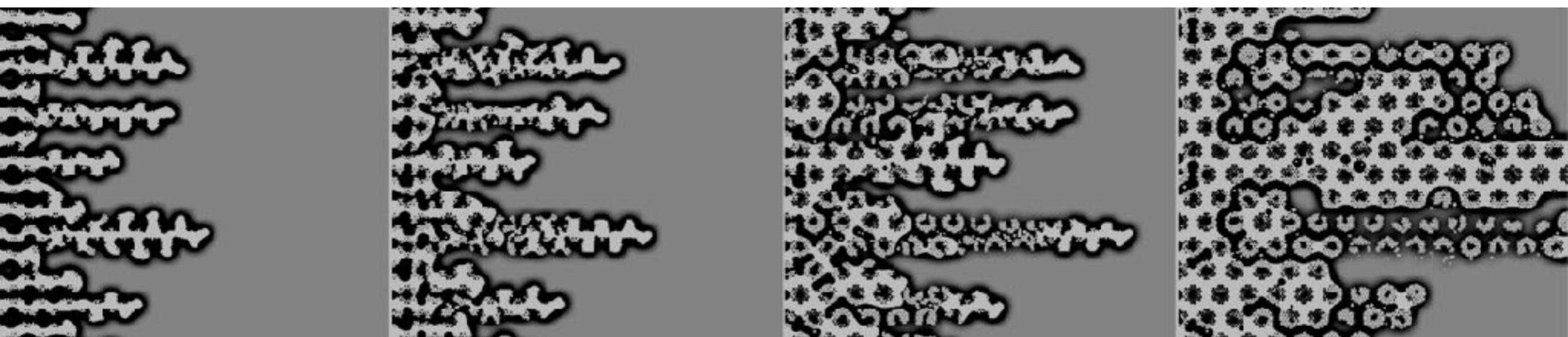


Pore Scale Modelling of Multiphase Flow in Heterogeneous Granular Materials



Yixiang Gan

School of Civil Engineering



The University of Sydney, Australia



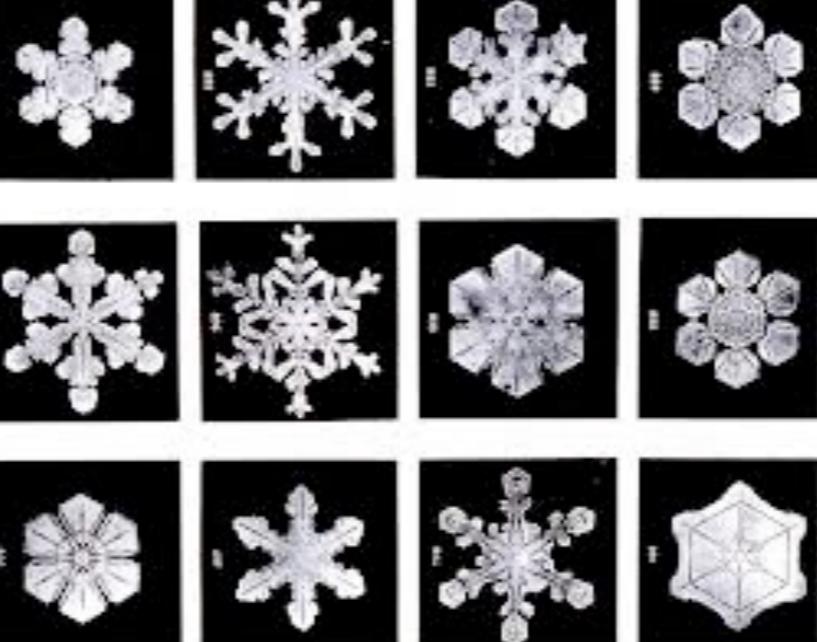
Email: yixiang.gan@sydney.edu.au



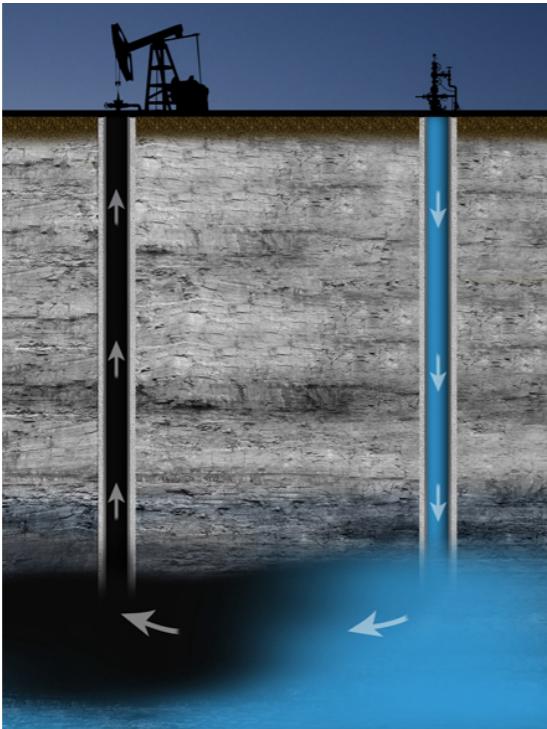
Twitter: [@drgan](https://twitter.com/drgan)



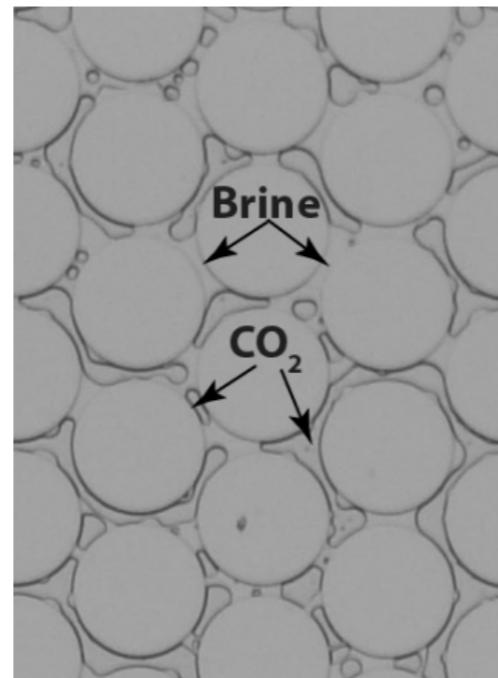
Website: drgan.org



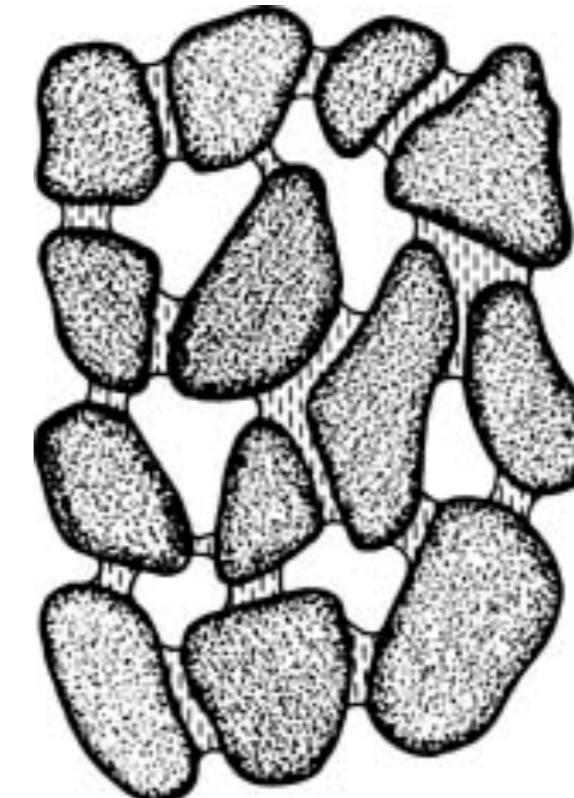
Background



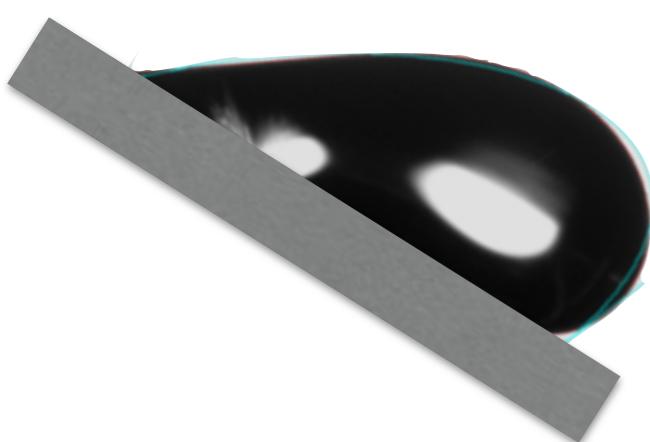
oil recovery



carbon storage



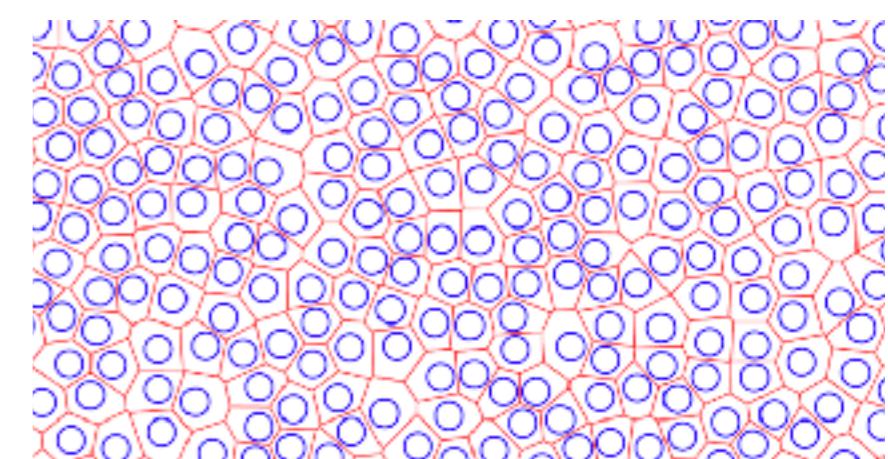
soil mechanics



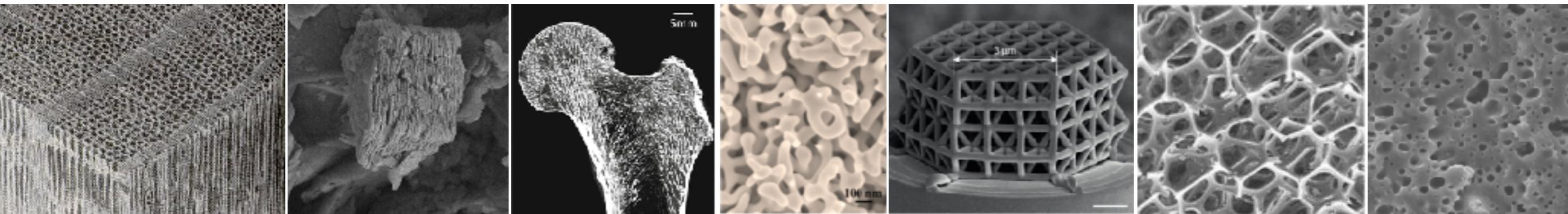
Multiphase Flow
in Porous Media

Wettability,
Contact Angle Dynamics

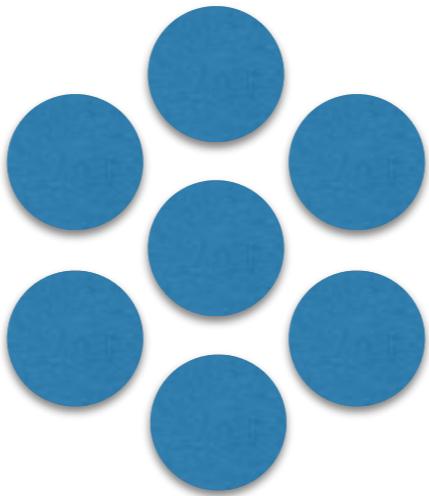
Heterogenous
Microstructure



Heterogeneity in Porous Media

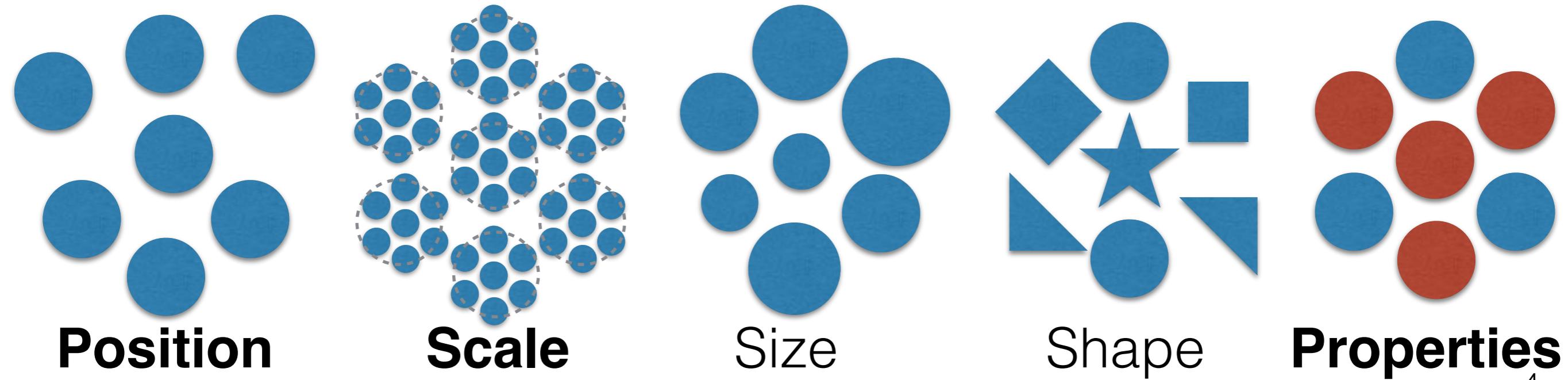


“Homogeneous”



“Homogeneous media are all alike; every heterogeneous medium is heterogeneous in its own way.” – “Anna Karenina Principle” by Leo Tolstoy

“Heterogeneous”



