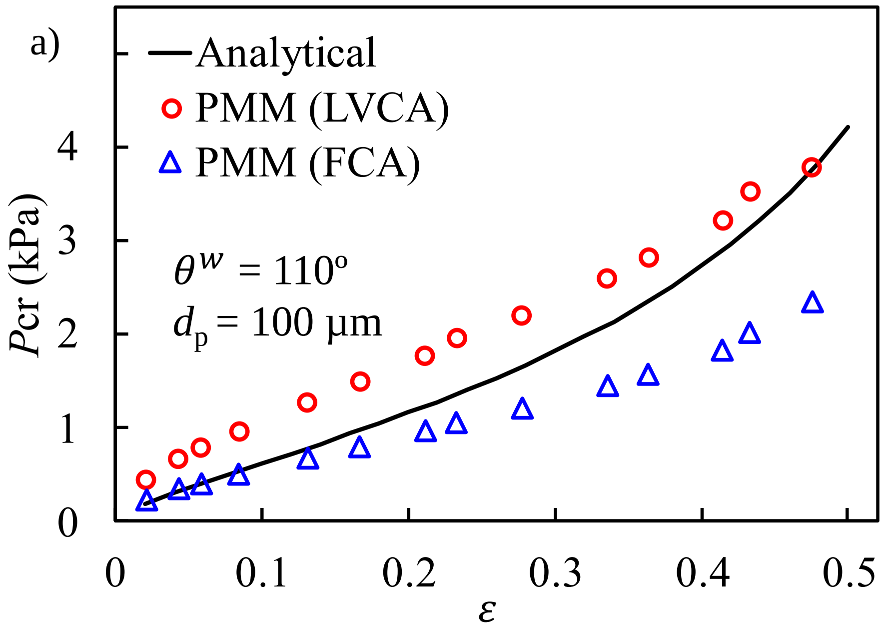
Triple contact line (TCL)

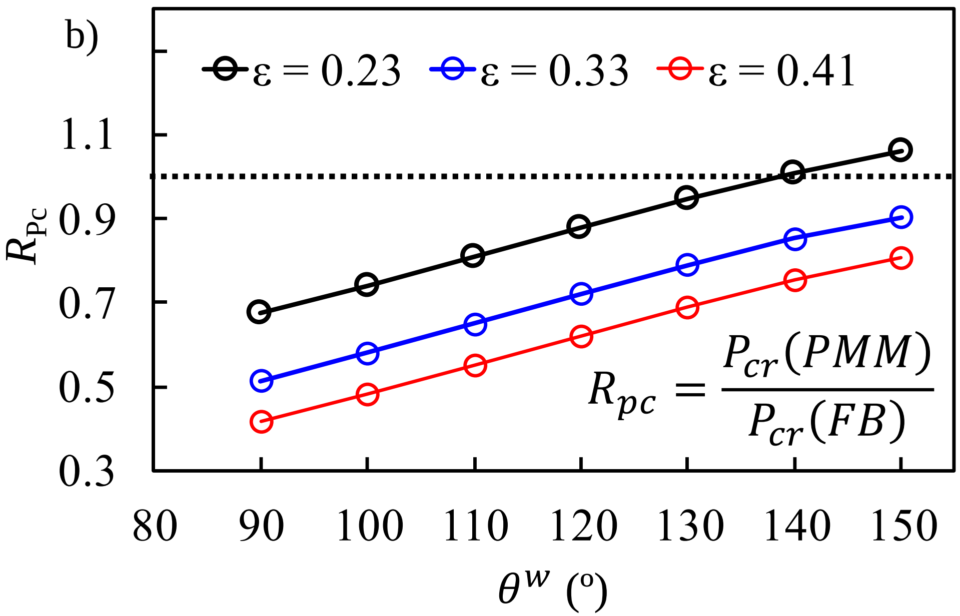


$P_c = 900$ Pa $\quad d_p = 100\ \mu$m , $\varepsilon = 0.23, \theta^w = 110°$

- TCL has a 3-D wavy profile rather than being a horizontal circle
- Immersion angle changes along the TCL around the particle because the AWI has a 3D shape