Position

Scale

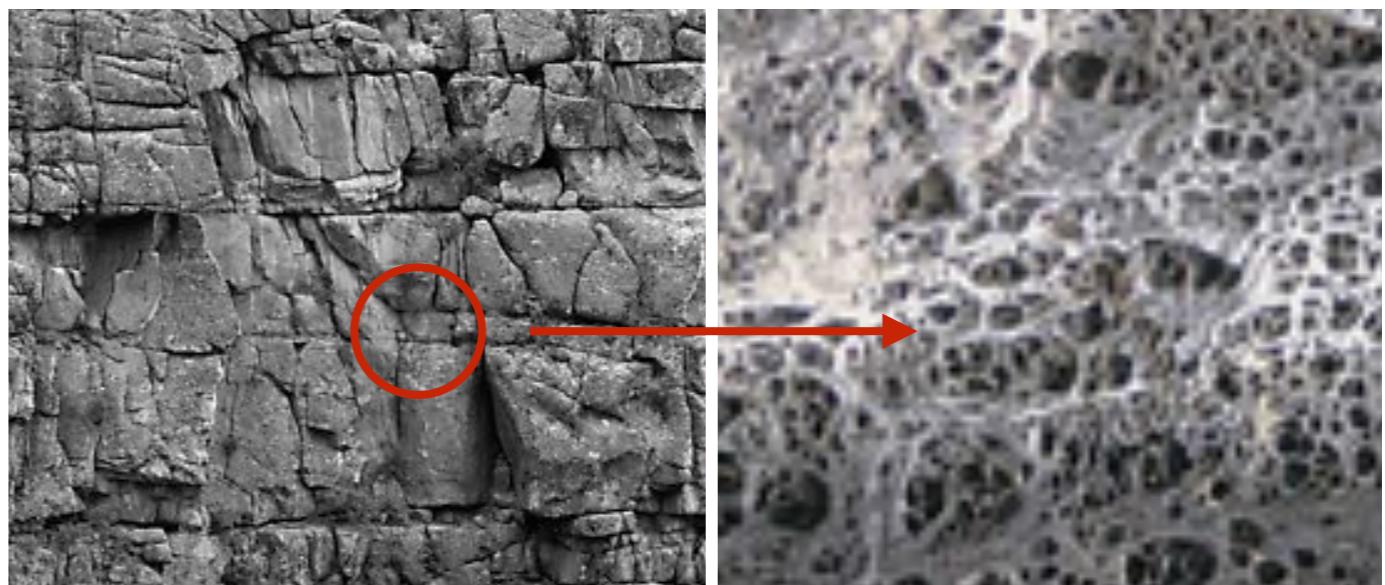
Size

Shape

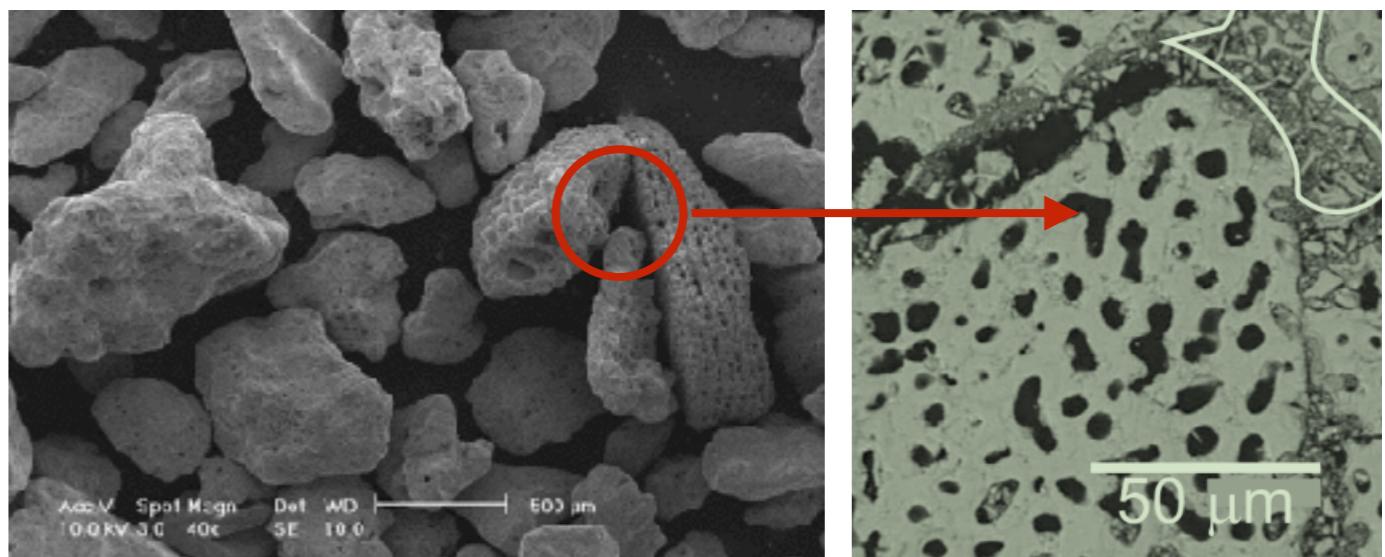
Properties

Hierarchical Porous Media

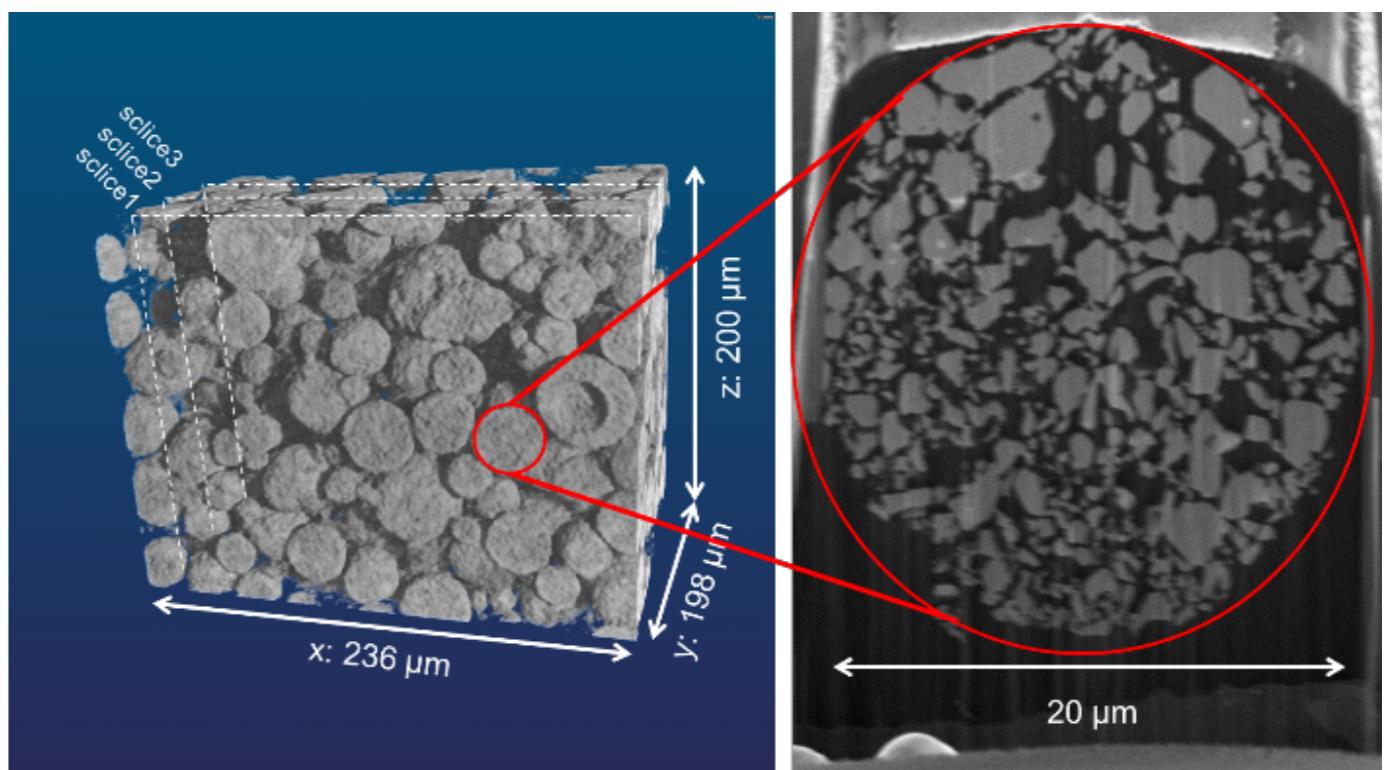
- fractured rocks



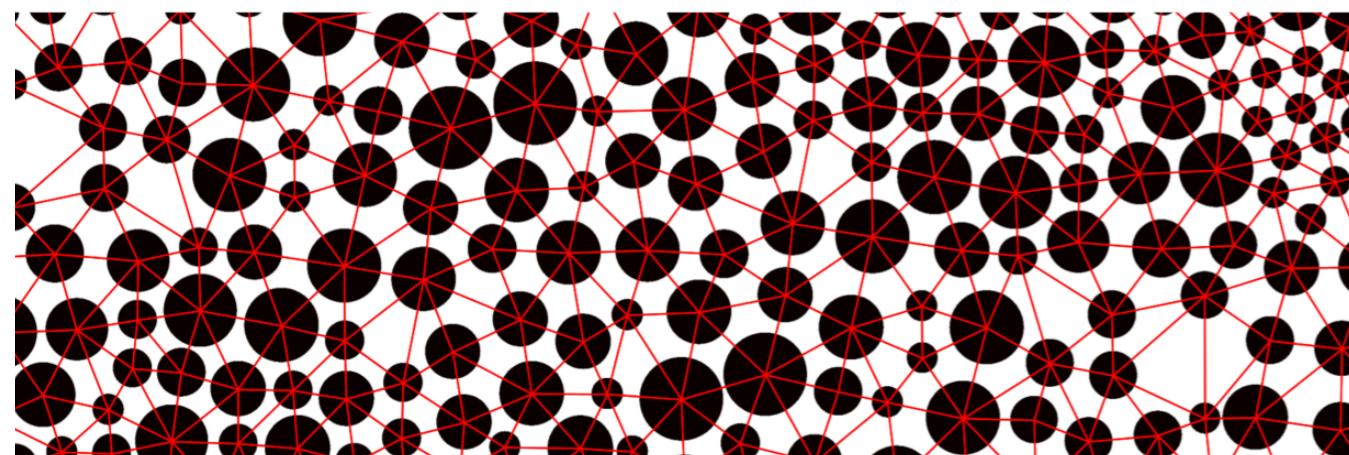
- carbonate sand



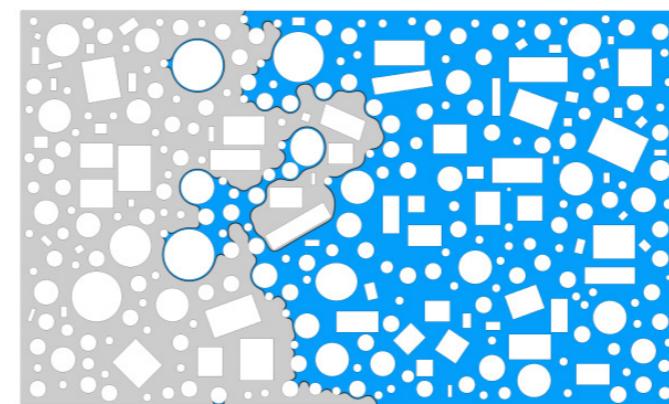
- Li-ion battery cathode materials



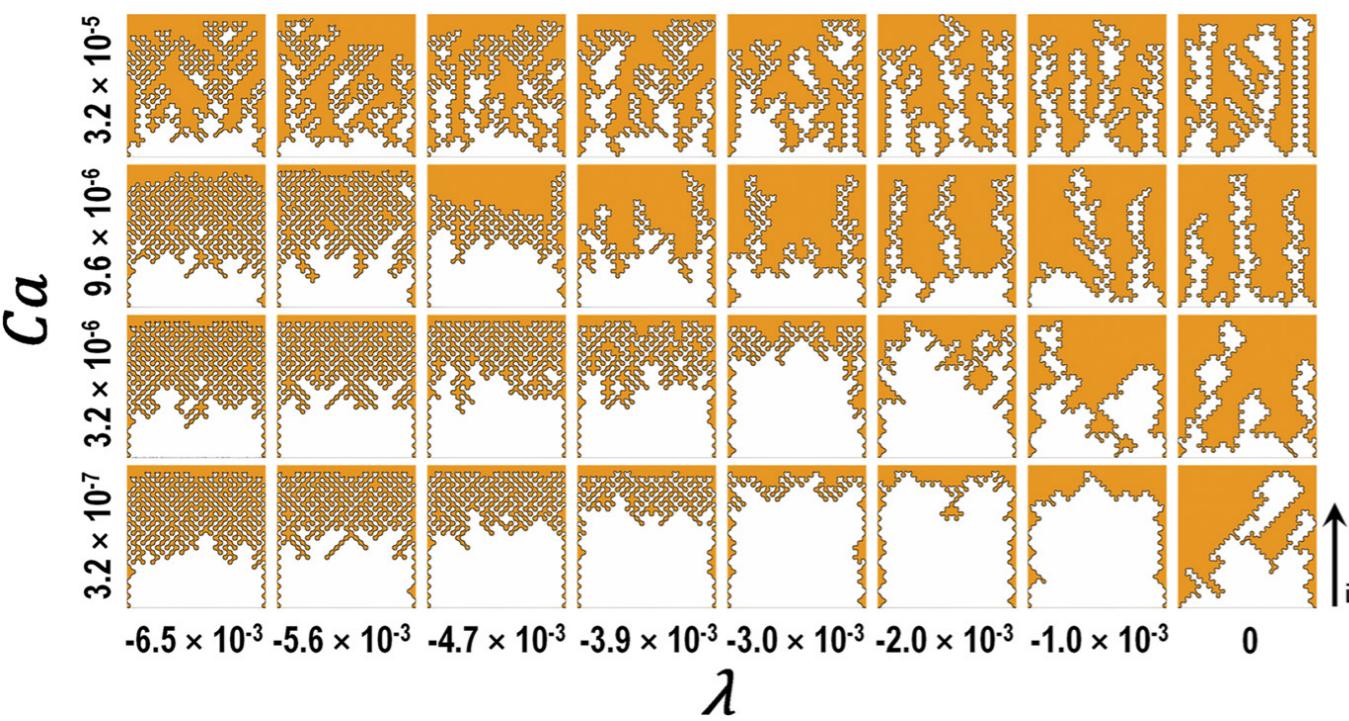
Heterogeneity in Porous Media



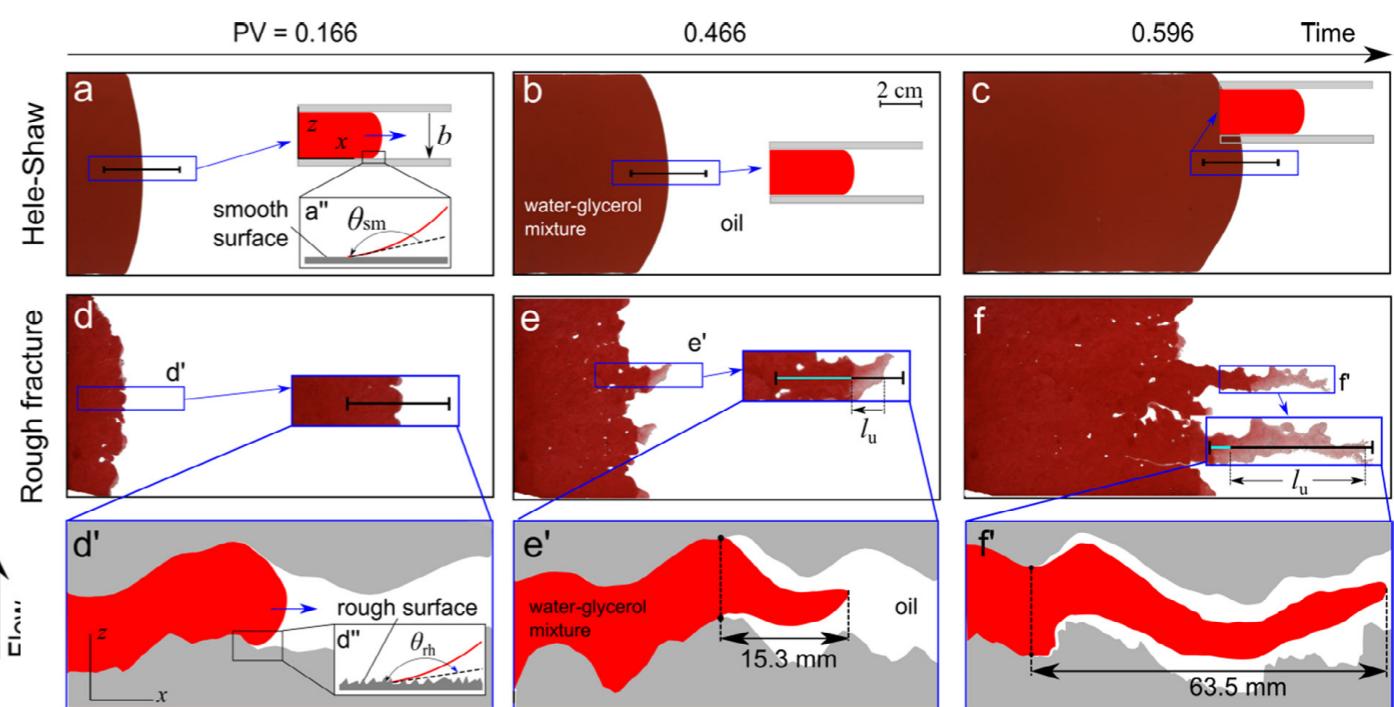
Spatially correlated heterogeneity, Borgman et al. (2017)



Obstacle shape, Cueto-Felgueroso et al. (2018)



Gradient structure, Rabbani et al. (2018)

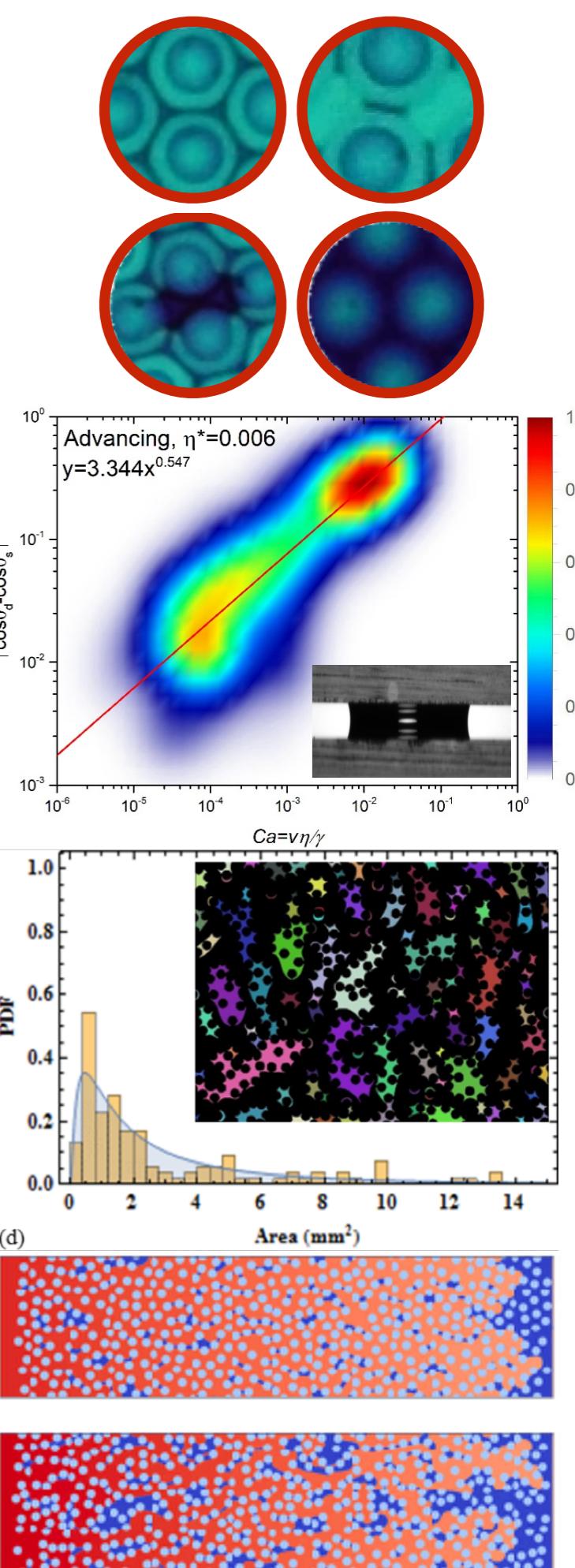


Morphology and roughness, Chen Y-F, et al. 2018

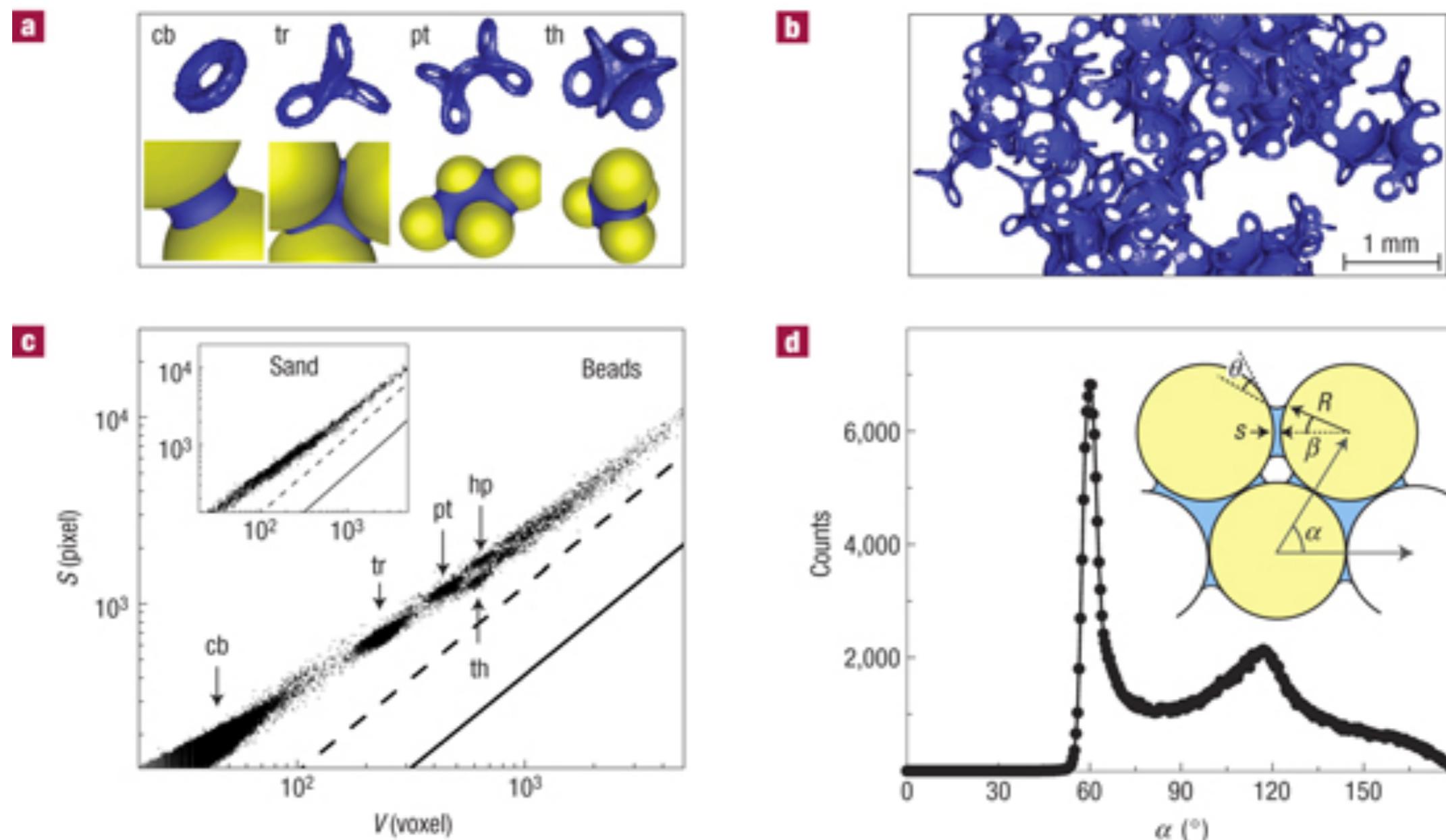
Outline

Multiphase flow in heterogenous porous media:

1. (Surface-scale) **Wettability**: contact angle dynamics including capillary bridge experiments, SPH and MD simulations;
2. (Pore-scale) **Topological disorder** porous structure, including drainage and injection;
3. (Multiple time scales) Effects of Cassie-Wenzel **wetting transition** in fluid displacement;
4. (Multiple length scales) **Hierarchical** porous structure.



Unsaturated granular media: liquid patches



Scheel, M. et al. Morphological clues to wet granular pile stability. Nat. Mater. 7, 189–93 (2008).

vs the state variable, degree of saturation:

$$S_r = \frac{V_w}{V_v}$$

Liquid penetration: wettability and injection rate

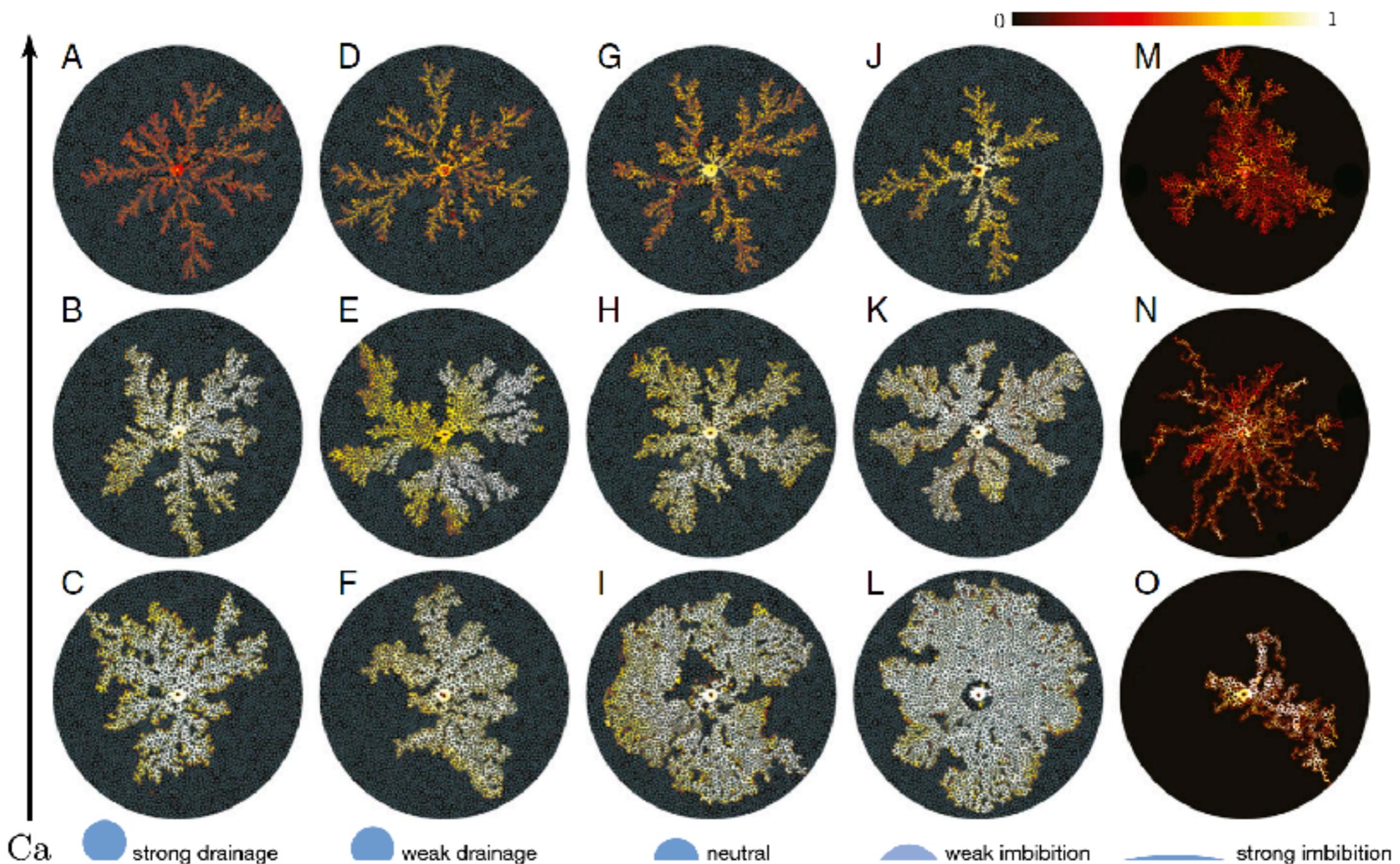
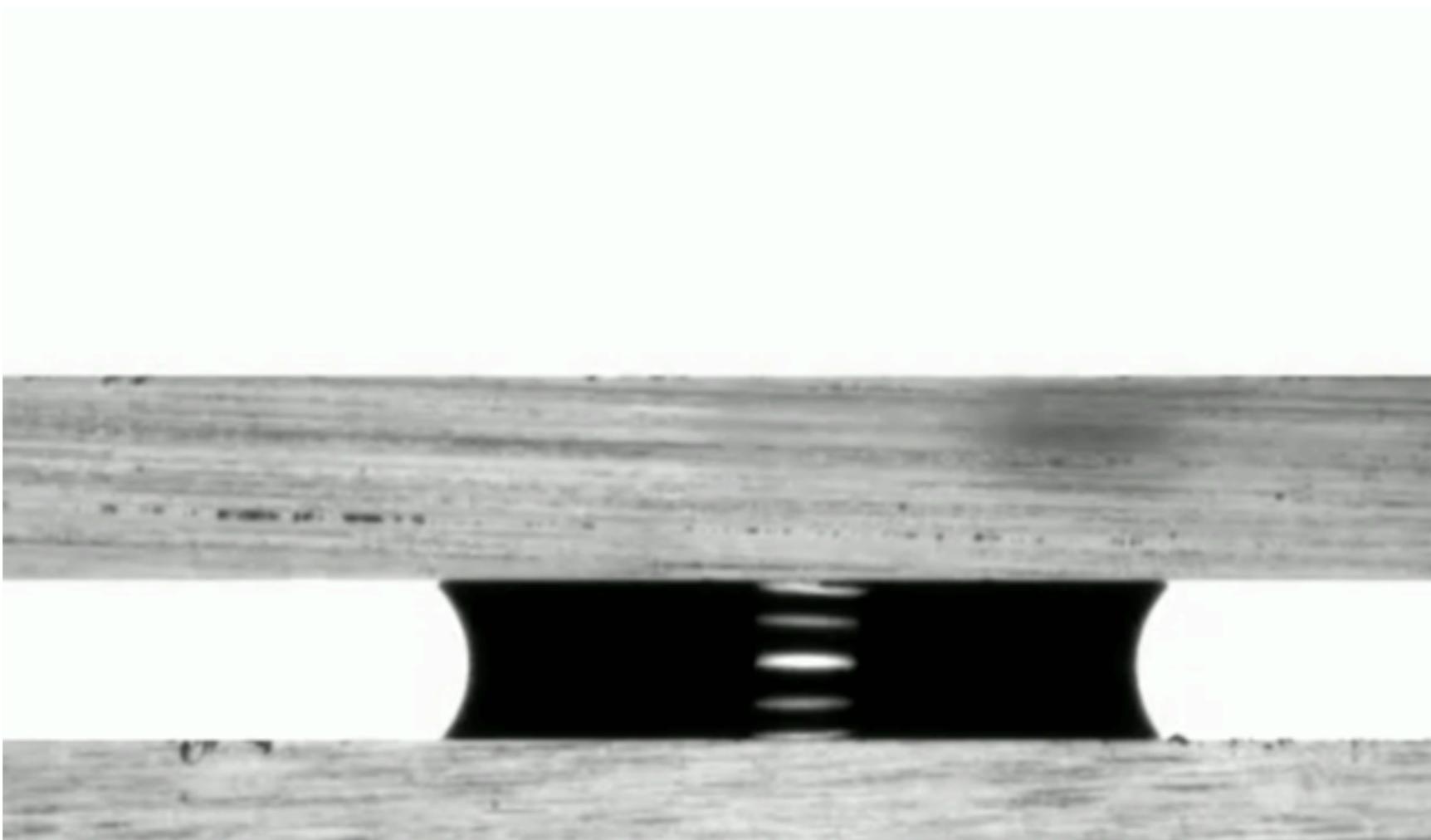
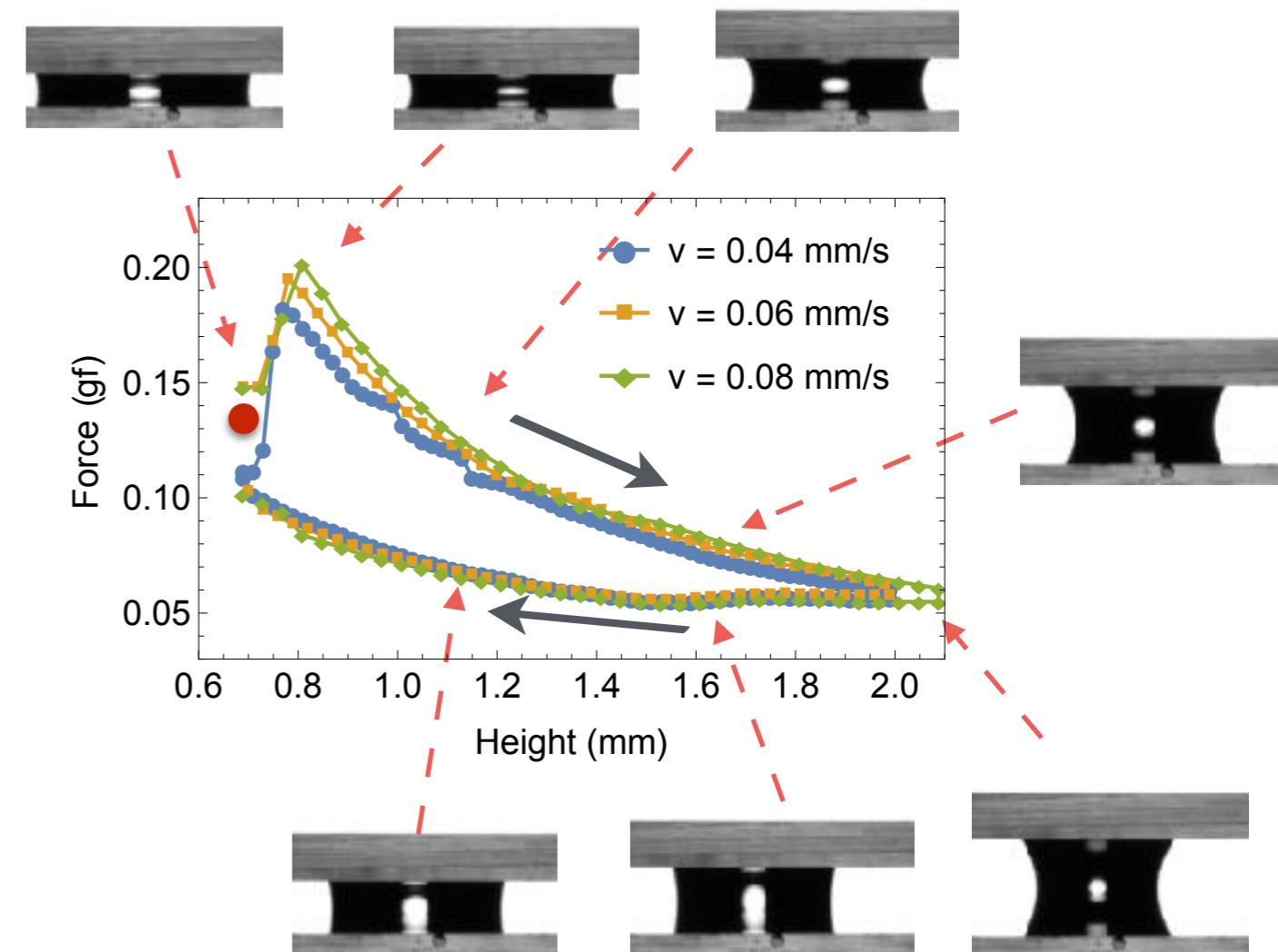
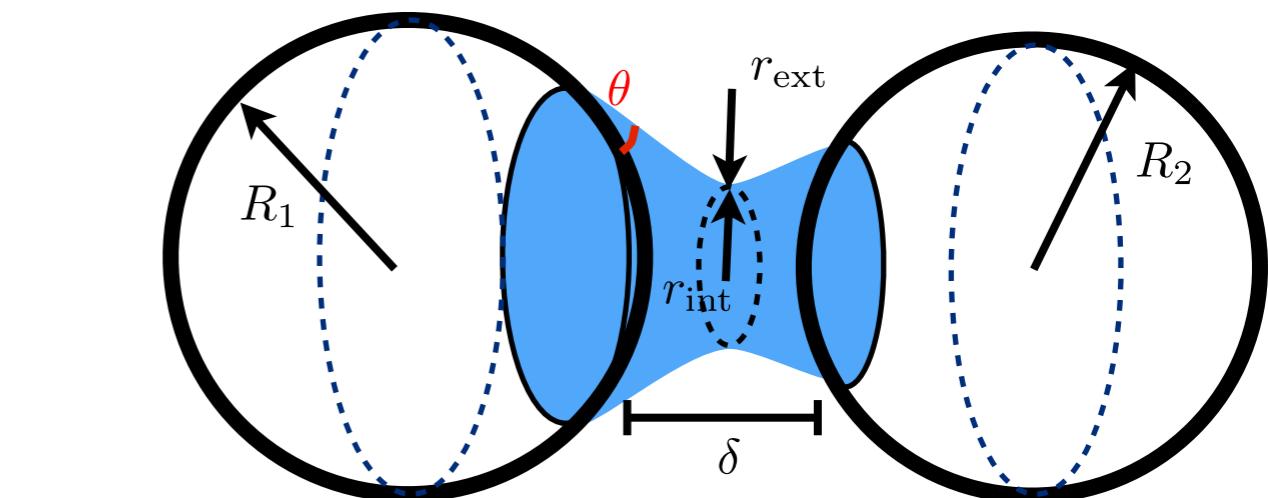
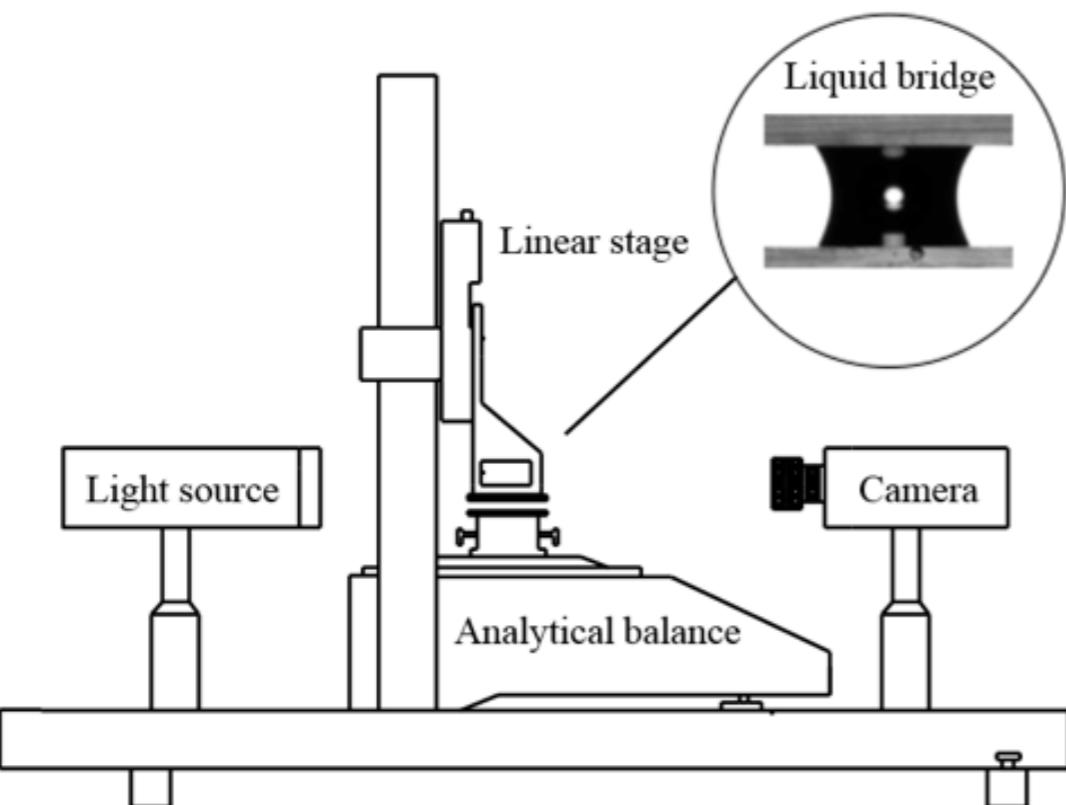
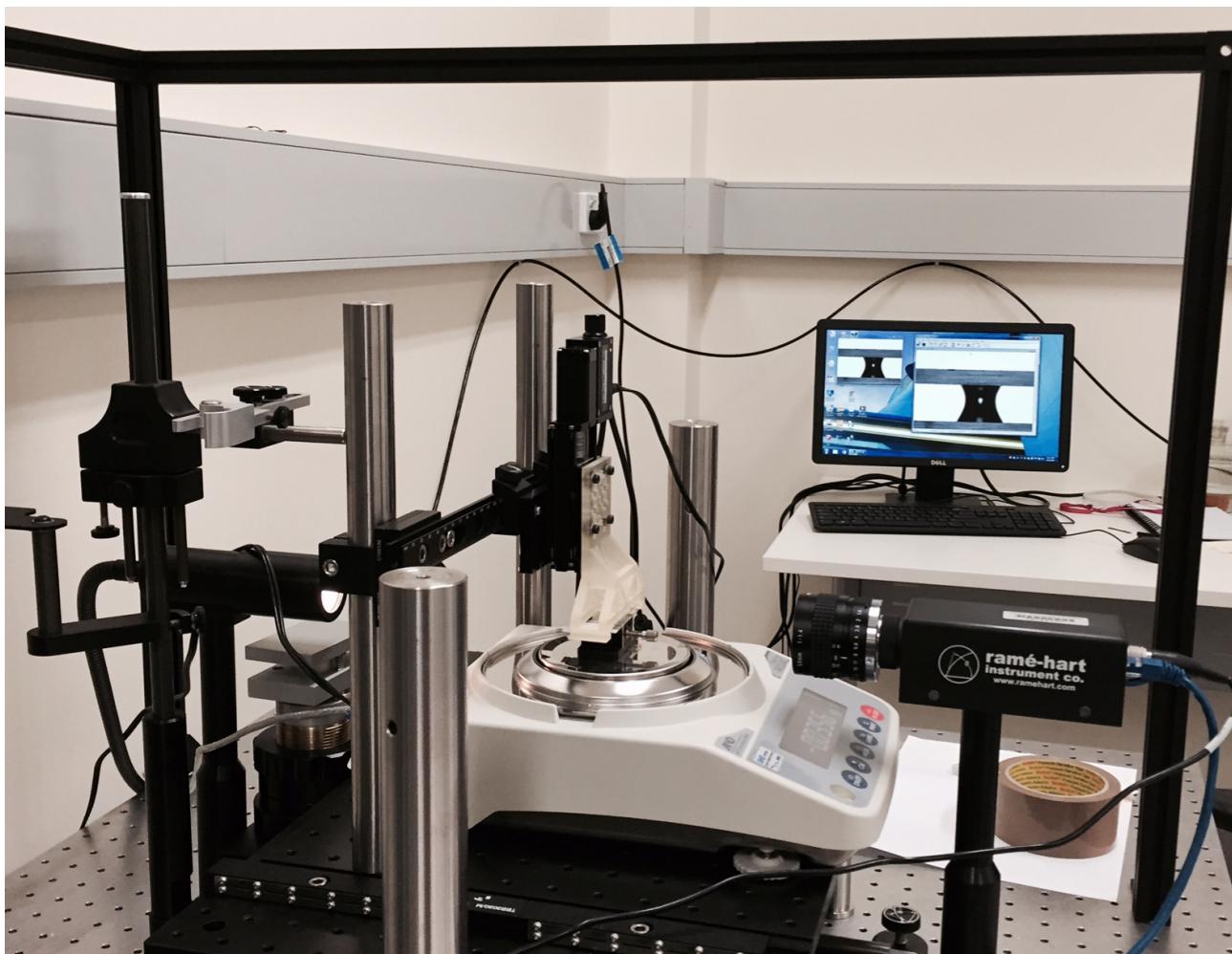


Fig. 2. Displacement patterns for different wettability conditions (left to right: $\theta = 150^\circ, 120^\circ, 90^\circ, 60^\circ, 7^\circ$) and capillary numbers (bottom to top: $Ca = 2.9 \times 10^{-3}, 2.9 \times 10^{-2}, 2.9 \times 10^{-1}$). These patterns correspond to the end of the experiment, which is when the invading fluid reaches the perimeter of the flow cell. The colormap shows the gap-averaged saturation of the invading water. The pattern of circular posts is overlaid on the experimental images and all images are oriented in the same way to aid visual comparison. Generally, the displacement becomes more efficient as the flow cell becomes more hydrophilic (i.e., decreasing θ), or as Ca decreases. These trends do not hold for strong imbibition (M–O), which has a very low displacement efficiency for all Ca .

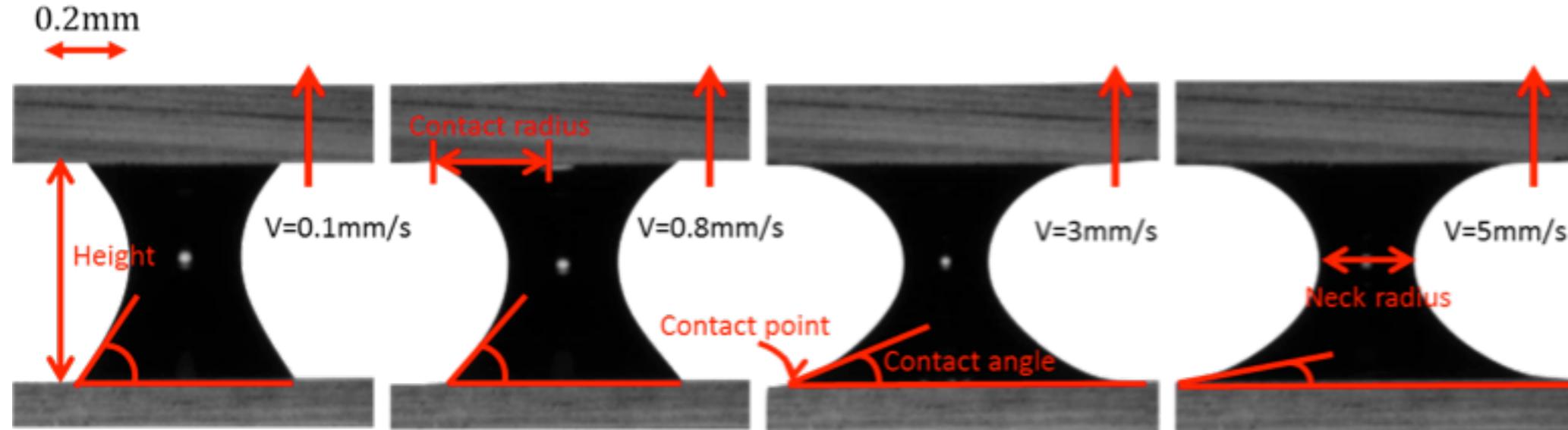
(1/4) Wettability: Contact Angle Dynamics



Contact angles dynamics (liquid bridge experiments)

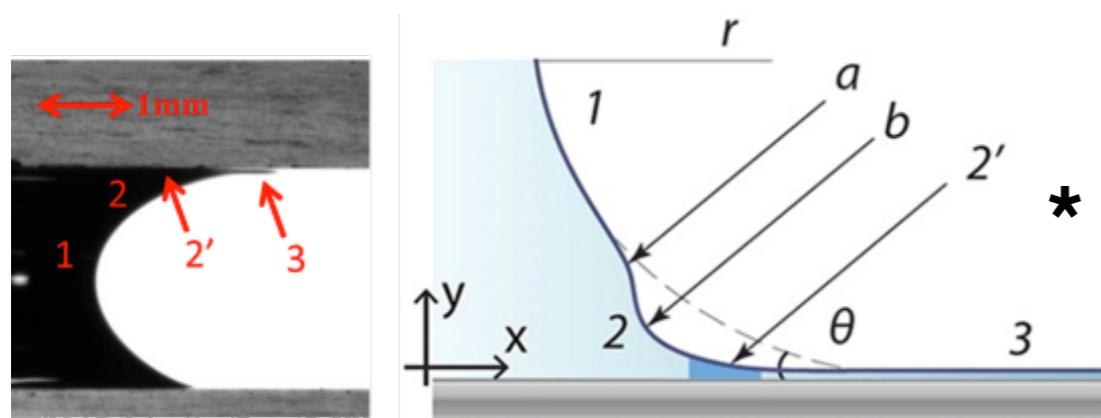


Contact angles dynamics (liquid bridge experiments)

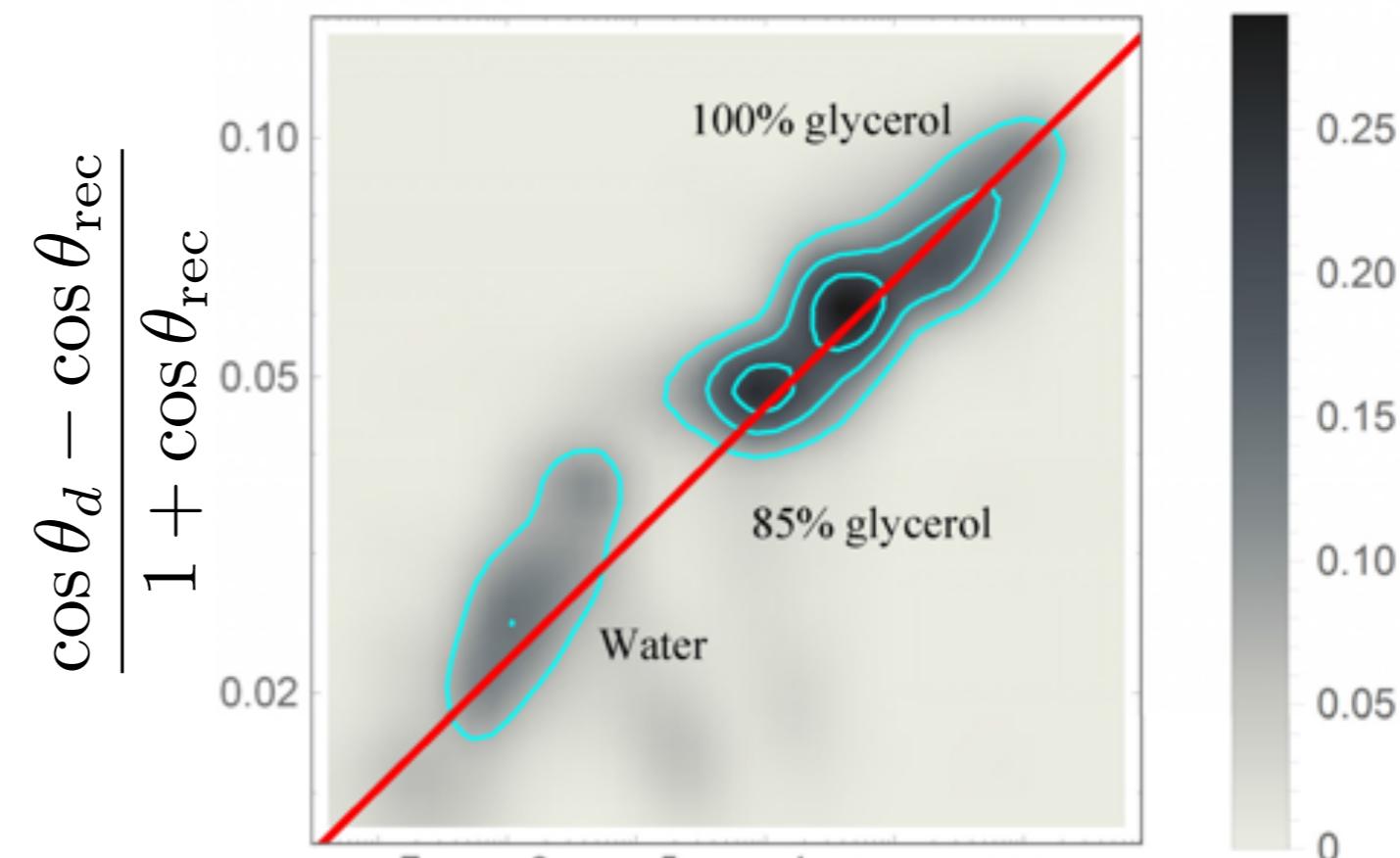


$$\cos \theta_d - \cos \theta_{\text{rec}} \propto (\text{Ca}^*)^\alpha$$

$$\cos \theta_{\text{adv}} - \cos \theta_d \propto (\text{Ca}^*)^\alpha$$



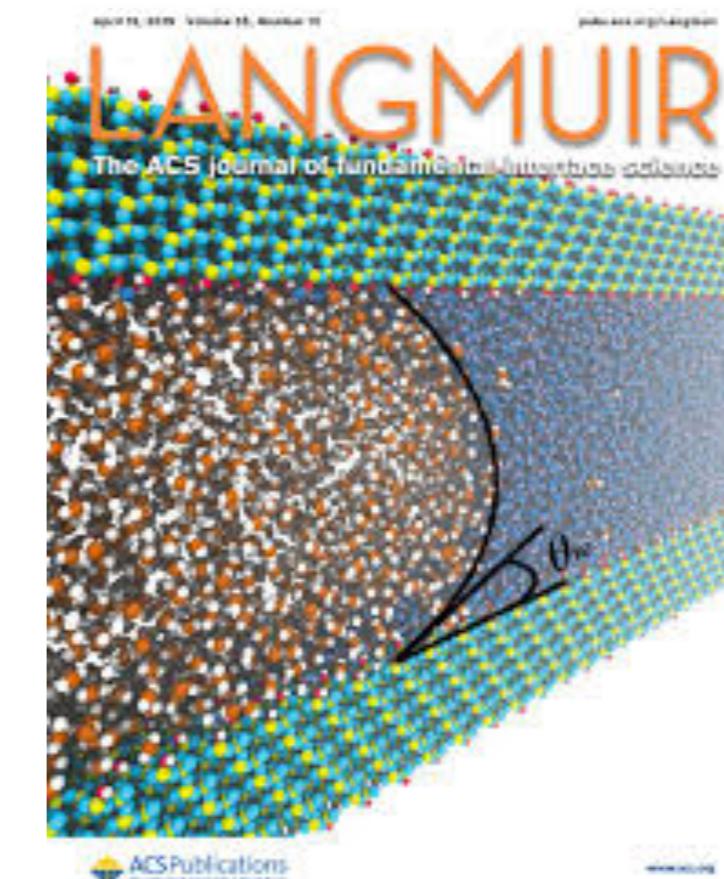
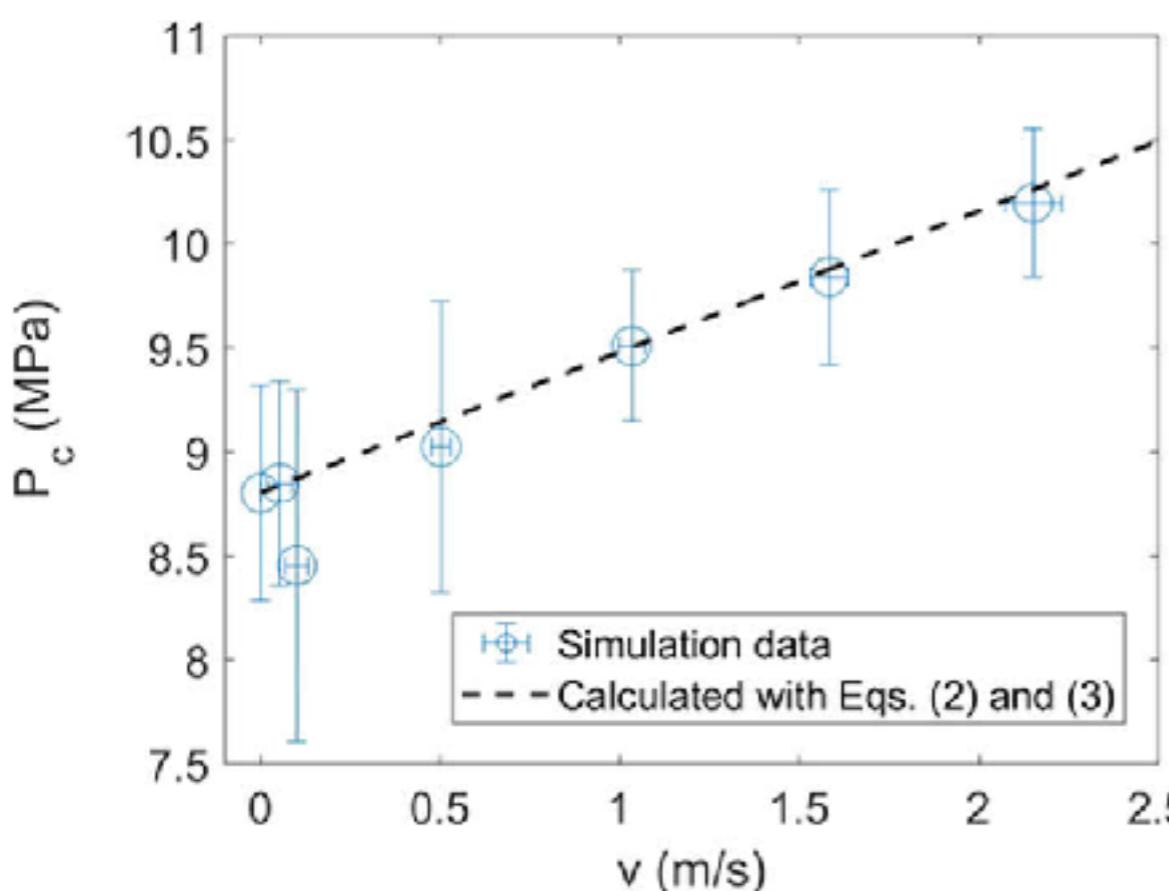
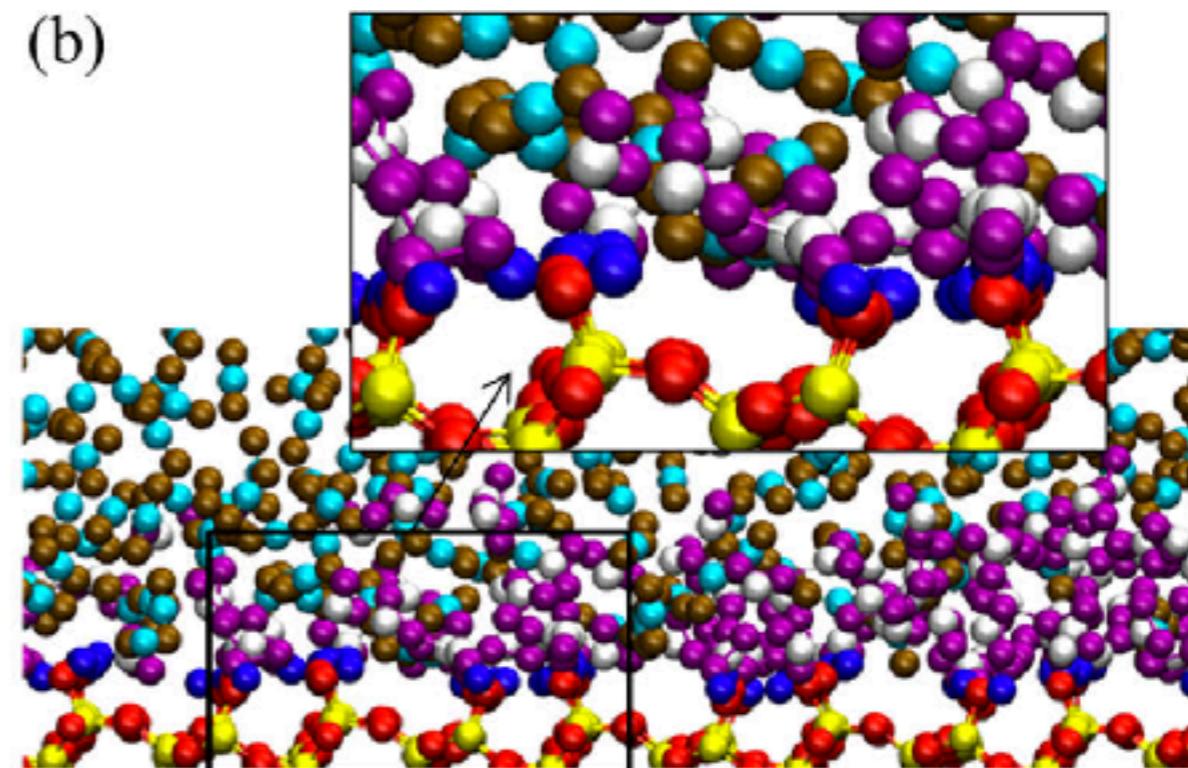
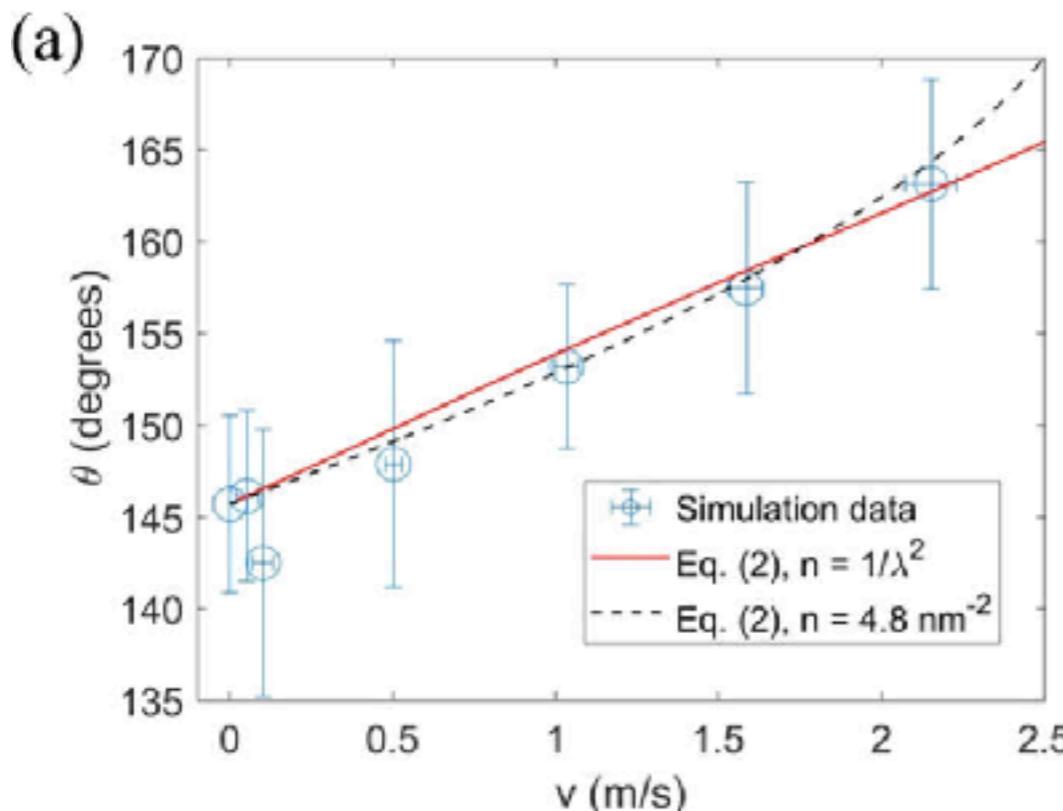
* Kuchin and Starov (2016) Hysteresis of contact angle of a meniscus inside a capillary with smooth homogeneous solid walls, Langmuir, 2016, 32 (21), pp 5333–5340.