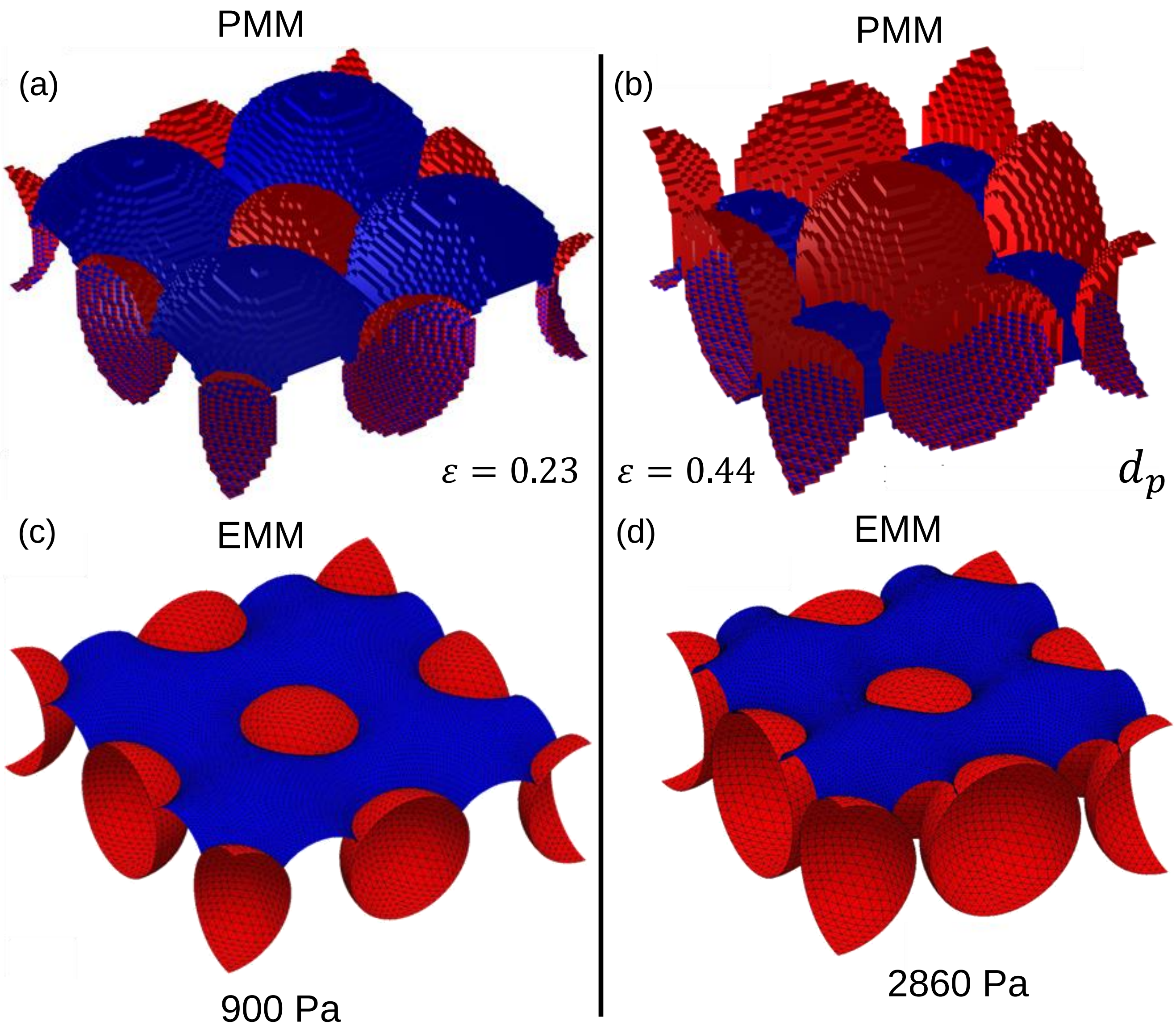
Impact of SVF and Contact Angle on Critical Pressure





Agreement between PMM (LVCA) and analytical simulation improve with increase of SVF due to reduction of waviness profile of TCL