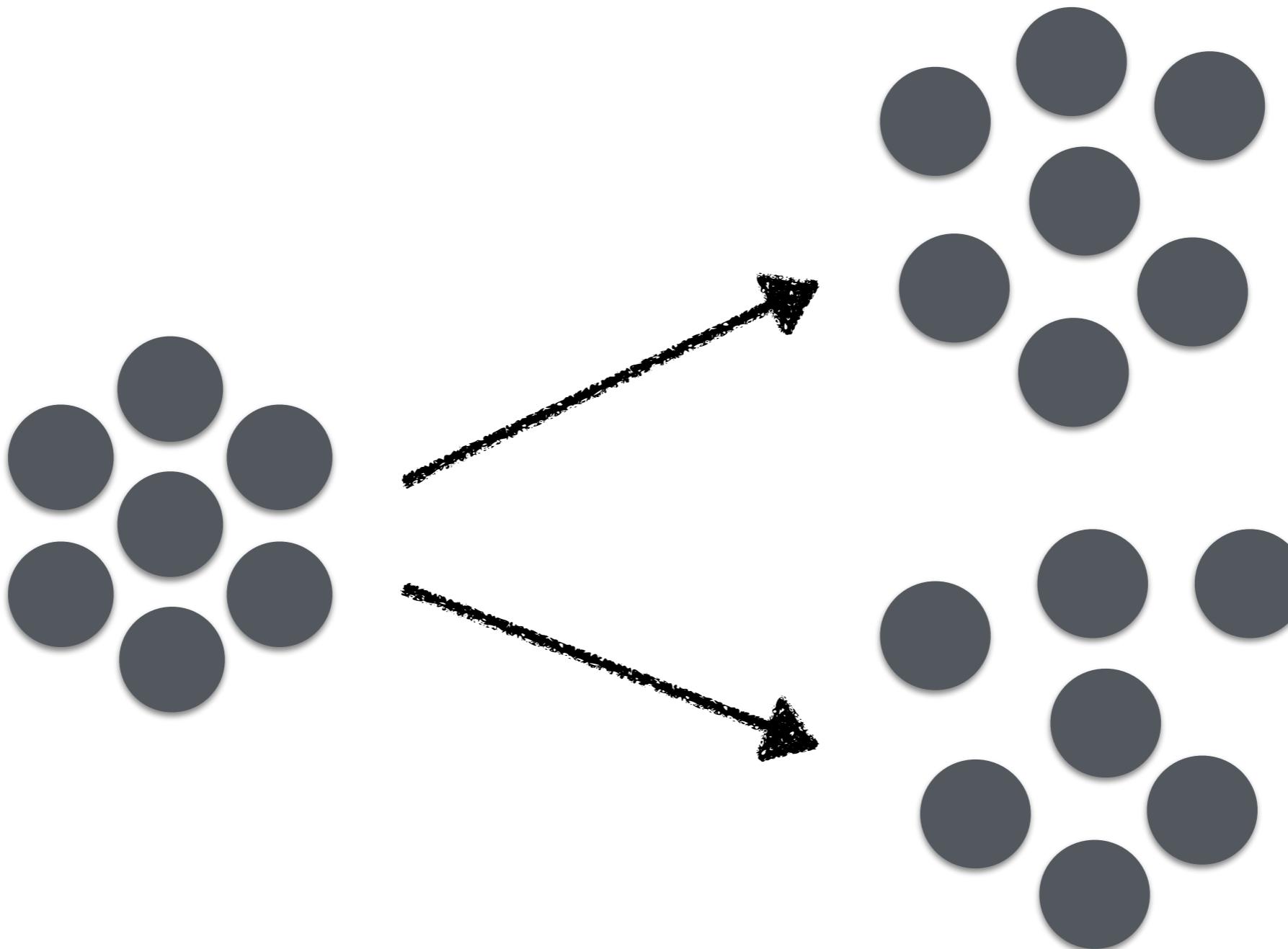
$$\text{Ca}^* = \frac{v\eta}{\gamma}$$

* Shi, Z., Zhang, Y., Liu, M., Hanaor, D.A. and Gan, Y. (2018). Dynamic contact angle hysteresis in liquid bridges. Colloids and Surfaces A. 555:365-371.

Supercritical CO₂: Wettability and dynamic behaviour

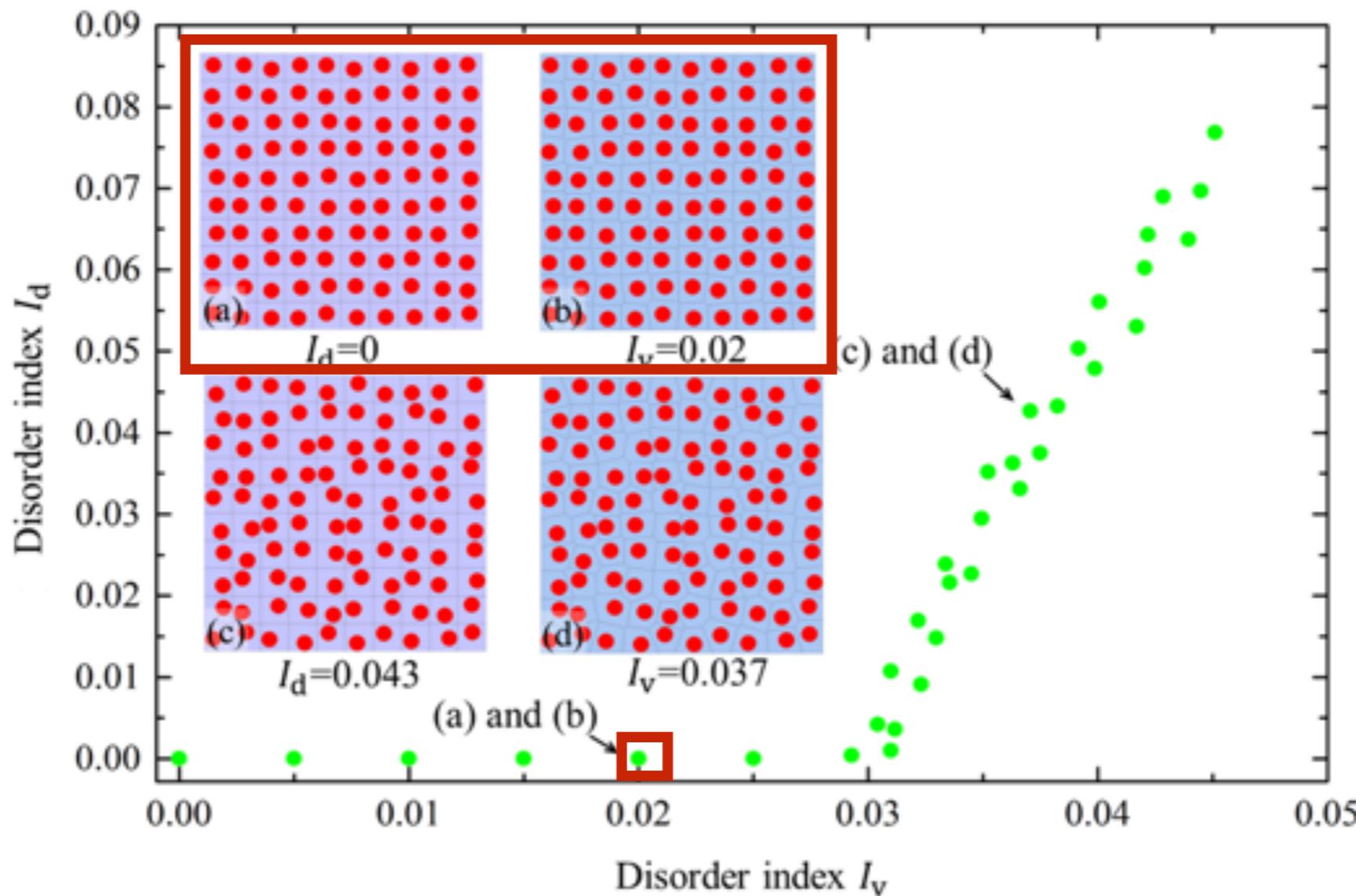


(2/4) Topological Disorder



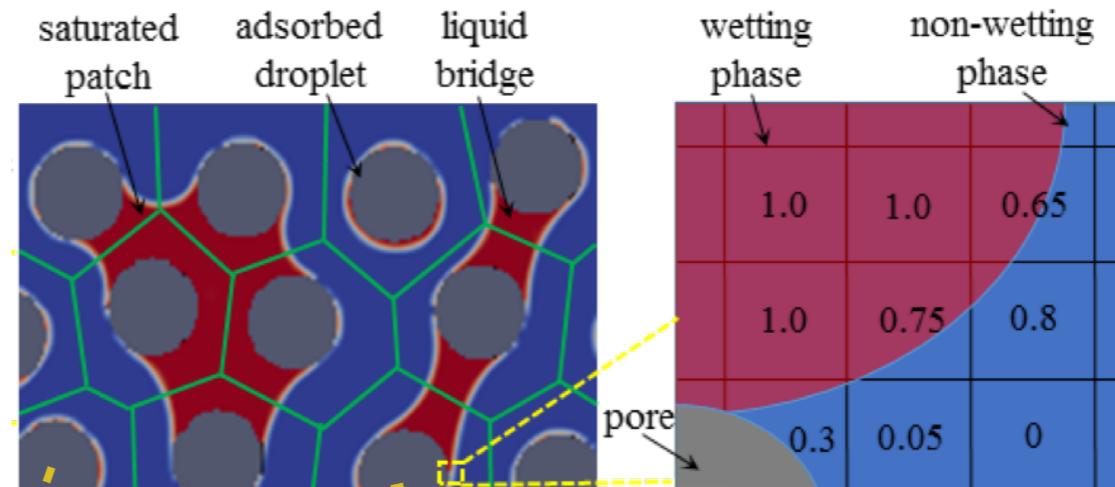
Topology: Disorder Index for Pore Space

$$I_V = [\langle \phi_i^2 \rangle - \phi^2]^{1/2}$$

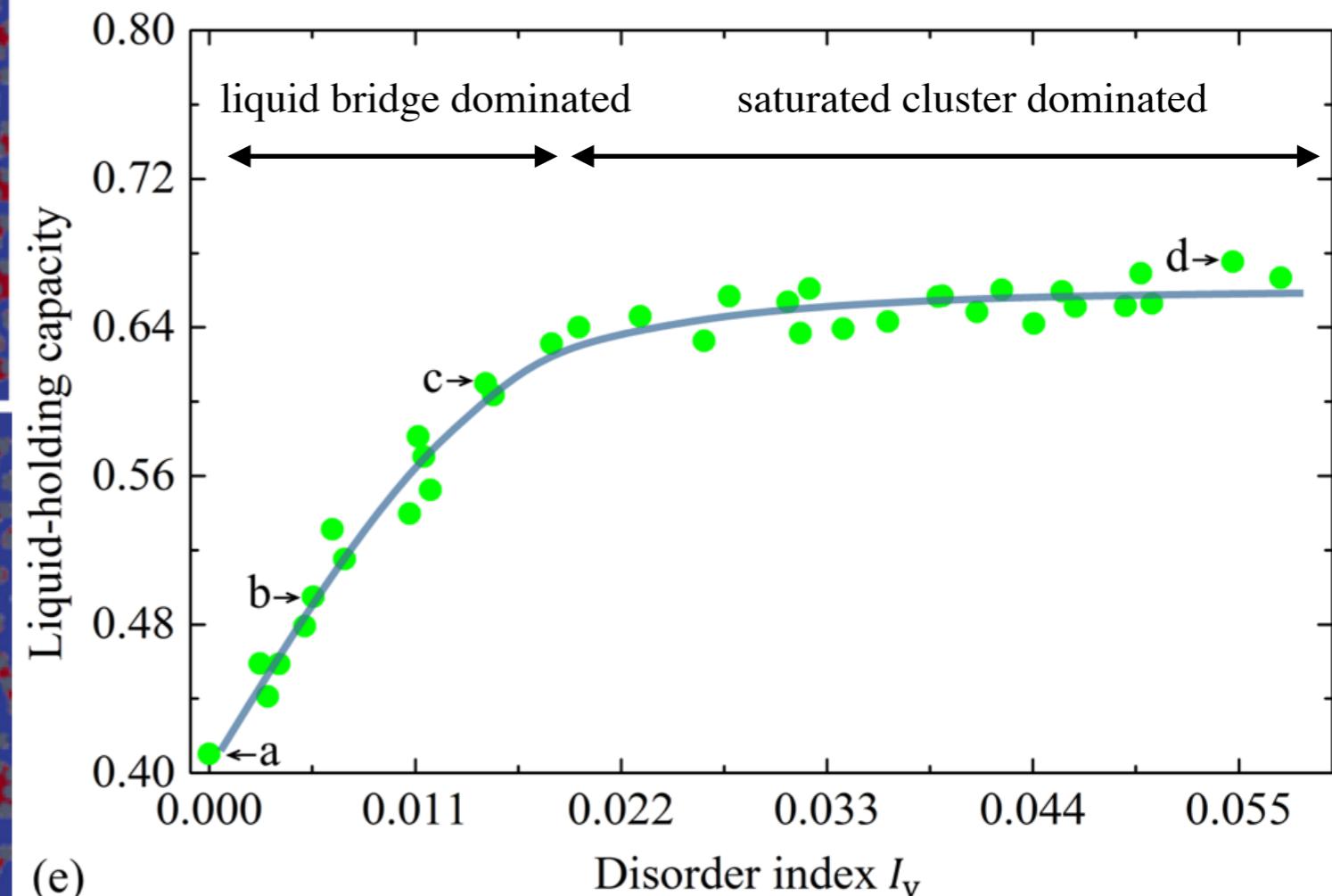
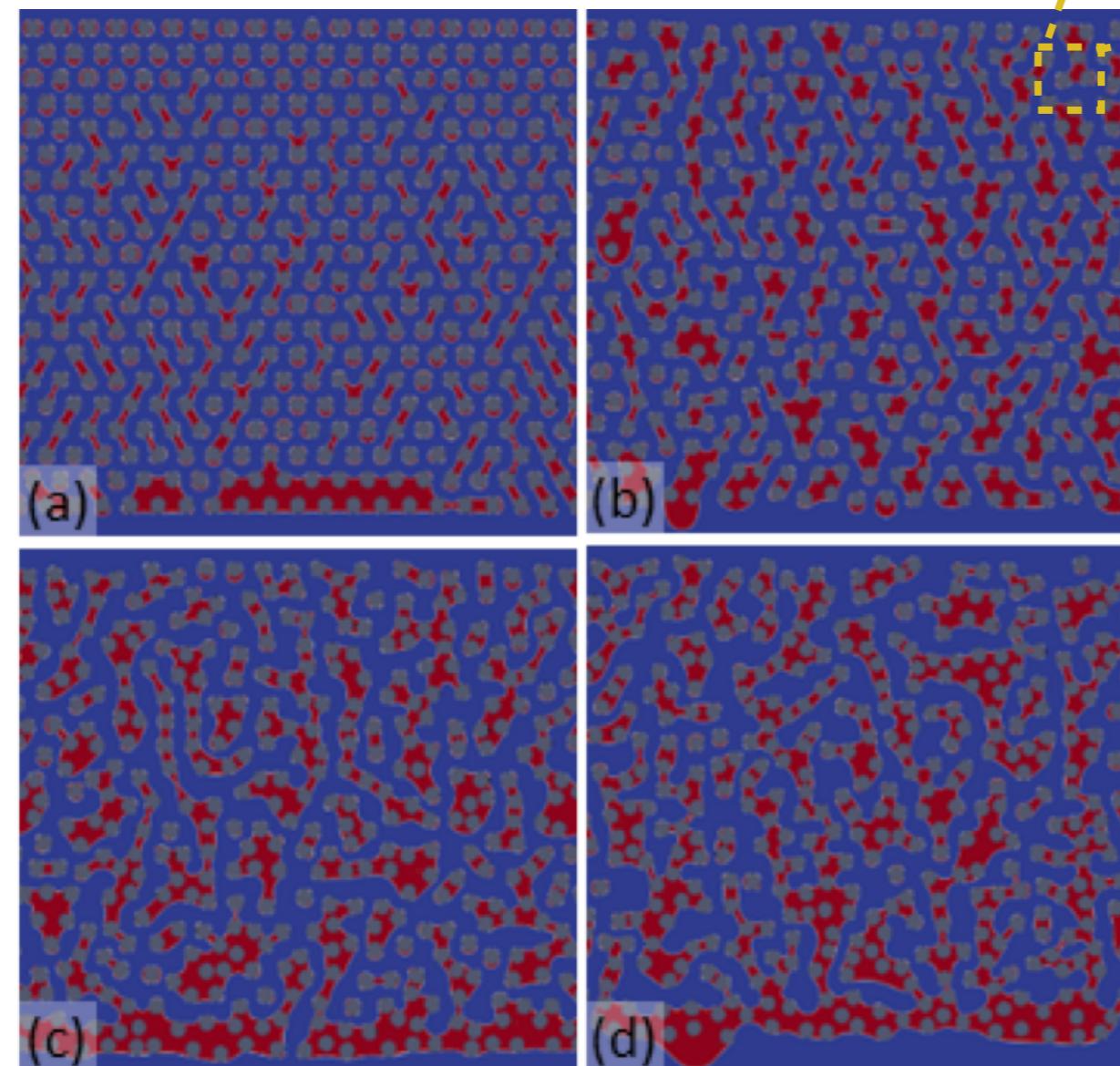


Disorder index (I_d) originally defined in Laubie et al. (2017) Phys. Rev. Lett., and the modified index (I_v) is formulated based on the Voronoi tessellation of the pore space. Main difference between these two definition is in the “**small perturbation**” region, where I_v is sensitive to the local changes.

Drainage simulations: Disorder index



VOF method
in OpenFoam

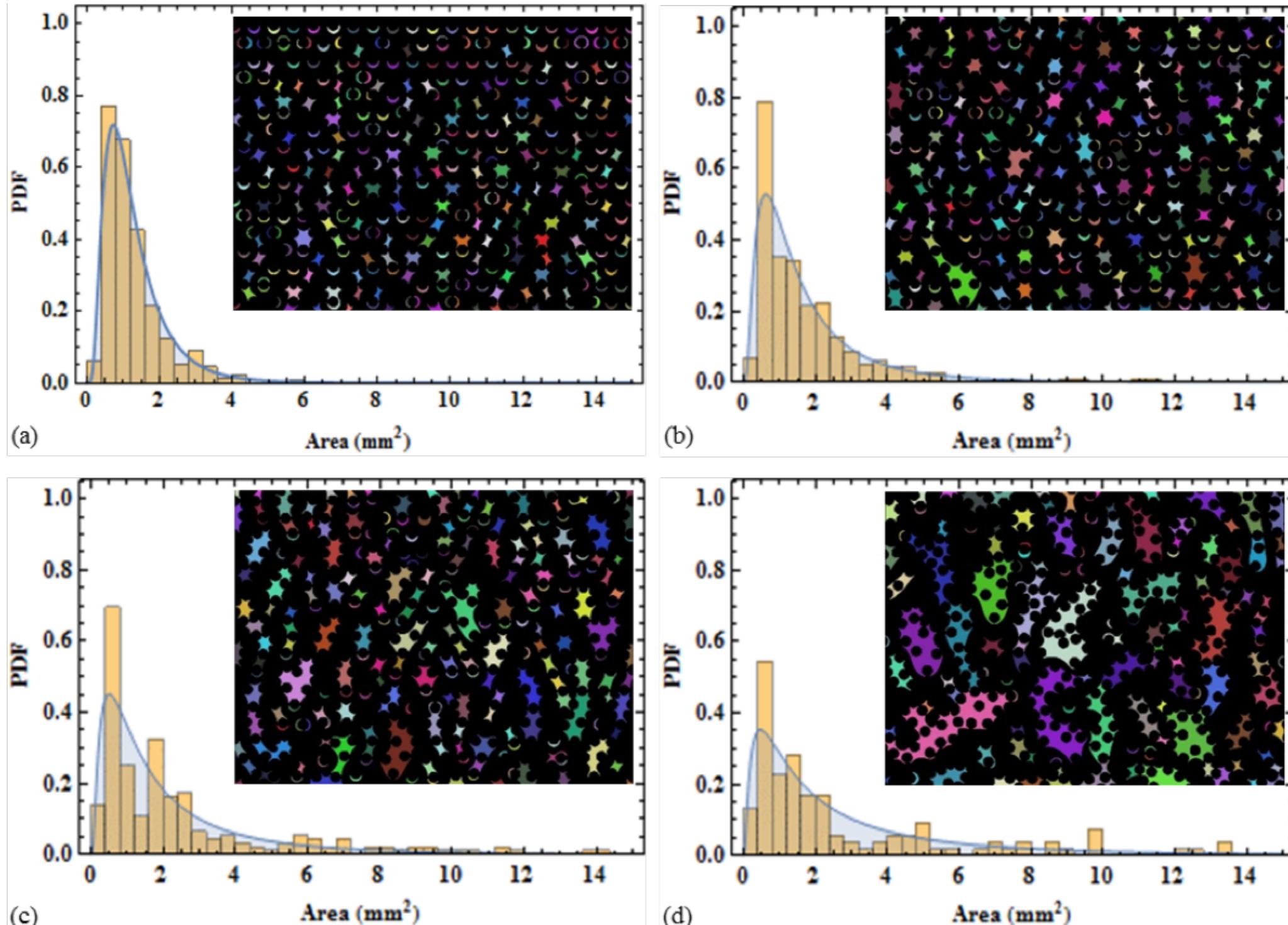


$$Bo = \frac{\Delta \rho g R^2}{\gamma} e \quad Ca = 0$$

* Cui, G., Liu, M., Dai, W., Gan, Y. (2019) Pore-scale Modelling of Gravity-driven Drainage in Disordered Porous Media. International Journal of Multiphase Flow. 114:19-27.

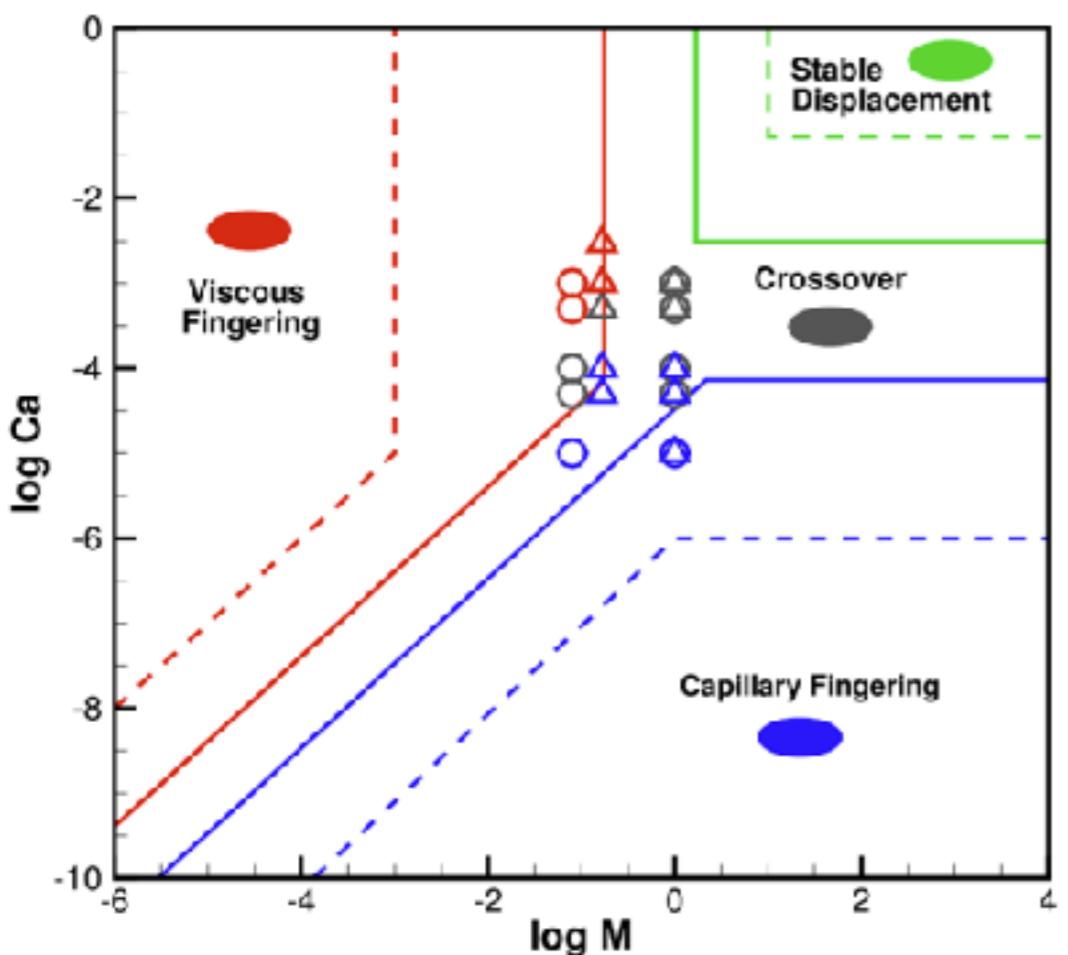
Drainage simulations: Saturated clusters

$$f(x, \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-\frac{(\ln x - \mu)^2}{2\sigma^2}}$$



Probability density function (PDF) and lognormal distribution of saturated zones area:
(a) $Iv=0$; (b) $Iv=0.0056$; (c) $Iv=0.015$; (d) $Iv=0.055$.

Liquid displacement simulations: Disorder

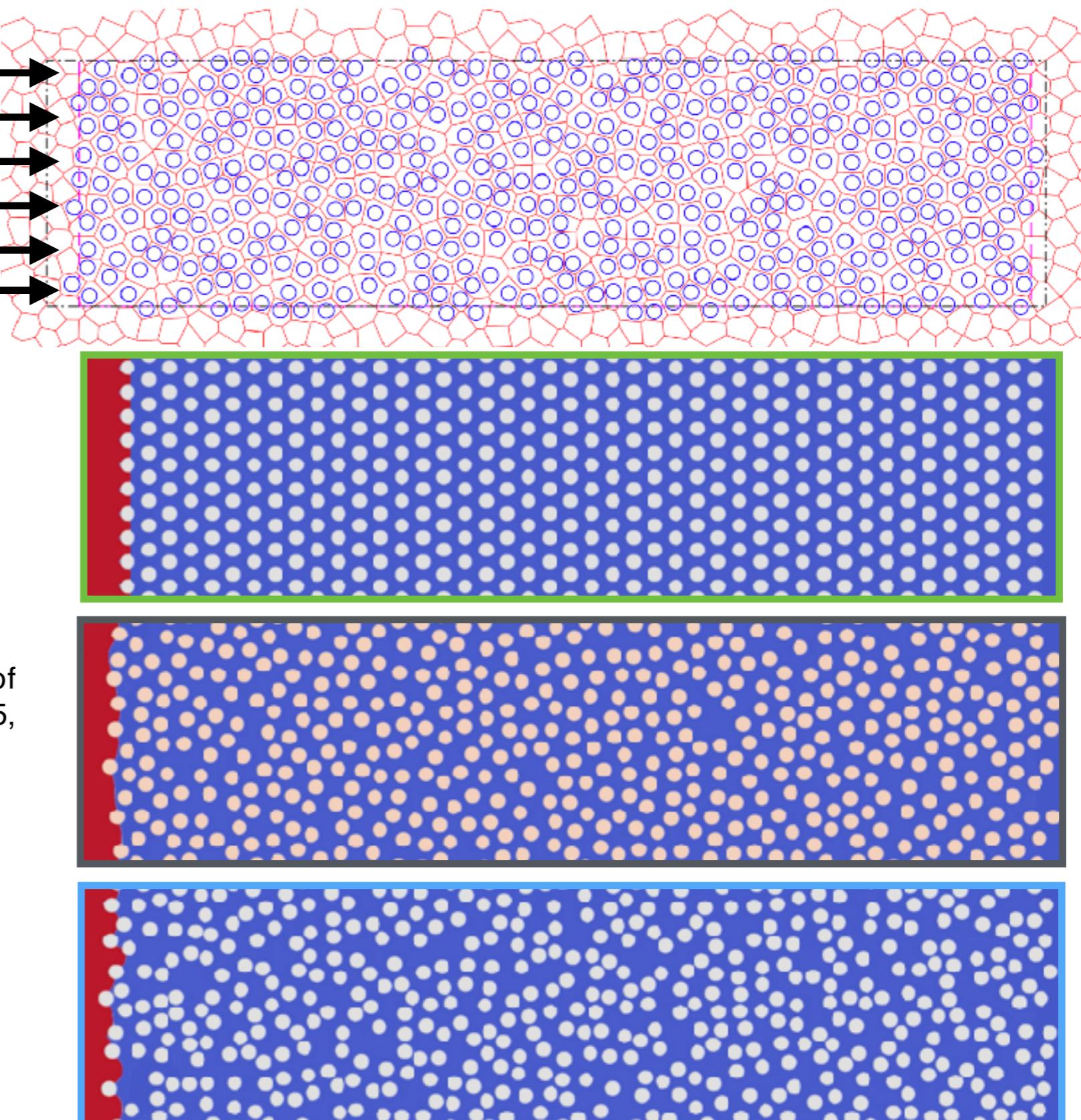


Displacement phase diagram as functions of viscosity ratio and Capillary number (Liu et al., 2015, Physics of Fluids).

$$Ca = \frac{V_{\text{inj}} \mu_{\text{def}}}{\gamma} = 0.0186$$

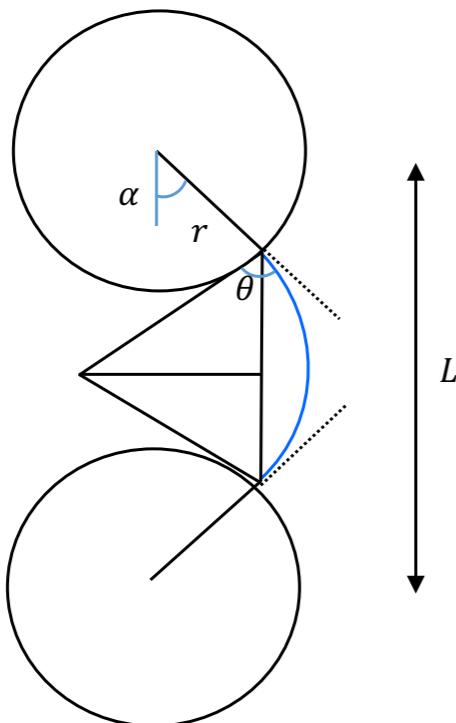
$$Bo = 0$$

$$M = 0.8$$

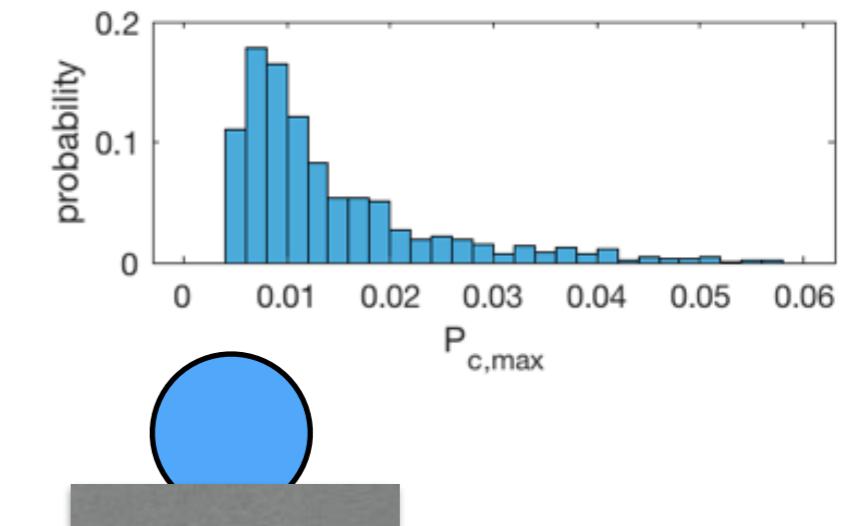
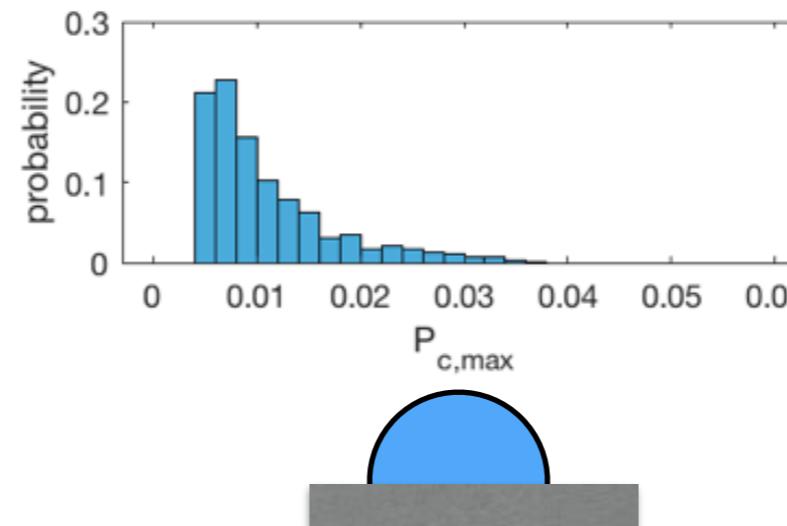
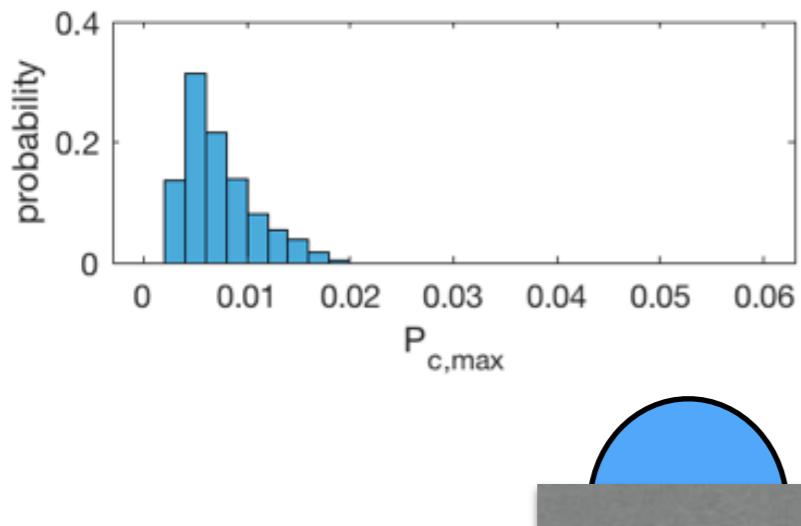
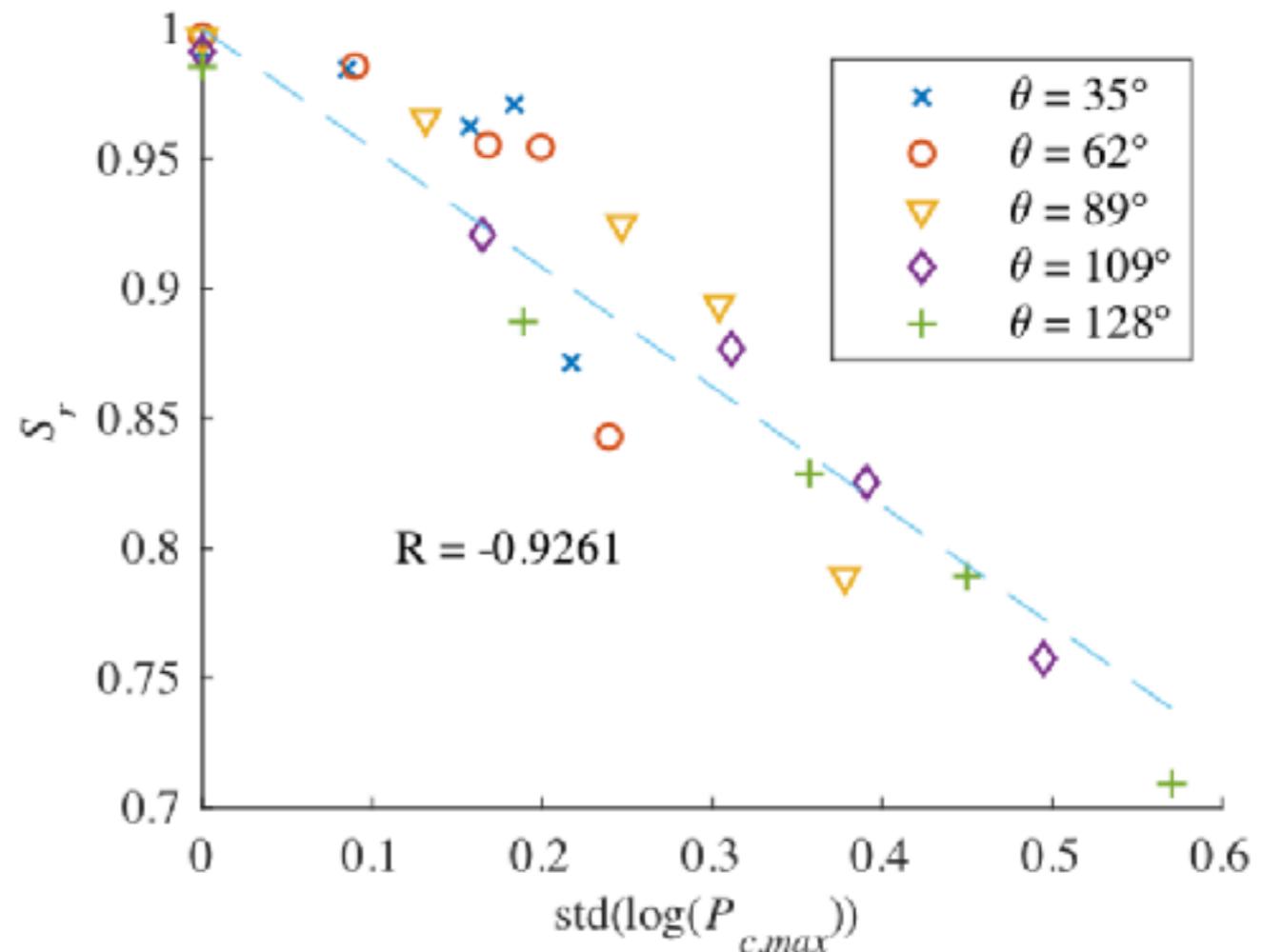


* Wang, Z., Chauhan, K., Pereira, J.M., Gan, Y. (2019) Disorder characterization of porous media and its effect on fluid displacement. Physical Review Fluids. 4, 034305.

Liquid displacement: Disorder and wettability



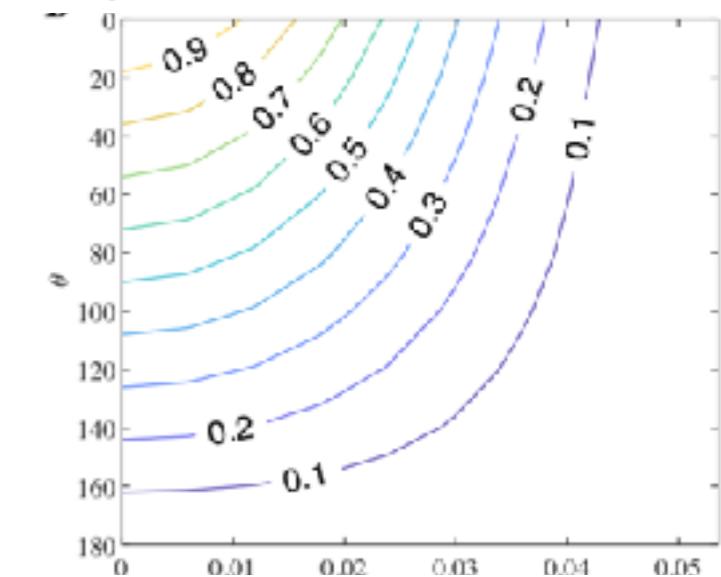
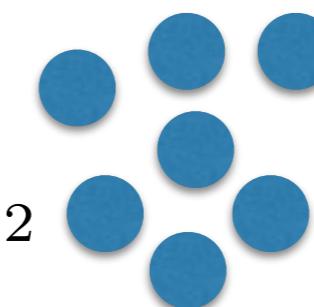
$$P_c = \frac{2\gamma \sin(\alpha + \theta - 90)}{L - 2r \cos(\alpha)}$$



Liquid displacement: Disorder and wettability



$$I_V = [\langle \phi_i^2 \rangle - \phi^2]^{1/2}$$



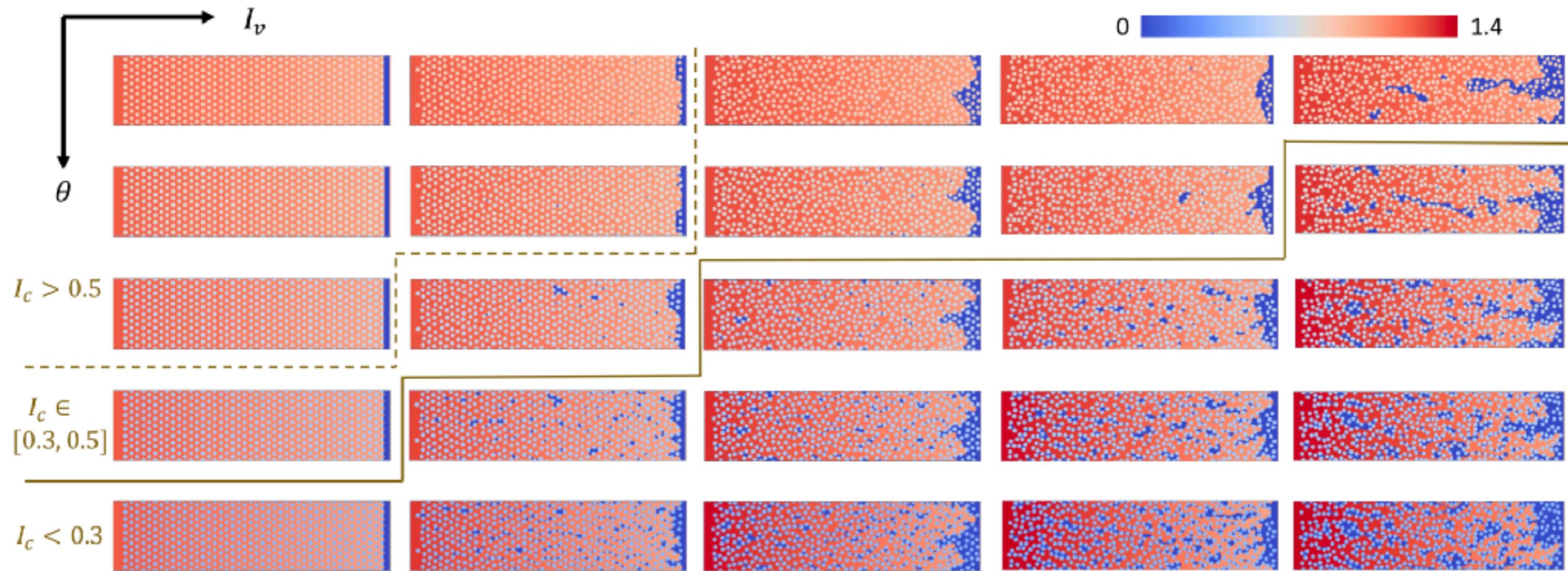
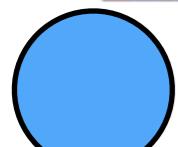
I_V

θ

$I_c > 0.5$

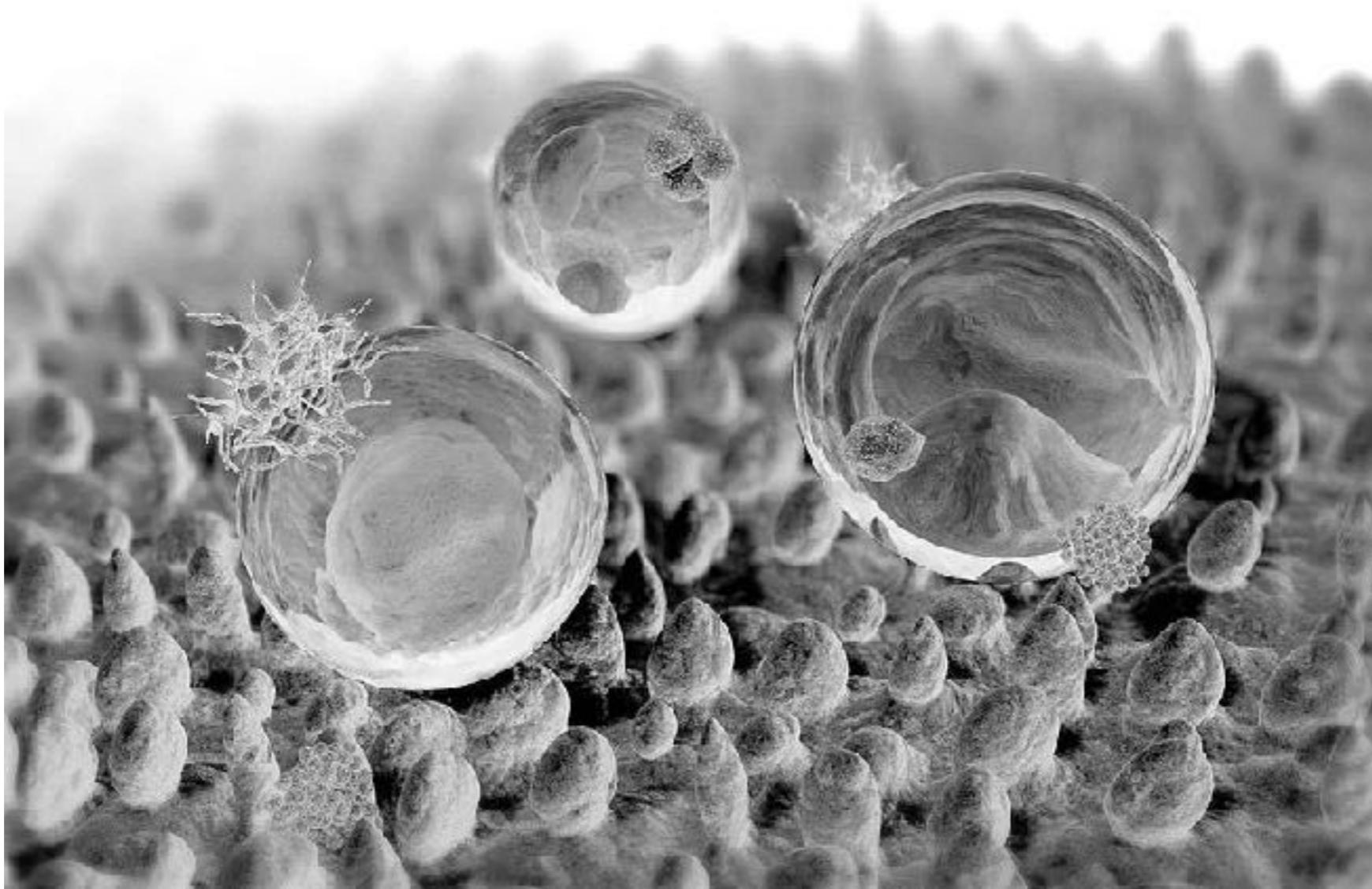
$I_c \in [0.3, 0.5]$

$I_c < 0.3$



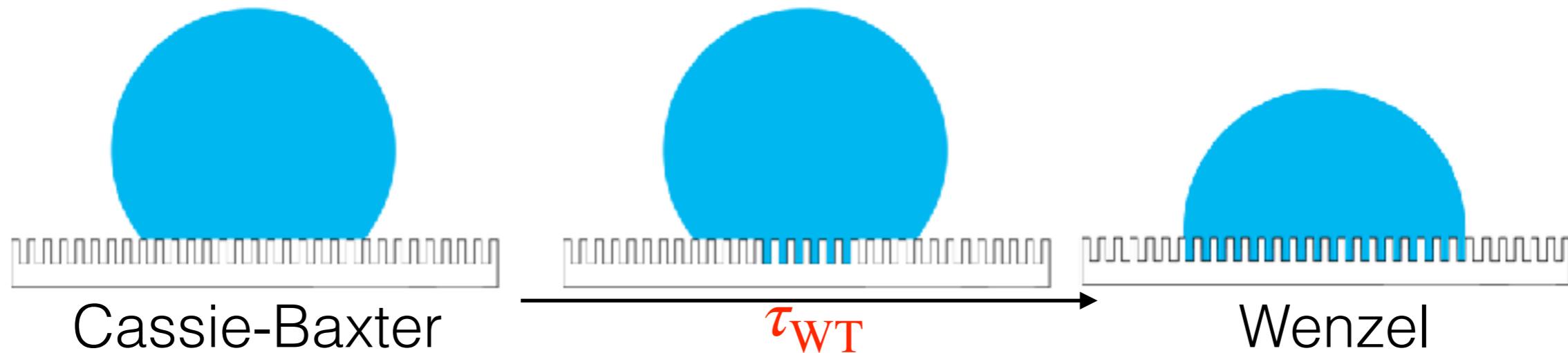
* Wang, Z., Chauhan, K., Pereira, J.M., Gan, Y. (2019) Disorder characterization of porous media and its effect on fluid displacement. Physical Review Fluids. 4, 034305.