3-D AWIs of PMM and EMM Simulations



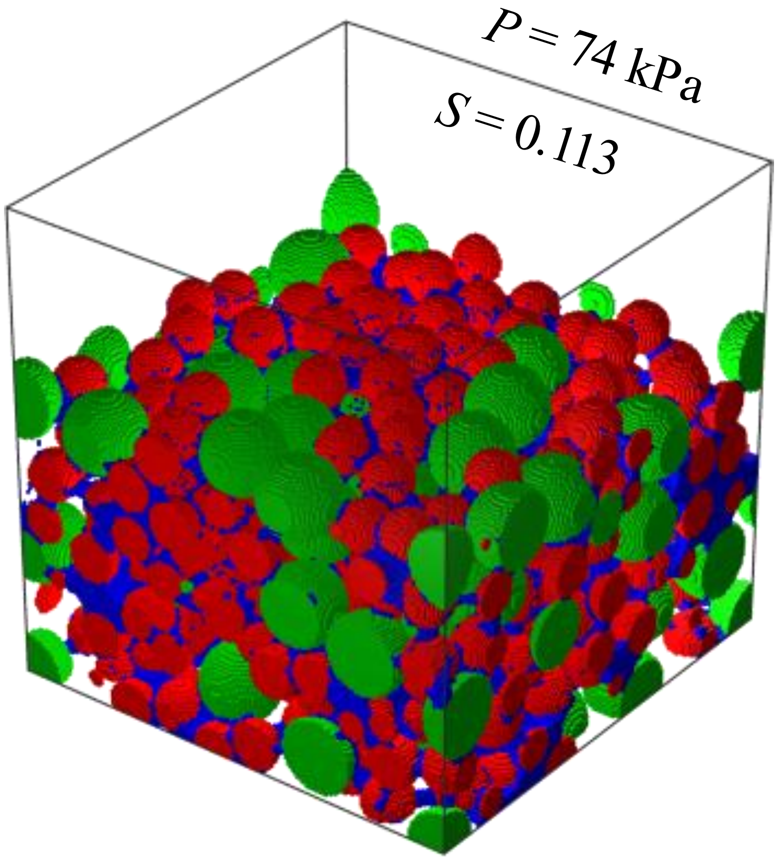
$d_p = 100\ \mu\text{m}\ \ \theta^w = 110°$

PMM cannot capture the physics of AWI coalescence and only predict burst failure

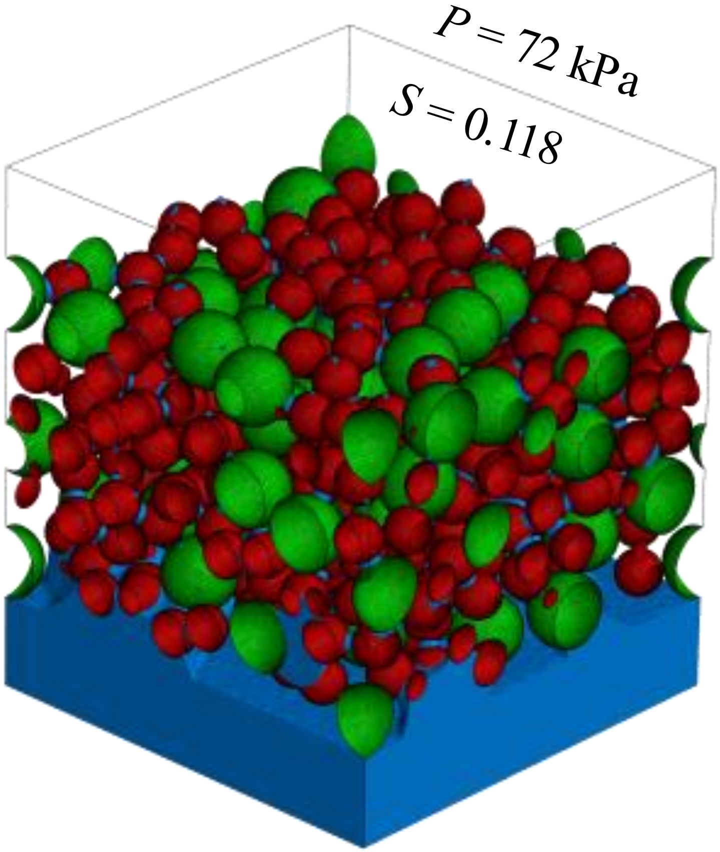
Comparison of PMM and VOF

Green: Particles $\theta_1{}^w = 80°, d_{p1} = 8\ \mu m$
Red: Particles $\theta_2{}^w = 60°, d_{p2} = 5\ \mu m$