(3/4) Wetting Transition



Effects of Wetting Transition

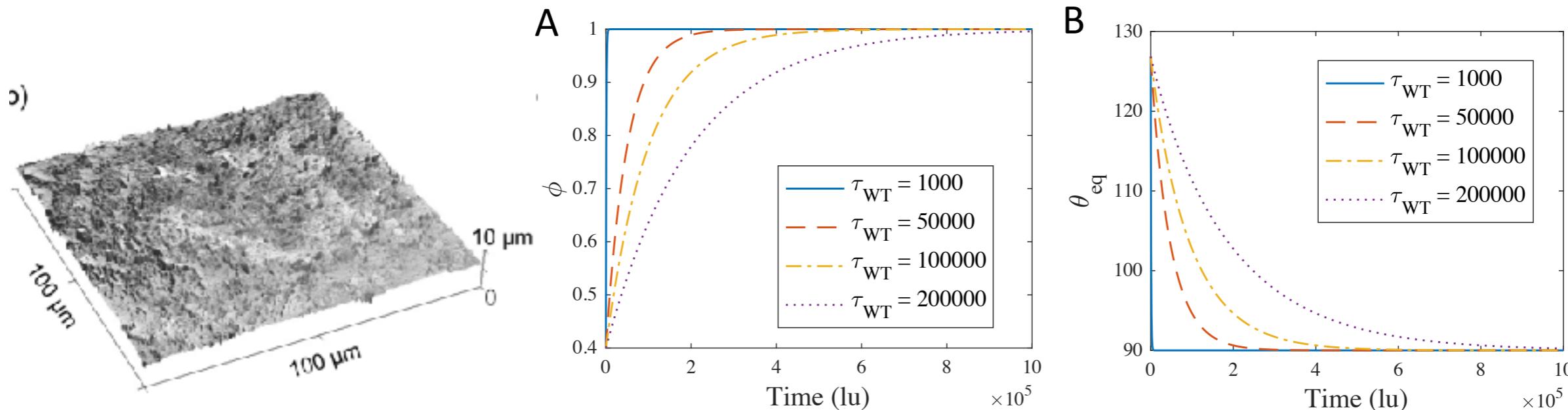
(1) Surface-scale: Cassie-Wenzel wetting transition time τ_{WT}



$$\cos \theta_{eq} = r_w \phi \cos \theta_0 + \phi - 1$$

↑ ↑ ↑
surface roughness intrinsic contact projected contact
ratio ($>= 1$) angle area

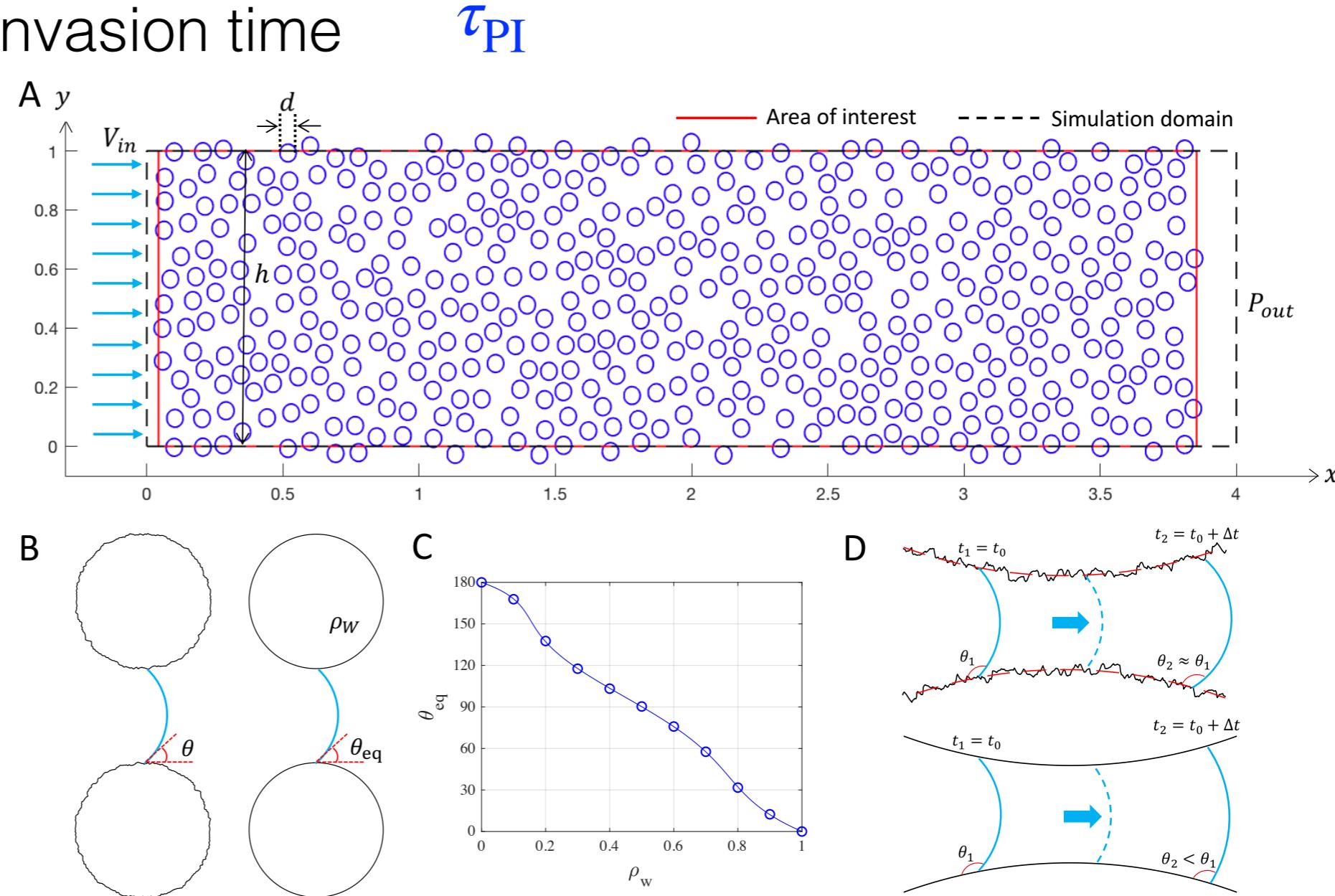
$$\phi = 1 + (\phi_0 - 1) e^{-\frac{t}{\tau_{WT}}}$$



Effects of Wetting Transition

(2) Pore-scale: Pore invasion time

$$\tau_{PI} = \frac{d}{V_{in}/\Phi}$$

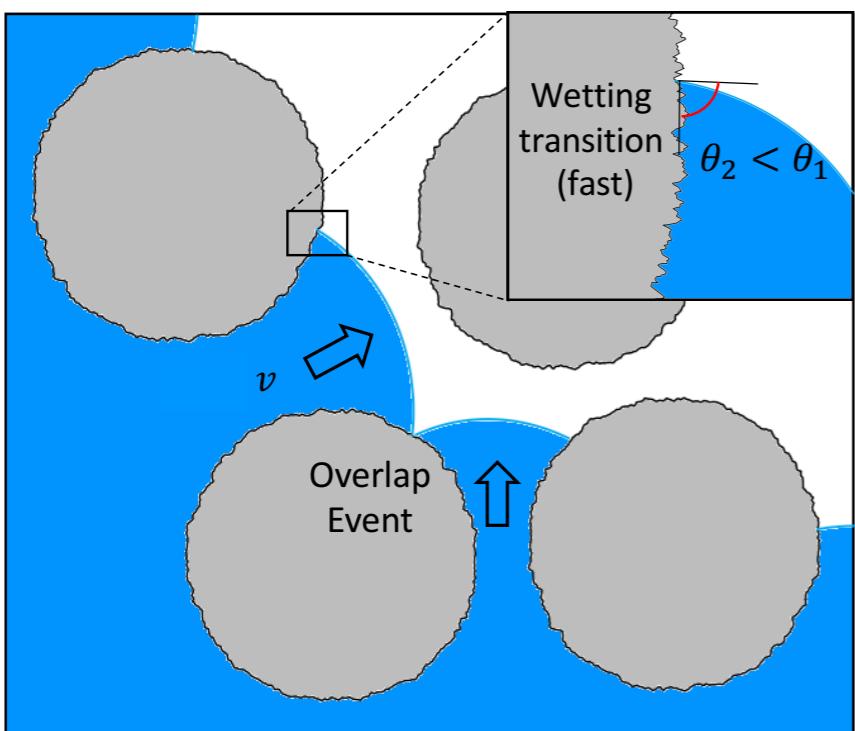
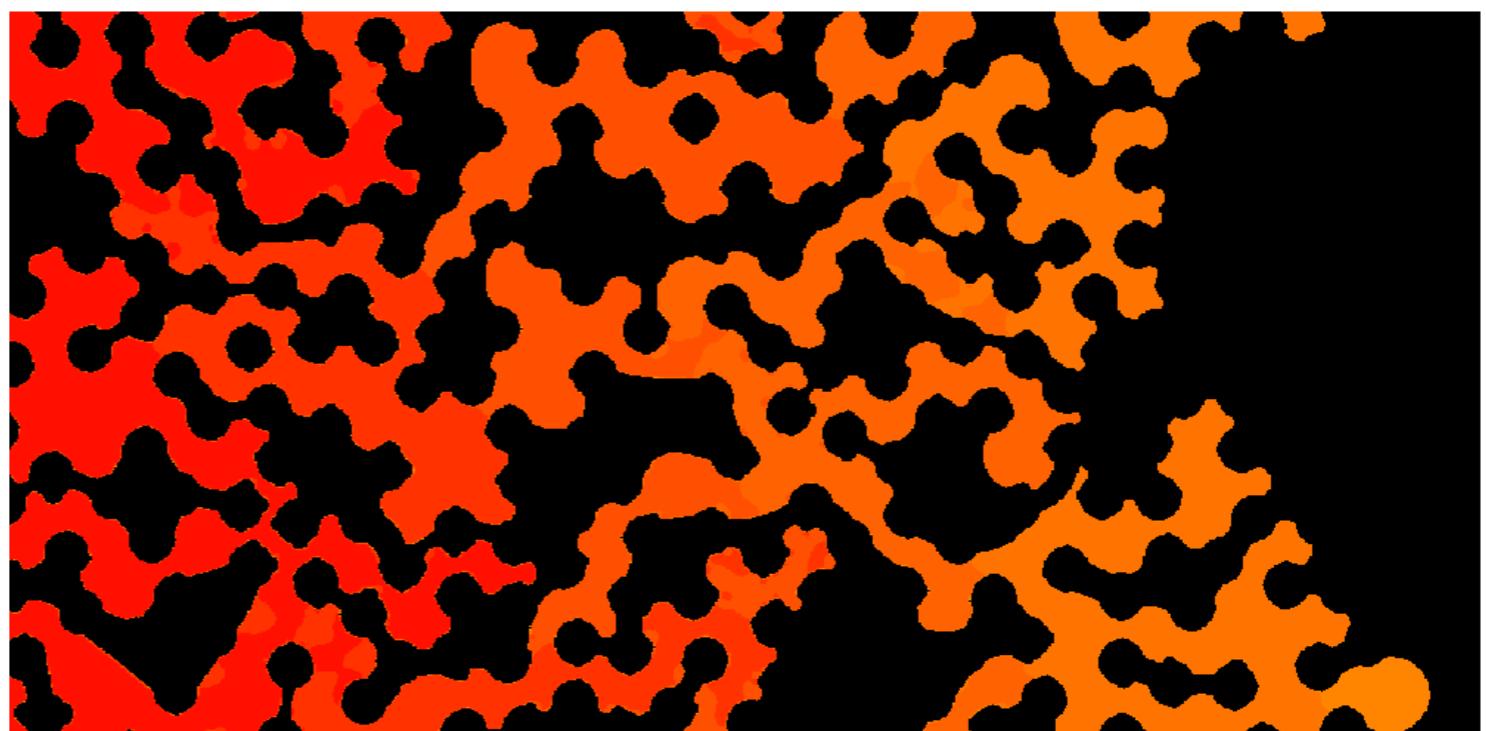
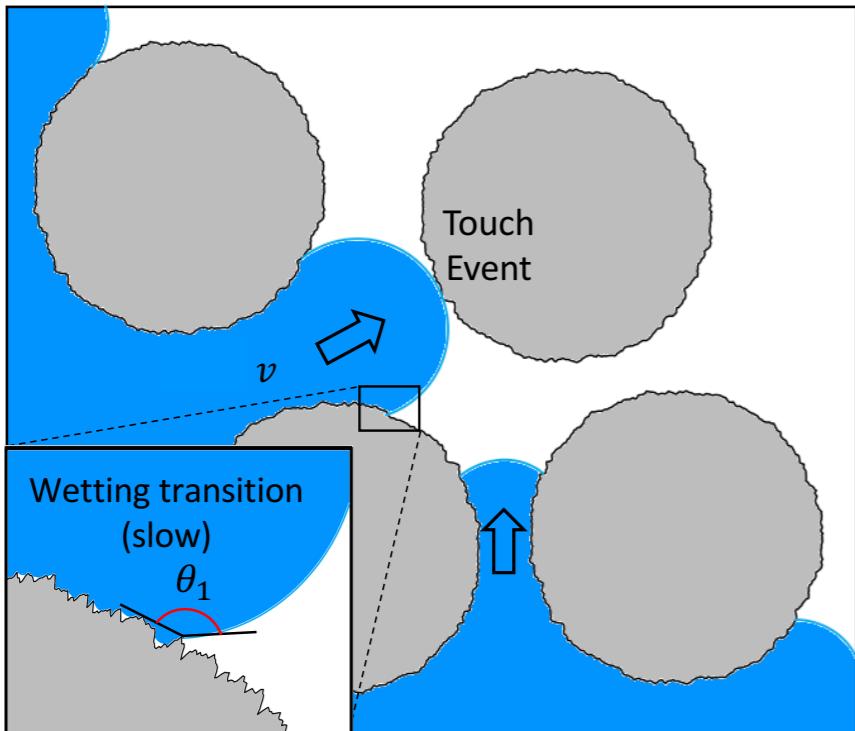


Ration of time scales of wetting transition and pore invasion:

$$D_y = \frac{\tau_{WT}}{\tau_{PI}}$$

invasion: slower —> faster
transition: faster —> slower

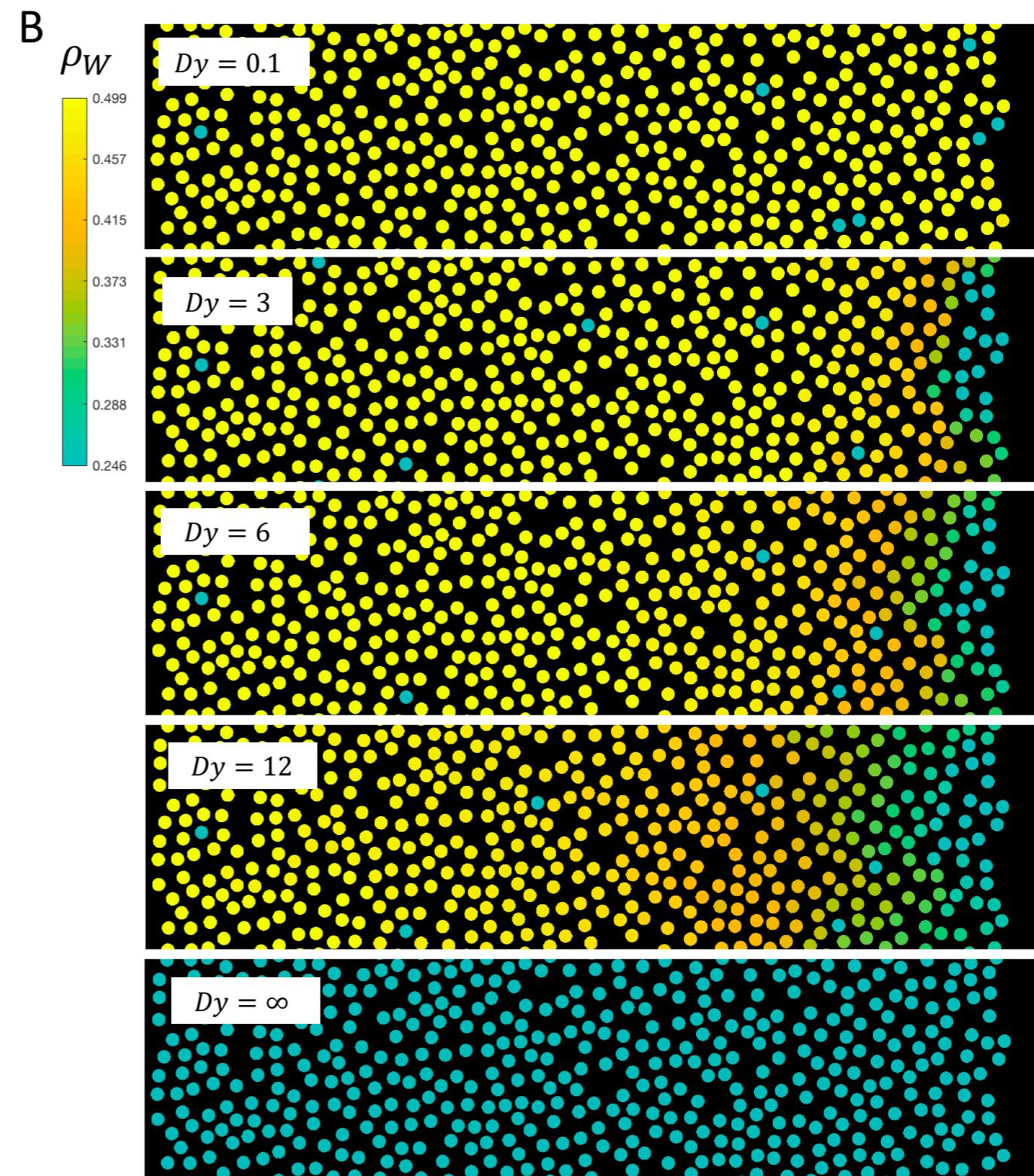
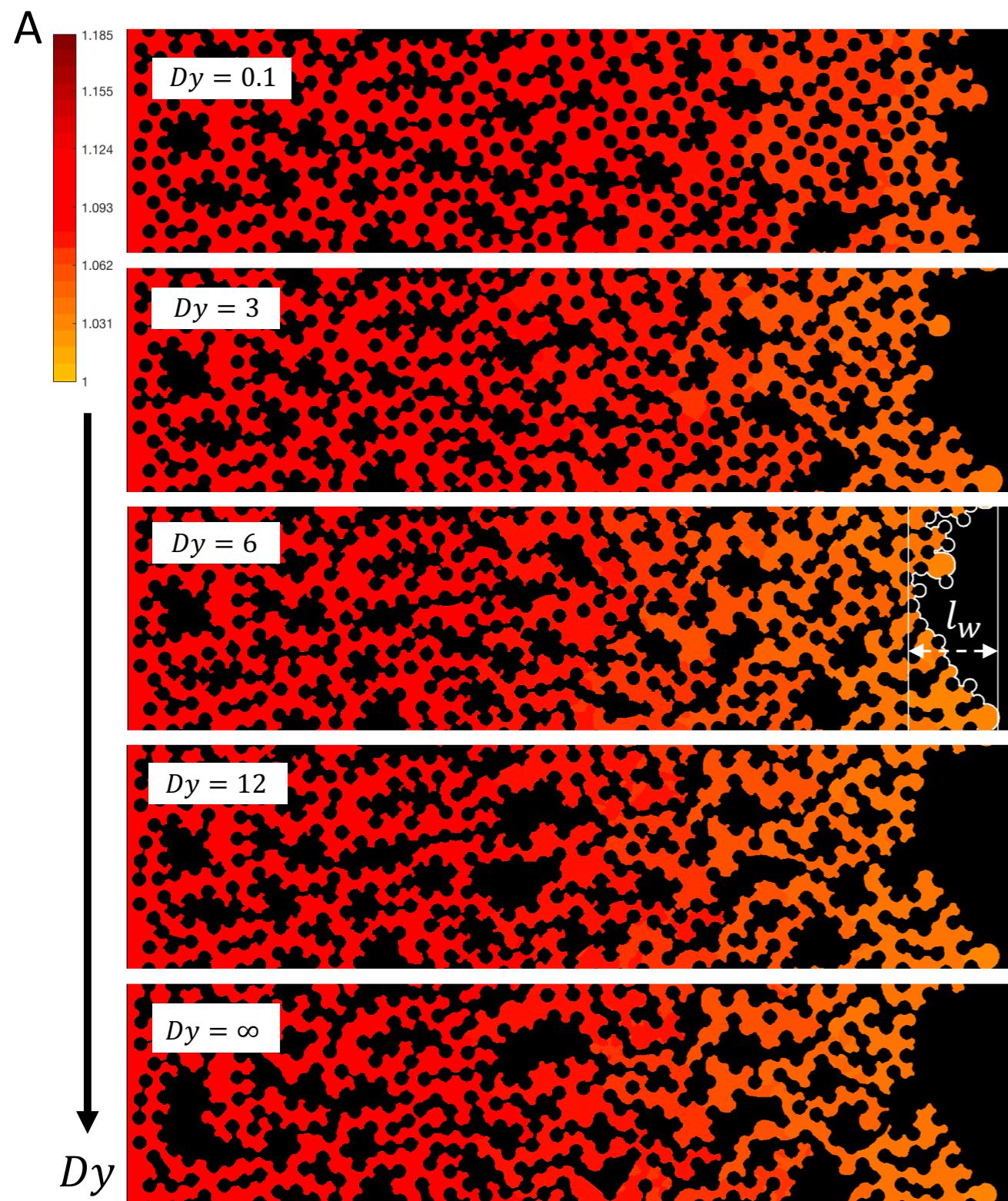
Effects of Wetting Transition: Displacement modes



$$D_y = \frac{\tau_{WT}}{\tau_{PI}}$$

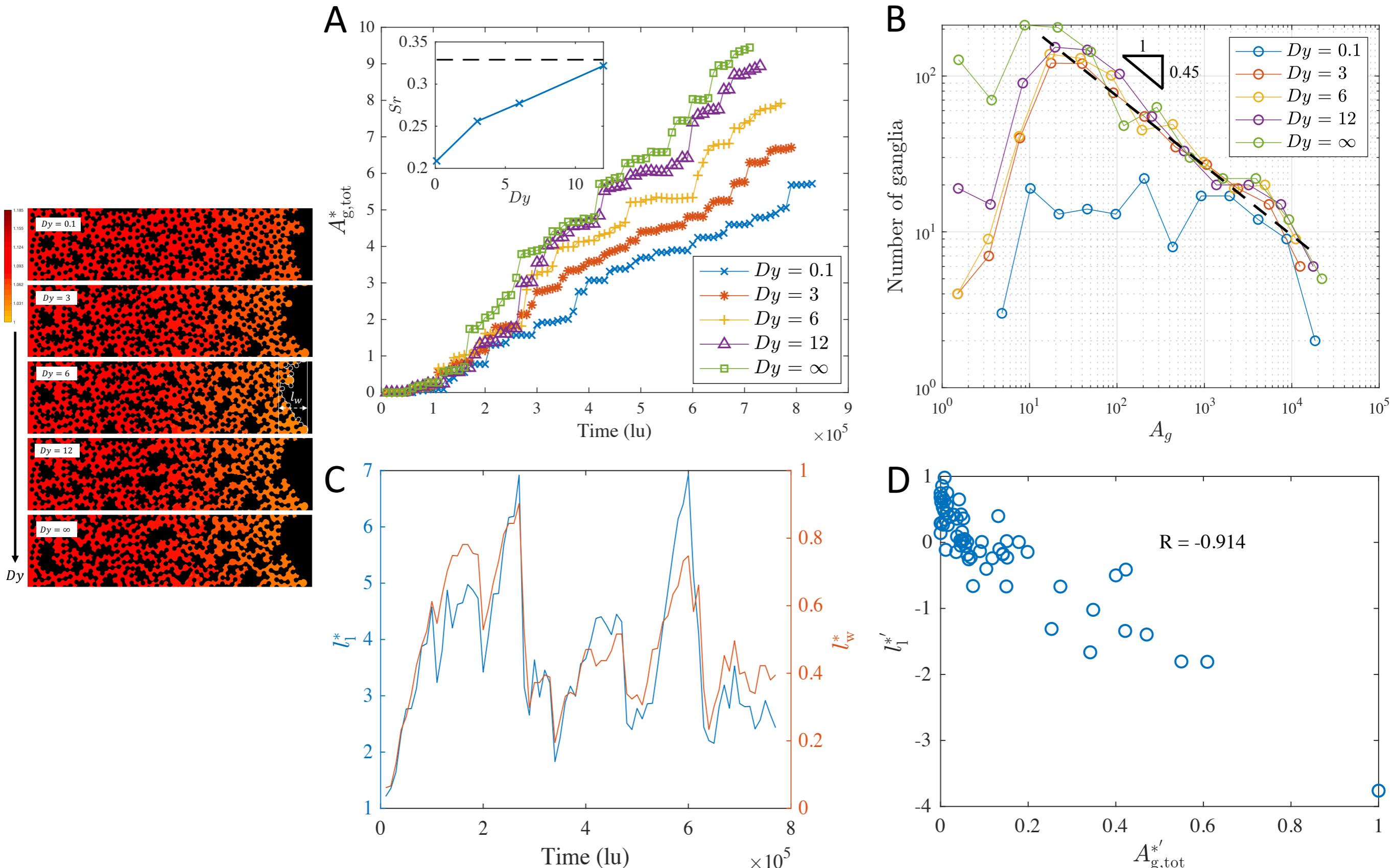
invasion: slower —→ faster
transition: faster —→ slower

Effects of Wetting Transition: Displacement patterns



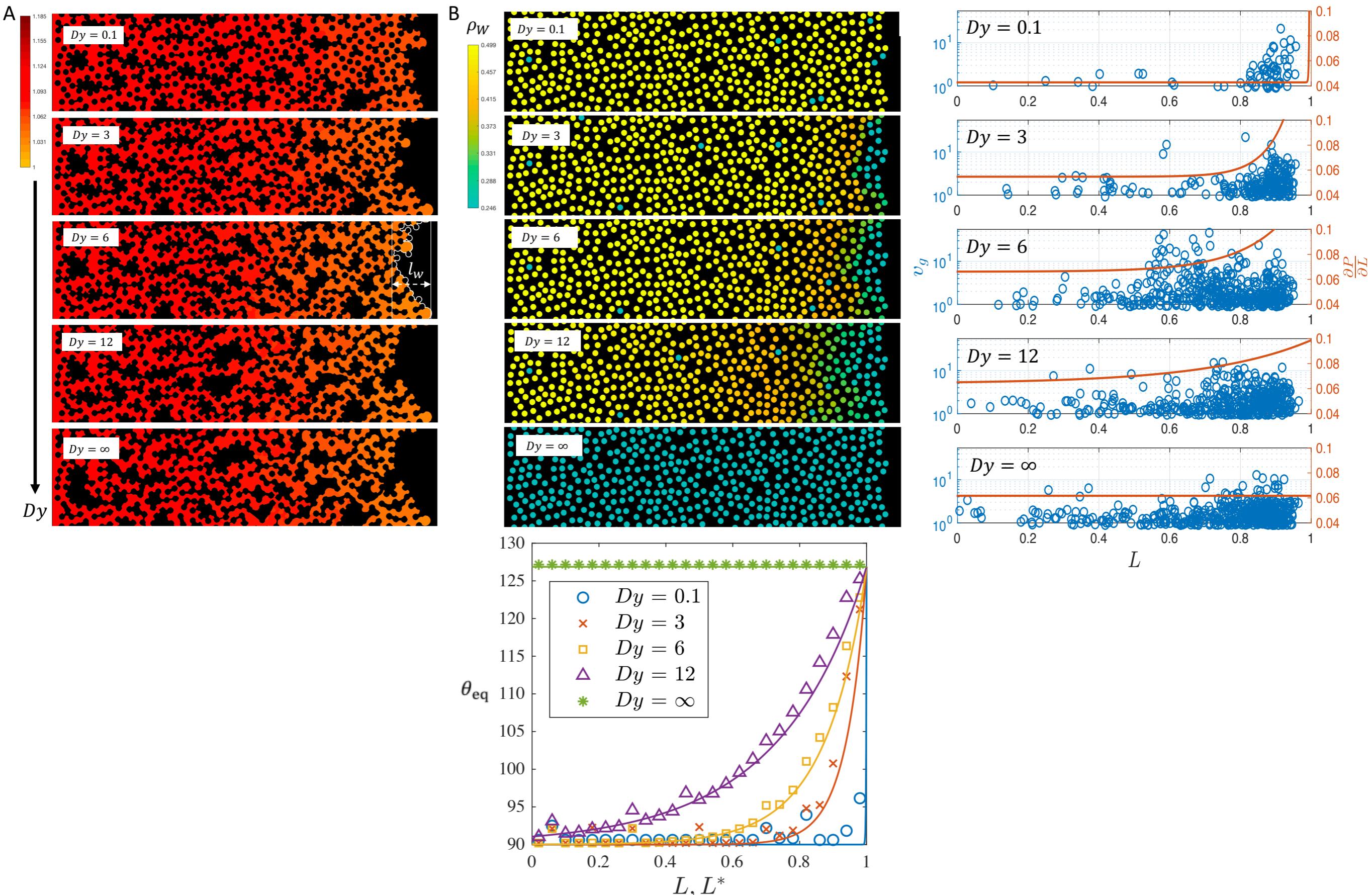
* Wang Z., Pereira, JM., Gan, Y. (2020) Effect of wetting transition during multiphase displacement in porous media. Langmuir, in press.

Effects of Wetting Transition: Ganglia mobilisation



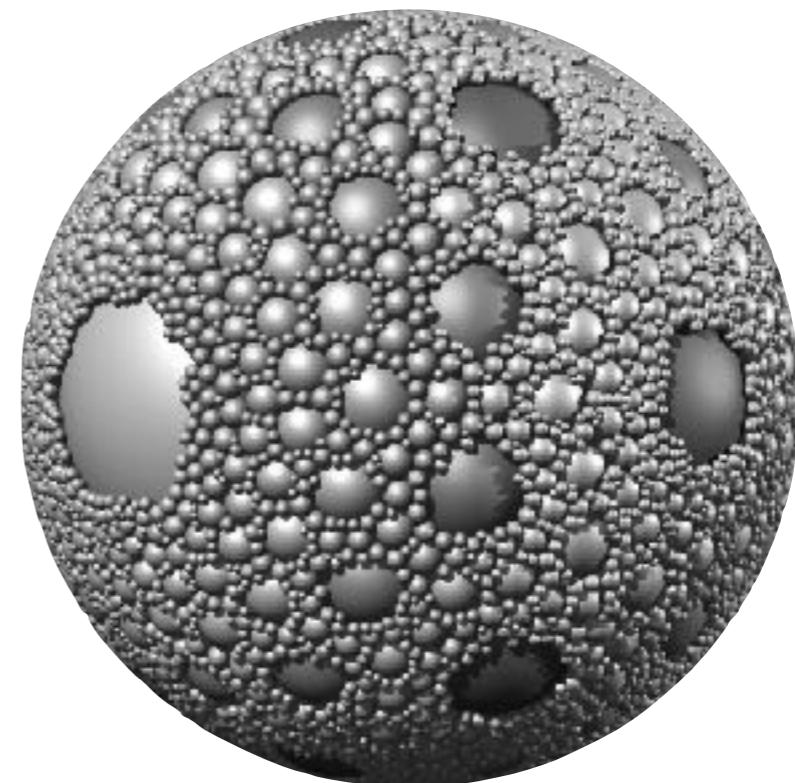
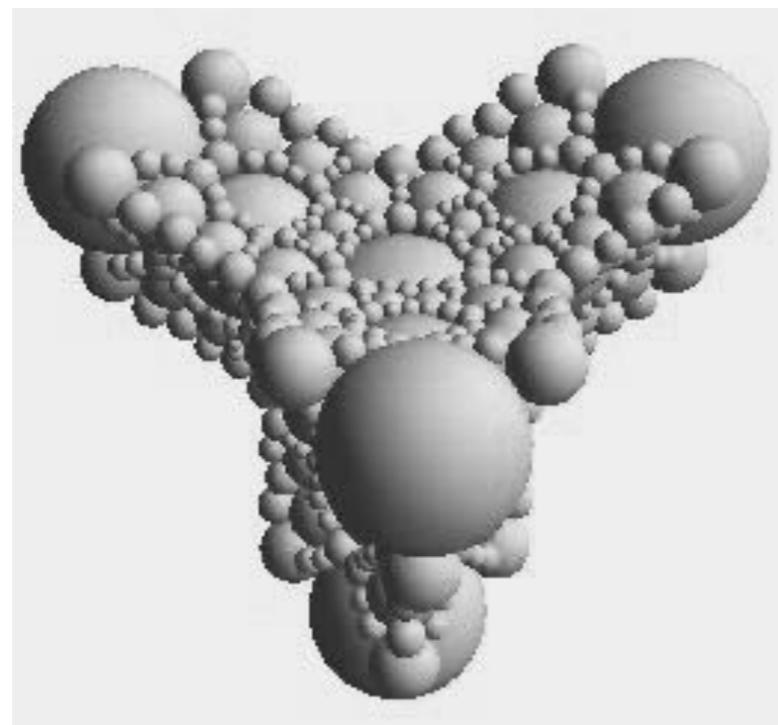
* Wang Z., Pereira, JM., Gan, Y. (2020) Effect of wetting transition during multiphase displacement in porous media. Langmuir, in press.

Effects of Wetting Transition: Ganglia mobilisation

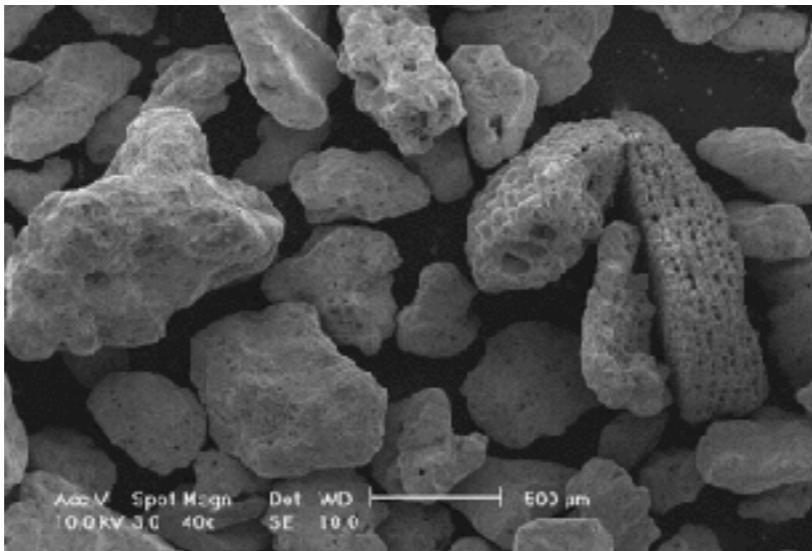


* Wang Z., Pereira, JM., Gan, Y. (2020) Effect of wetting transition during multiphase displacement in porous media. Langmuir, in press.

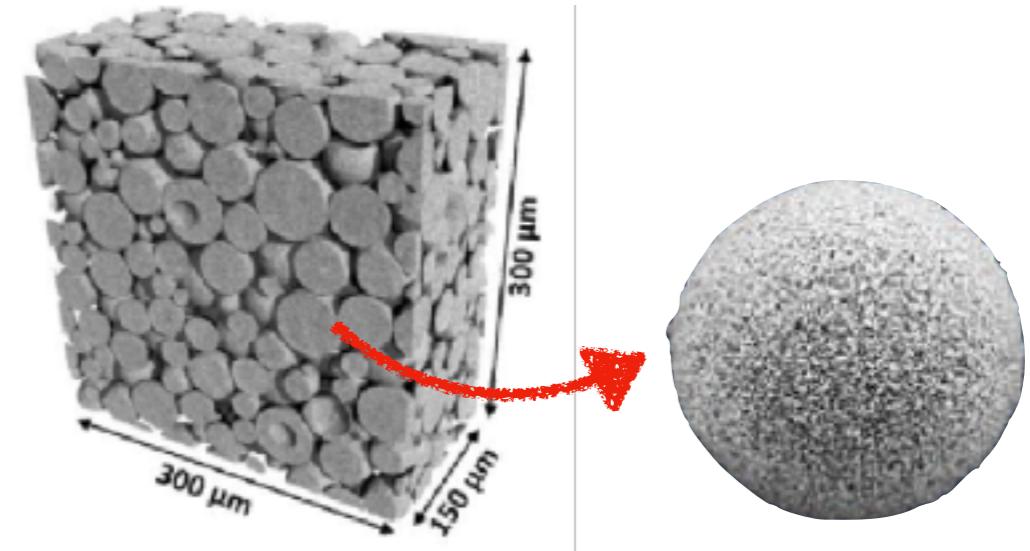
(4/4) Hierarchical Porous Structure



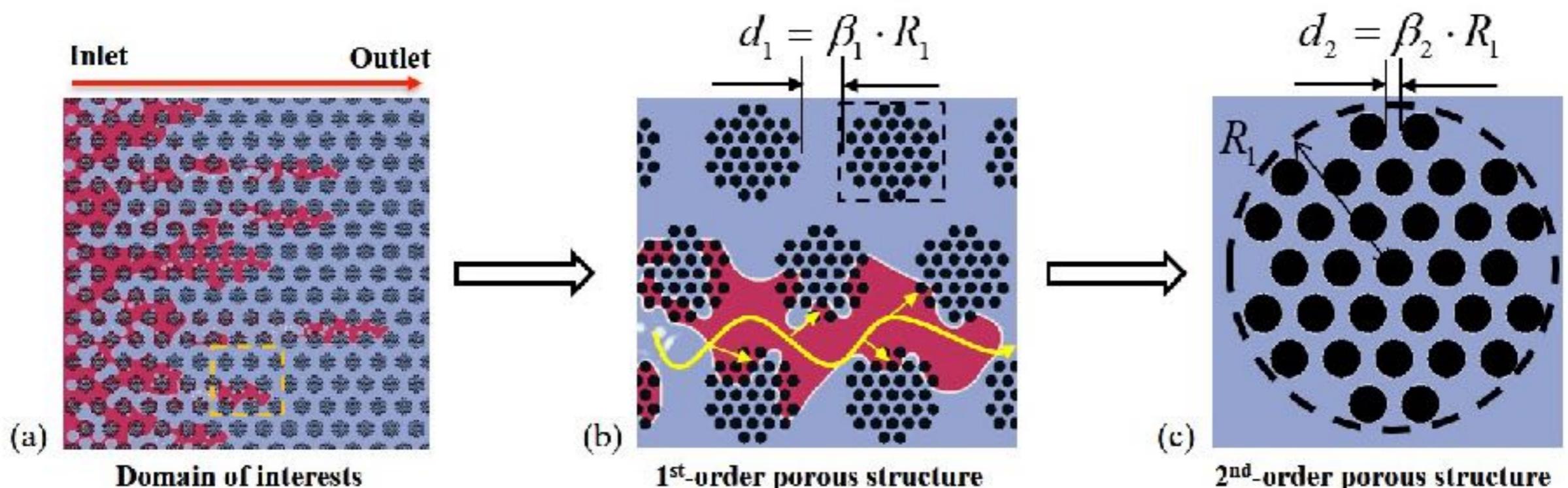
Modelling hierarchical porous media



calcareous sand



cathode active material in Li-ion batteries



$$M = \frac{1}{1000}$$

porosity

ϕ_1

obstacle size

R_1

throat size

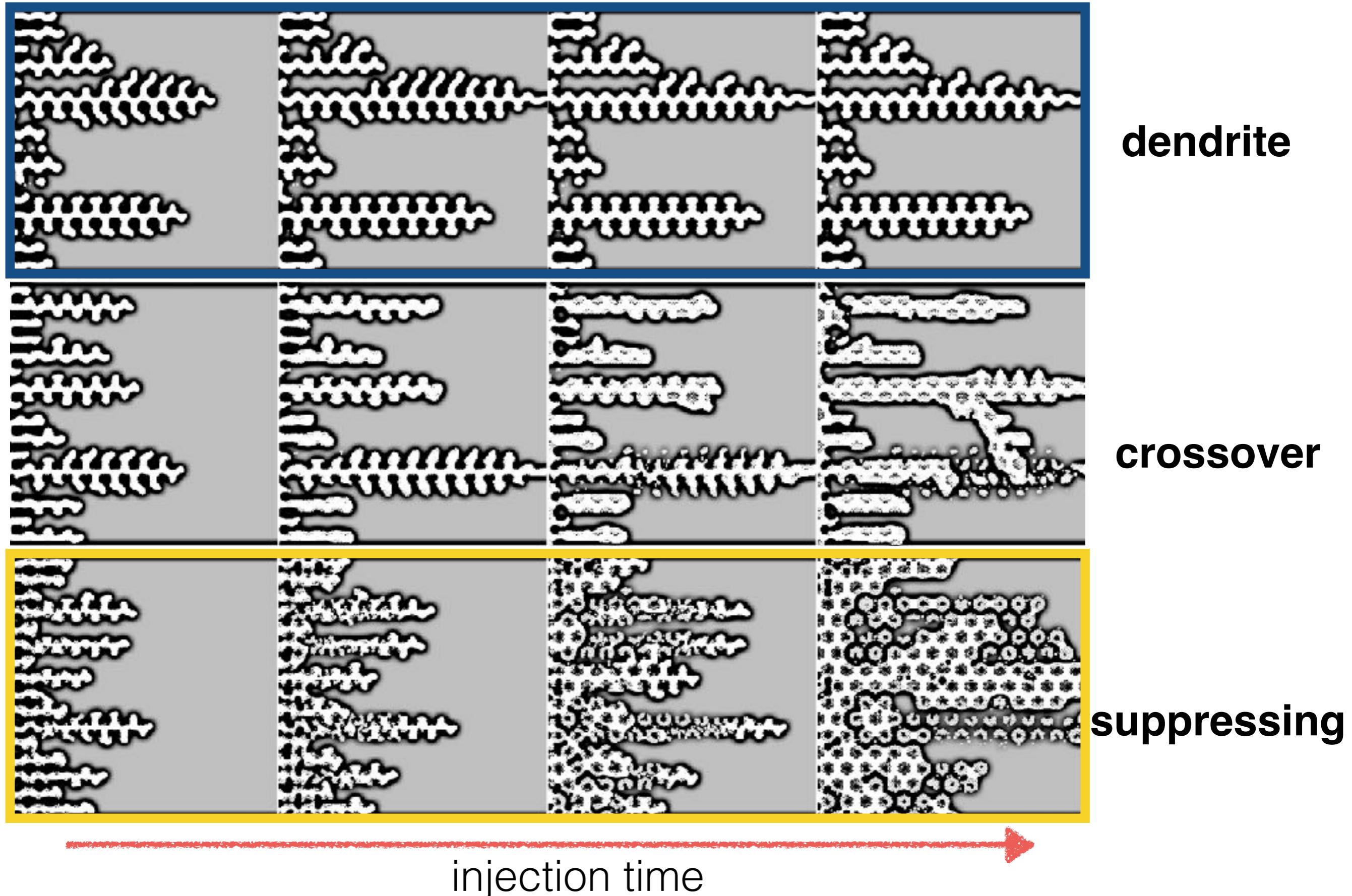
d_1

ϕ_2

R_2

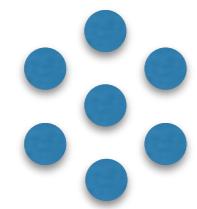
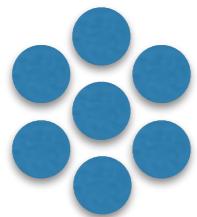
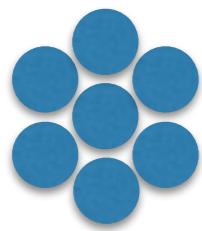
d_2

Hierarchical porous media: Fingering patterns

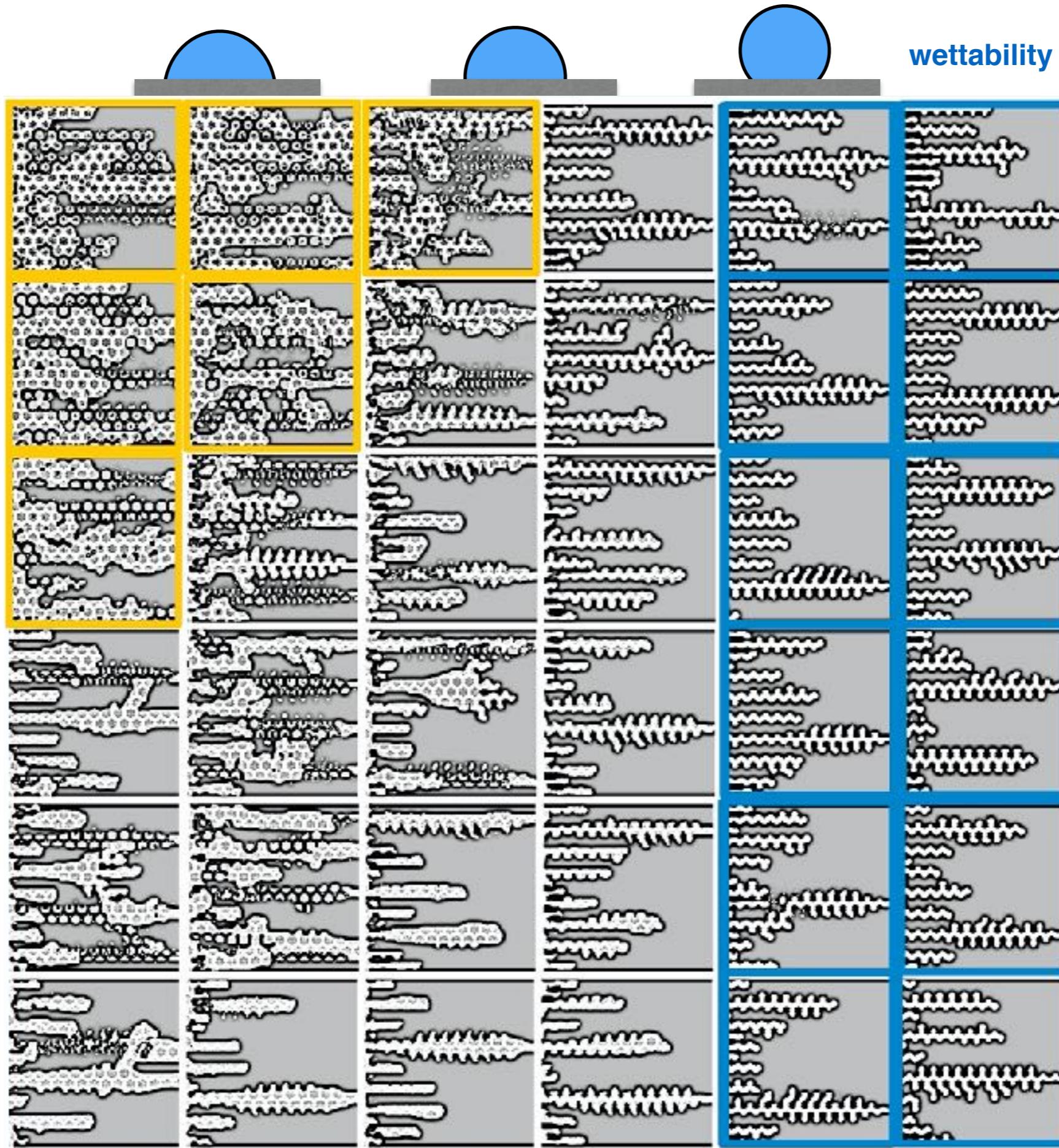


* Suo, S., Liu, M., Gan, Y. (2020) Fingering patterns in hierarchical porous media. Physical Review Fluids, in press.

Hierarchical porous media: Phase diagram (1/2)

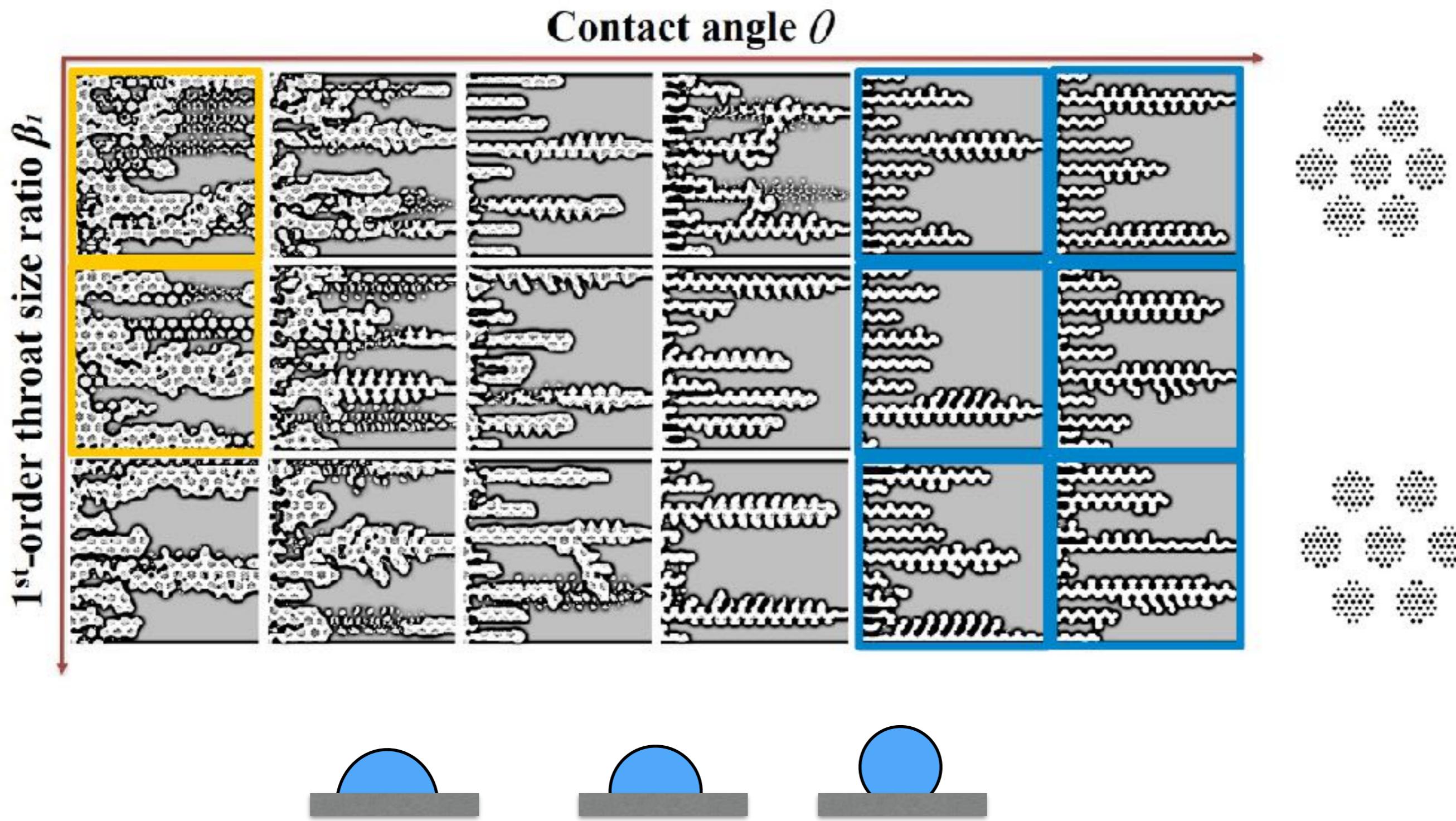


2nd order
throat size



wettability

Hierarchical porous media: Phase diagram (2/2)



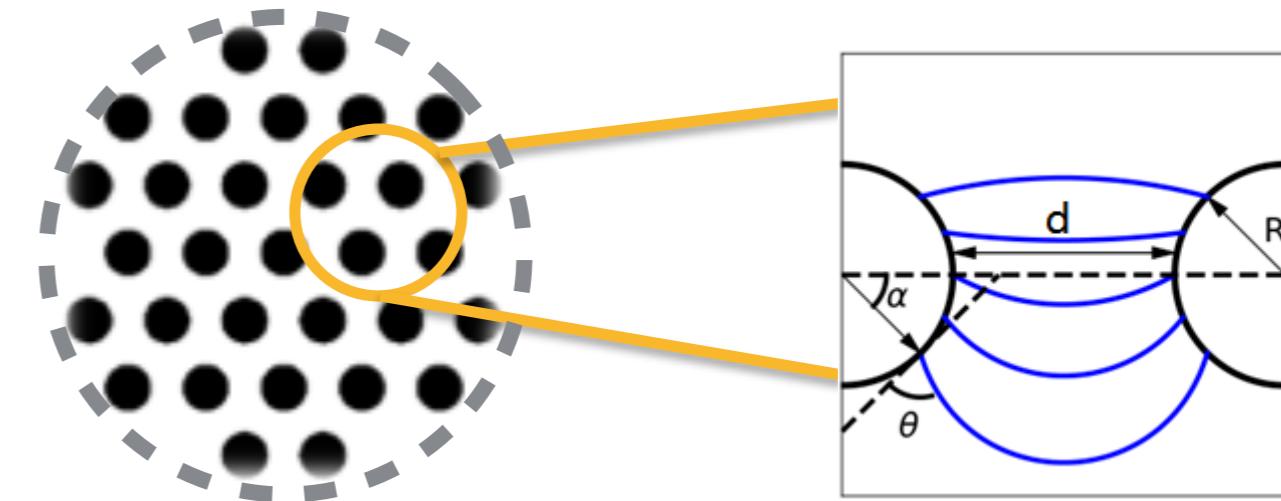
* Suo, S., Liu, M., Gan, Y. (2020) Fingering patterns in hierarchical porous media. Physical Review Fluids, in press.