Blue: Wetting phase (water)
Transparent: Non-wetting phase (air)



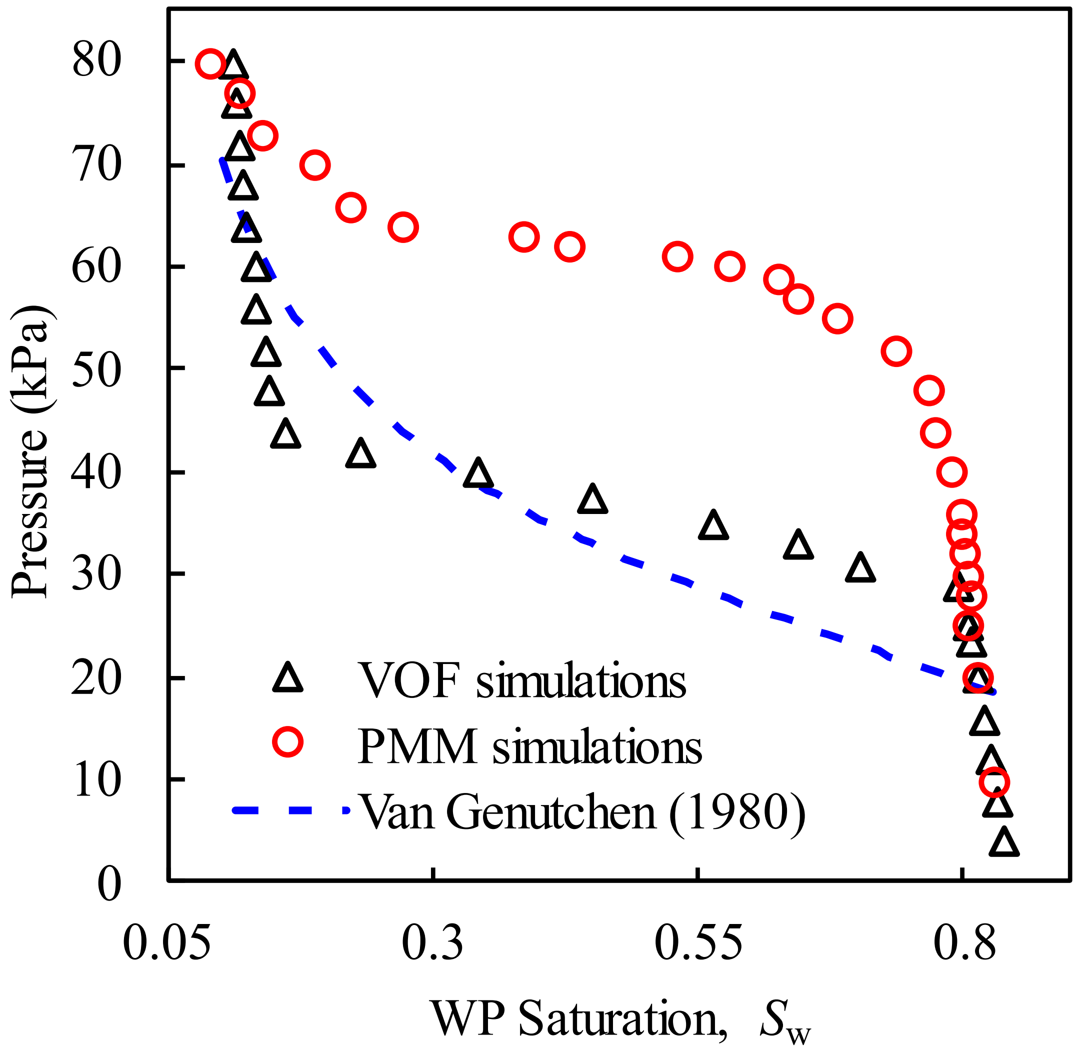
PMM



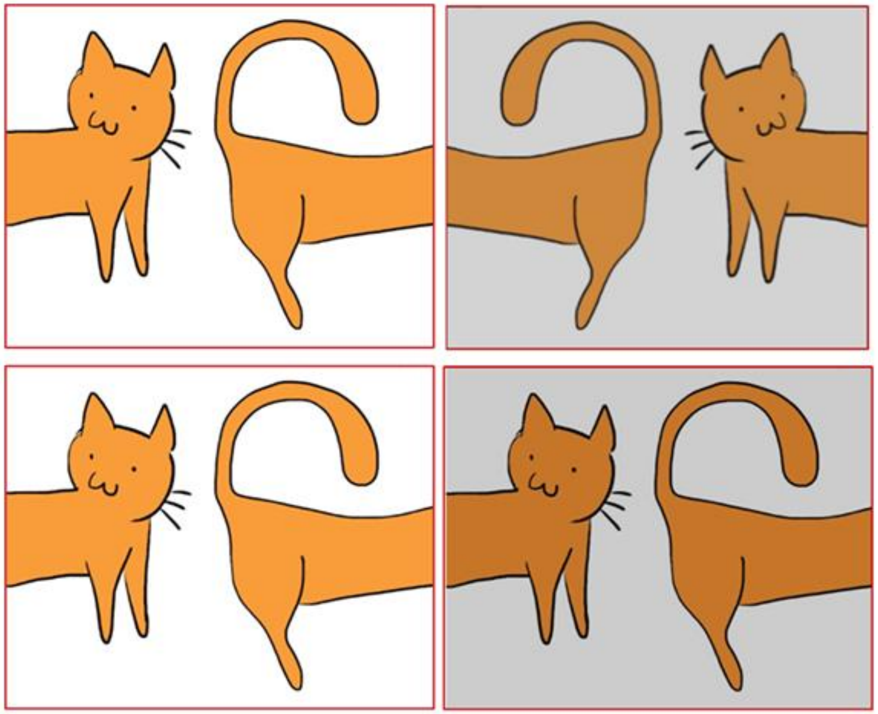
VOF

Comparison of PMM and VOF

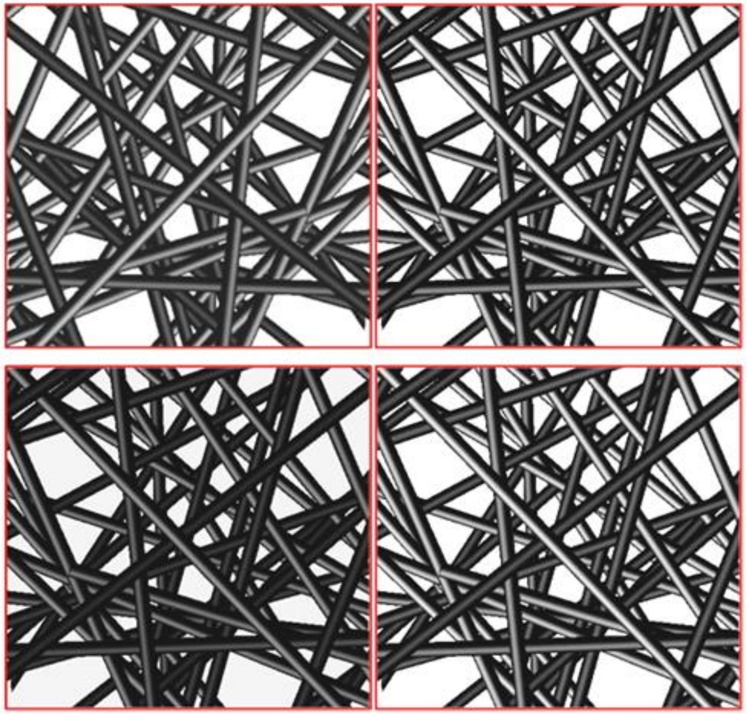
- PMM overestimate the intrusion pressure at high WP saturation
- PMM more accurate as the WP saturation decreases at higher intrusion pressure
    - *AWI is more circular rather than elongate for densely packed regions*



Boundary Conditions: Symmetry or Periodic



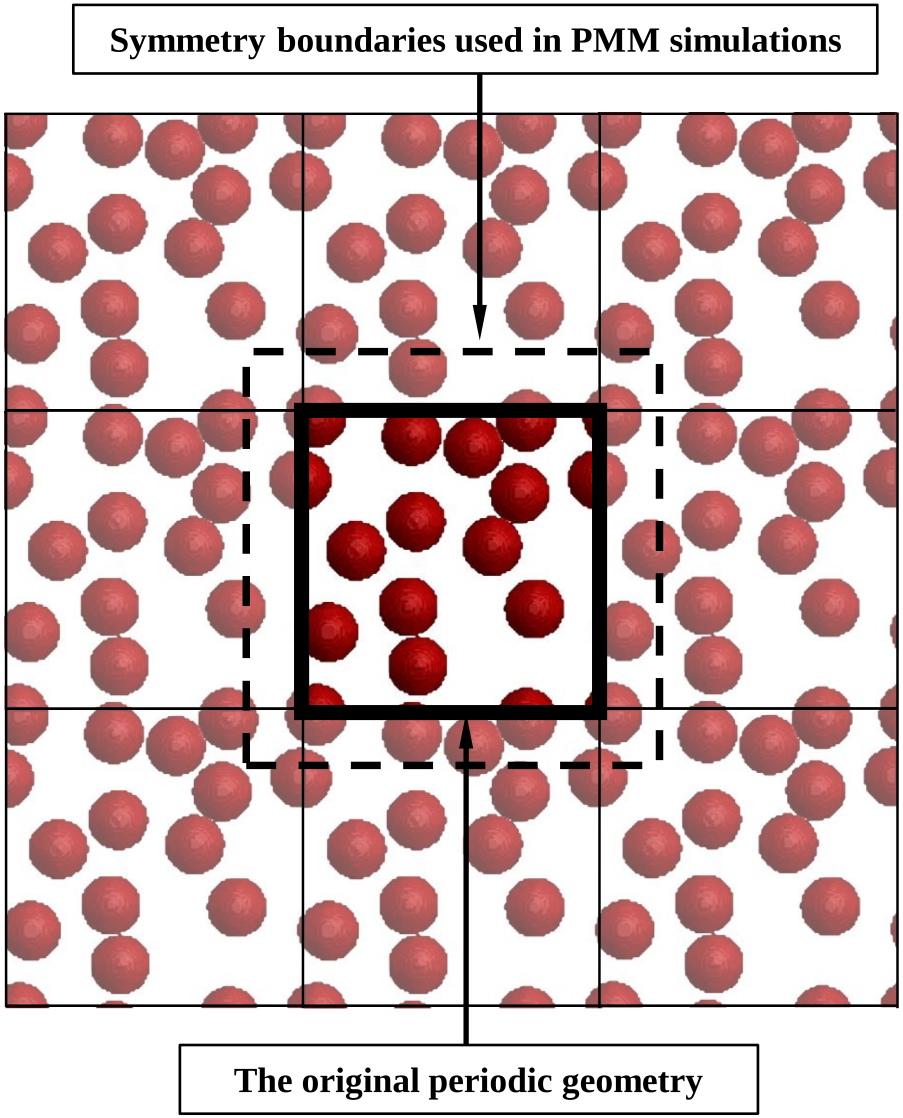
http://dingercatadventures.blogspot.com/2012/09/



The geometry of fibrous filters is neither symmetric nor periodic

Boundary Condition Treatment

- PMM inherently treat the lateral boundaries as symmetry boundaries even if the solid geometry is not symmetric
- Additional step is required to conduct accurate PMM simulation
  - ❖ *Copy the periodic image of the solid geometry across the periodic boundaries*
  - ❖ *Cropped a larger domain and performed the PMM simulation*
  - ❖ *Post-processing was only conducted for voxel that were inside the original domain*
- Error at boundaries do not propagate error deep into the domain in the PMM simulation



Conclusions

- PMM simulations reasonably accurate in densely packed particle beds, where interface coalescence is not prevalent
- PMM overestimate the intrusion pressure for a given wetting phase saturation
- PMM simulations are many orders of magnitude faster than their traditional counterparts
- PMM only predict the burst failure of AWI

- Acknowledgement:

  - *Financial support from North Carolina Collaboratory Program is gratefully acknowledged.*