Dimensionless analysis

- Driving pressure

$$P_{\text{ext}} = \frac{v_{\text{in}} \cdot \eta_{\text{in}}}{k_1} \cdot d_1$$

$$P_c = \frac{\gamma}{d} \cdot \frac{\cos(\theta - \alpha)}{1 + 2 \cdot R/d \cdot (1 - \cos(\alpha))}$$

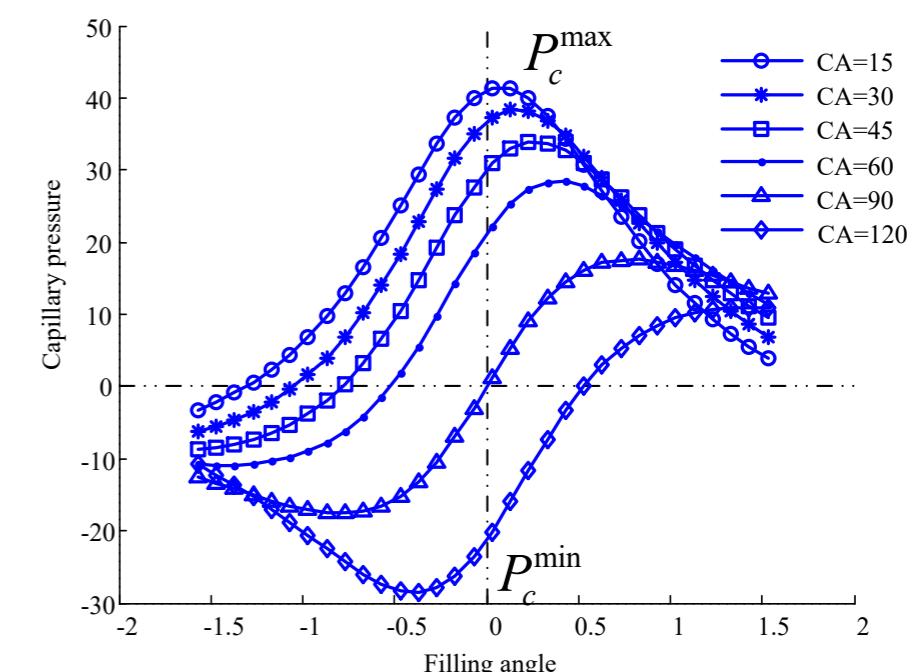


ϕ_1	ϕ_2
R_1	R_2
d_1	d_2

- Interaction duration

$$T_1 = \frac{\phi_1 \cdot d_1}{v_{\text{in}}}$$

$$T_2 = \frac{\eta_{\text{in}} \cdot \phi_2 \cdot d_2^2}{2 \cdot k_2 \cdot P_c^*}$$

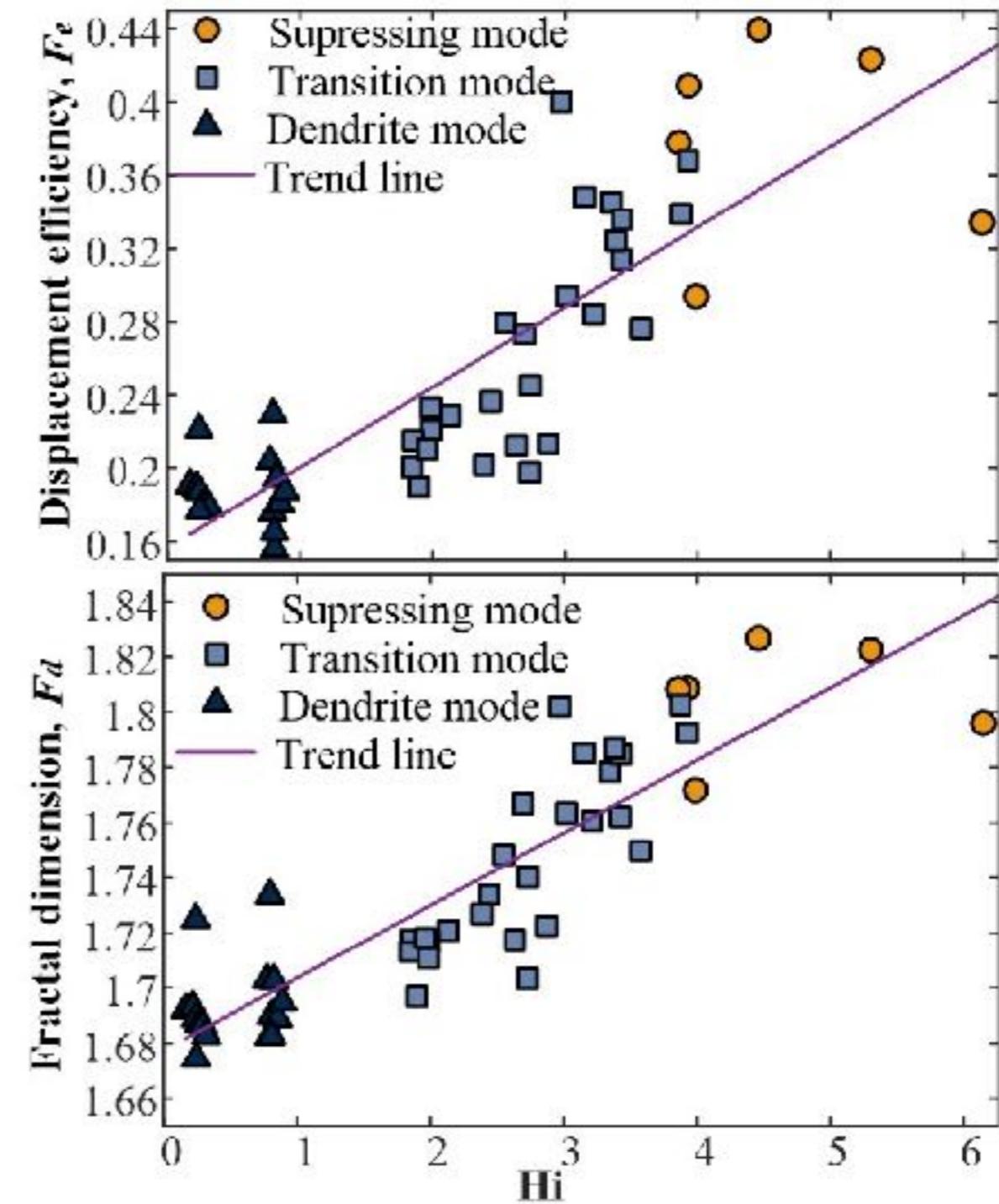
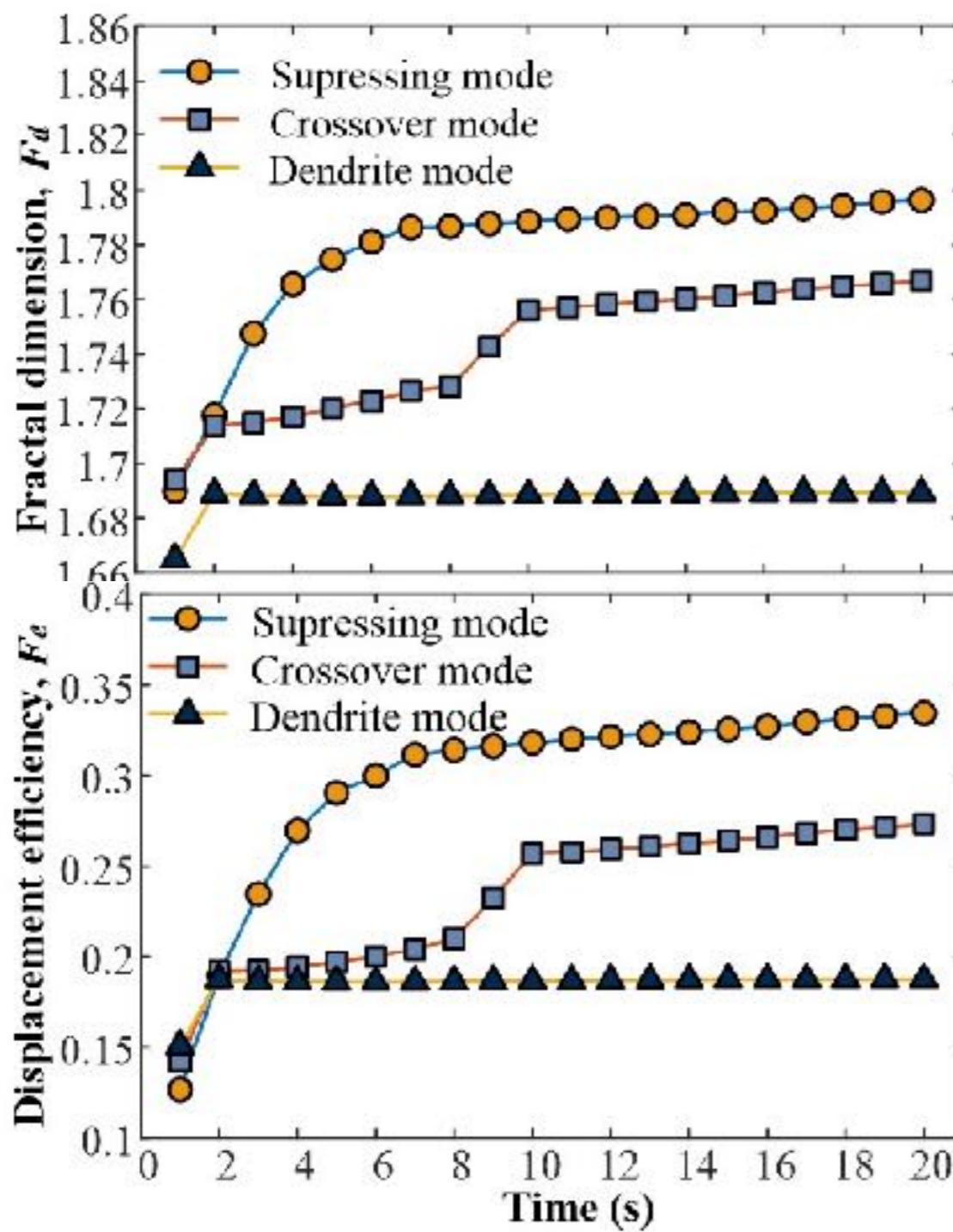


- Non-dimensional number, Hi

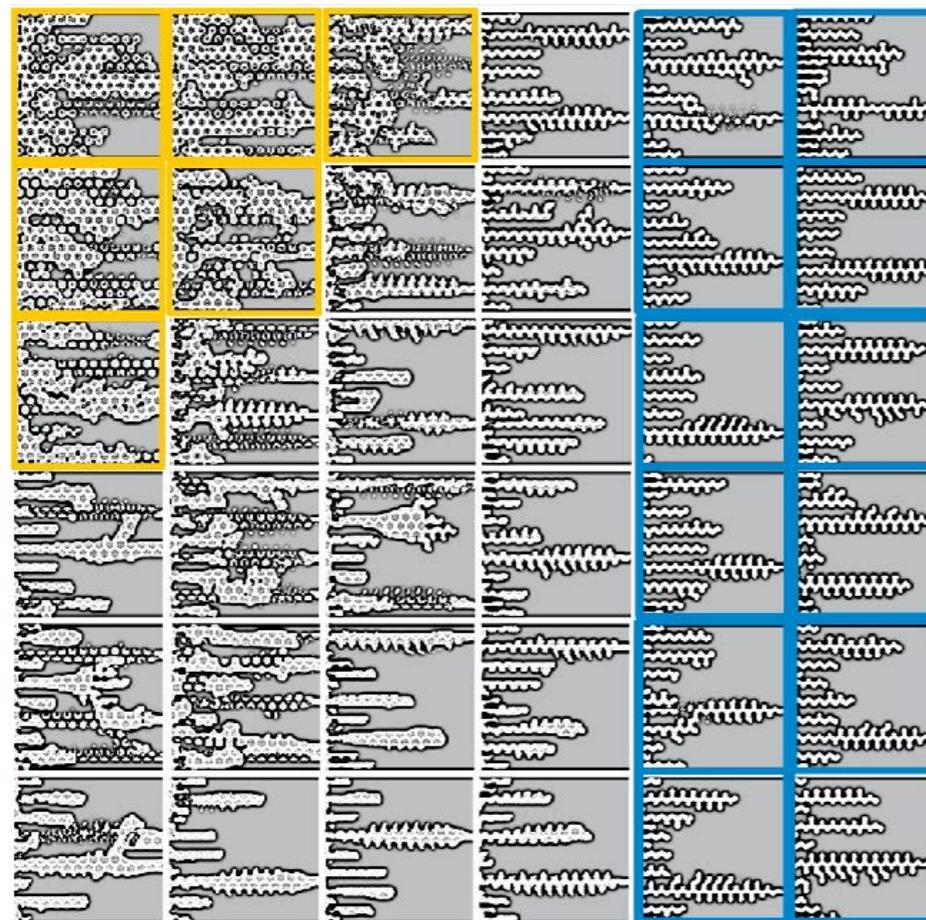
$$\text{Hi} = R_p \cdot R_T = \frac{P_{\text{ext}}}{P_{c,\min}} \cdot \frac{T_1}{T_2} = 2 \cdot \frac{P_c^*}{P_{c,\min}} \cdot \frac{\phi_1}{\phi_2} \cdot \frac{k_2}{k_1} \cdot \left(\frac{d_1}{d_2} \right)^2$$

* Suo, S., Liu, M., Gan, Y. (2020) Fingering patterns in hierarchical porous media. Physical Review Fluids, in press.

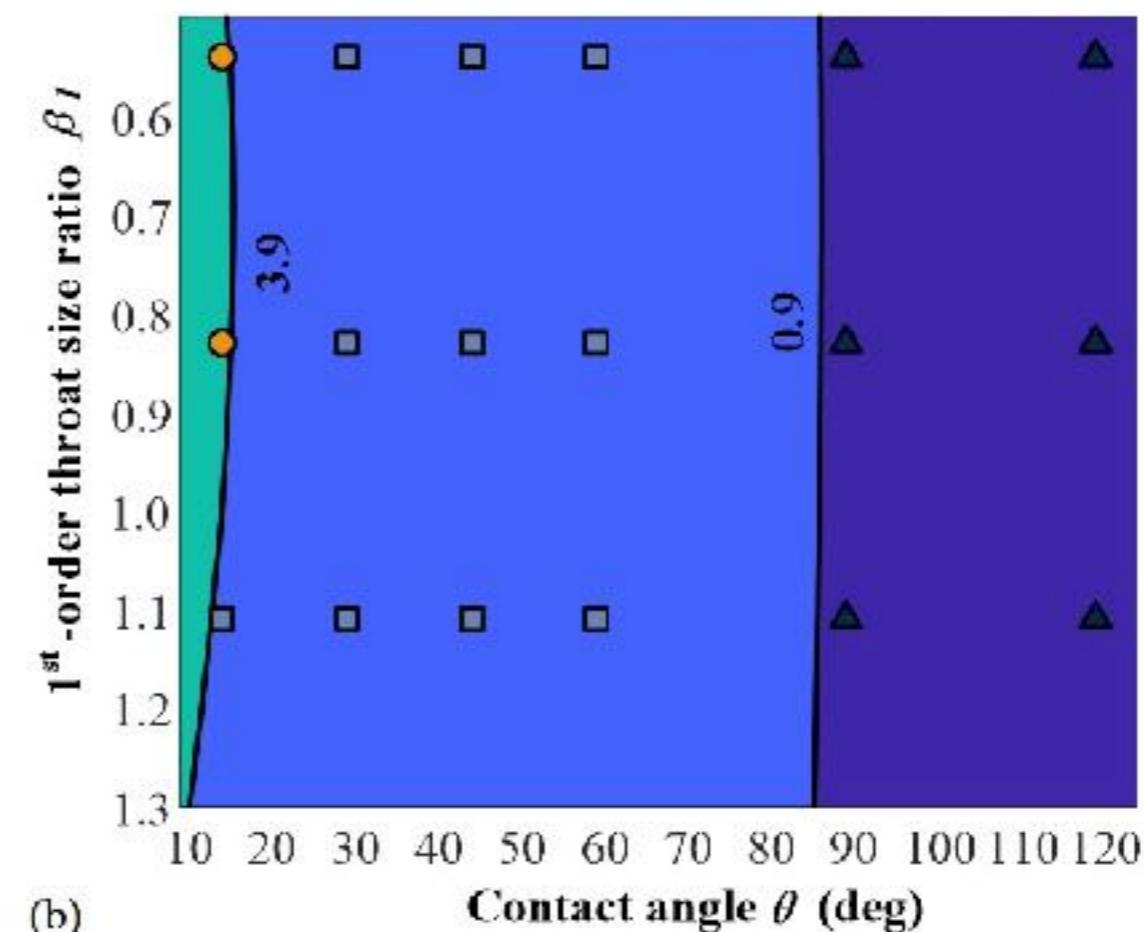
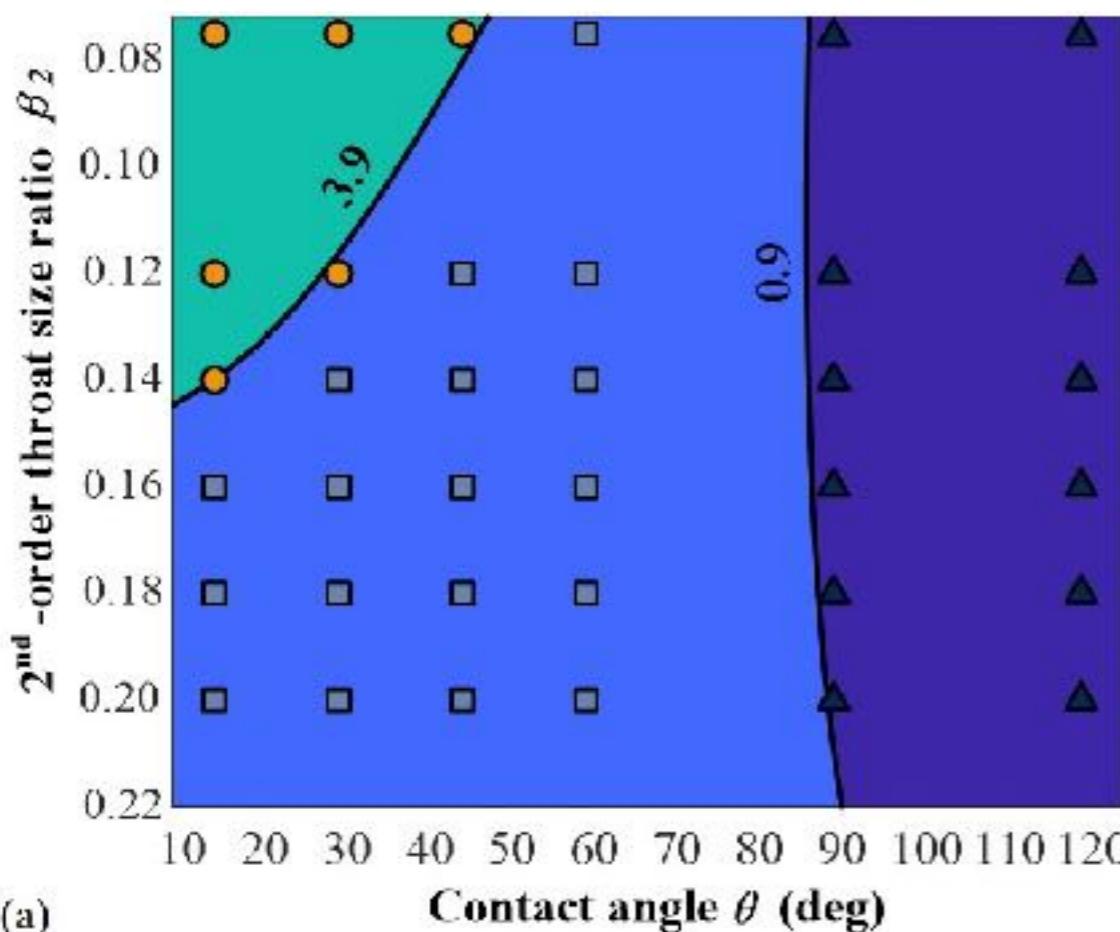
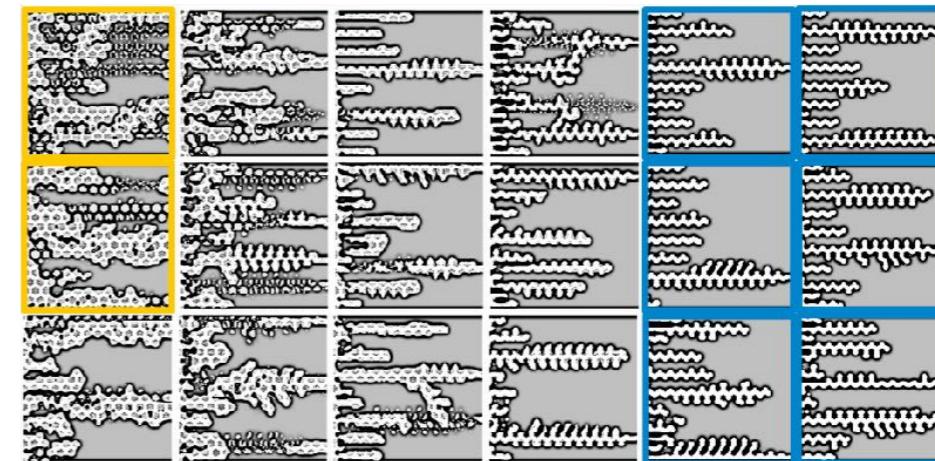
Index for Hierarchical Porous Structure



Index for Hierarchical Structure: Predictions

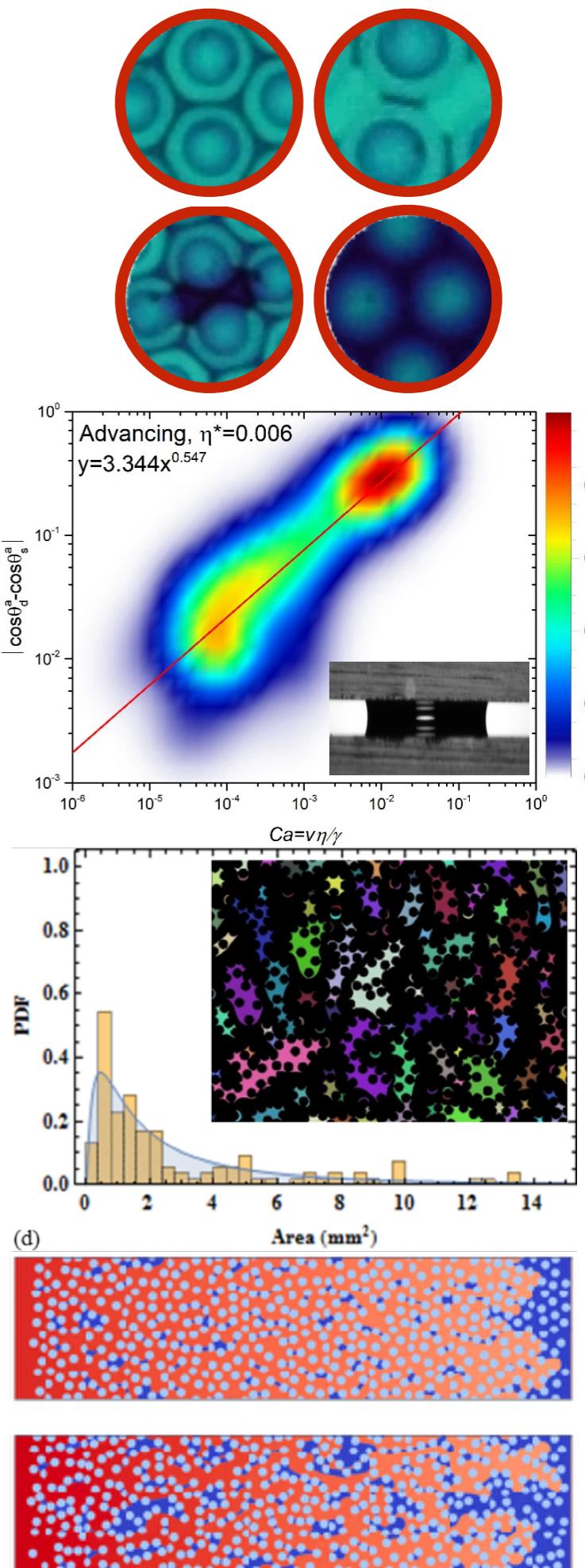


$$Hi = R_p \cdot R_T = \frac{P_{ext}}{P_{c,min}} \cdot \frac{T_1}{T_2} = 2 \cdot \frac{P_c^*}{P_{c,min}} \cdot \frac{\phi_1}{\phi_2} \cdot \frac{k_2}{k_1} \cdot \left(\frac{d_1}{d_2} \right)^2$$

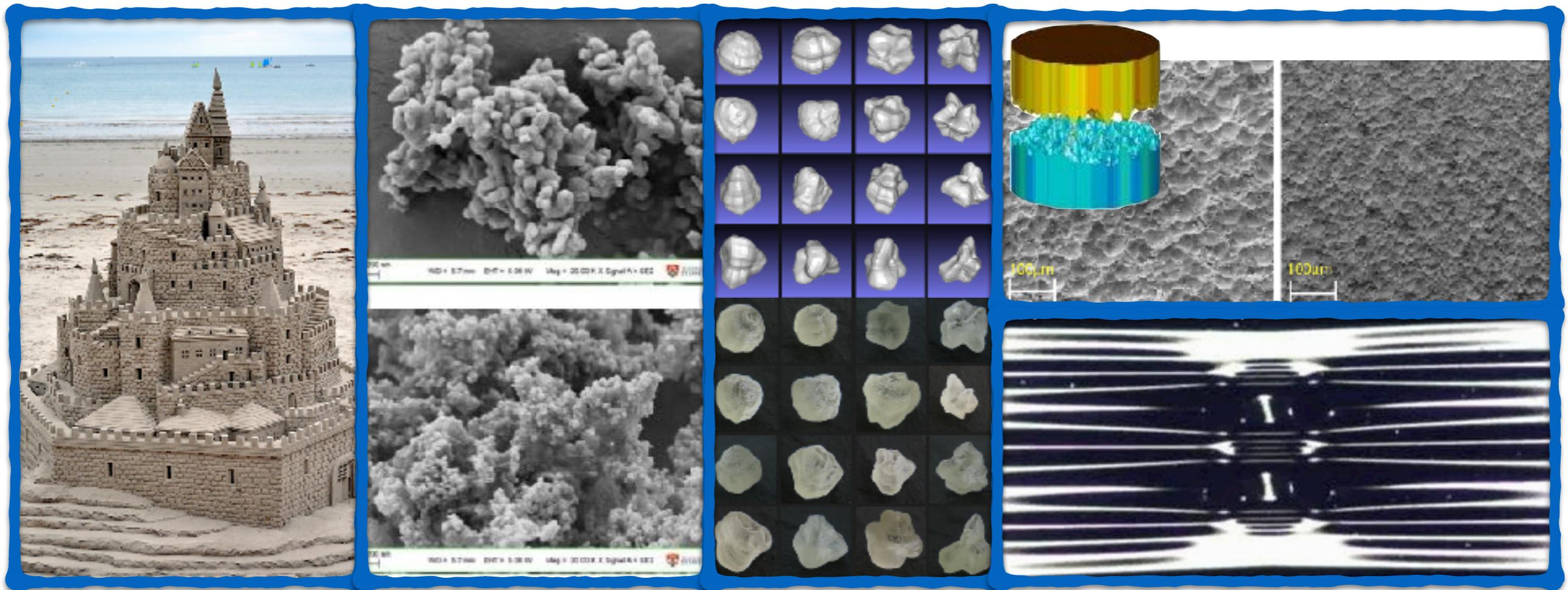


Conclusions

- **Heterogenous porous media:** disorder index, wetting transition, and hierarchical structure.
- **Porous topology** determines fingering patterns in hierarchical porous media, jointly with the surface wettability features.
- **Phase diagram** of fingering patterns and transitions from the dendrite to the suppressing modes in hierarchical porous media, captured by the newly proposed scaling number, **Hi**.
- Mechanism of the **fingering mode transition** implies an effective method to suppress / control the viscous fingering by adjusting hierarchical porous topology, wettability and rate of fluid displacement.



Thank you!



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