SCEJ 55th Autumn Meeting
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Meso-macro modeling of slip casting

鋳込み成形のメソ・マクロ連携モデリング

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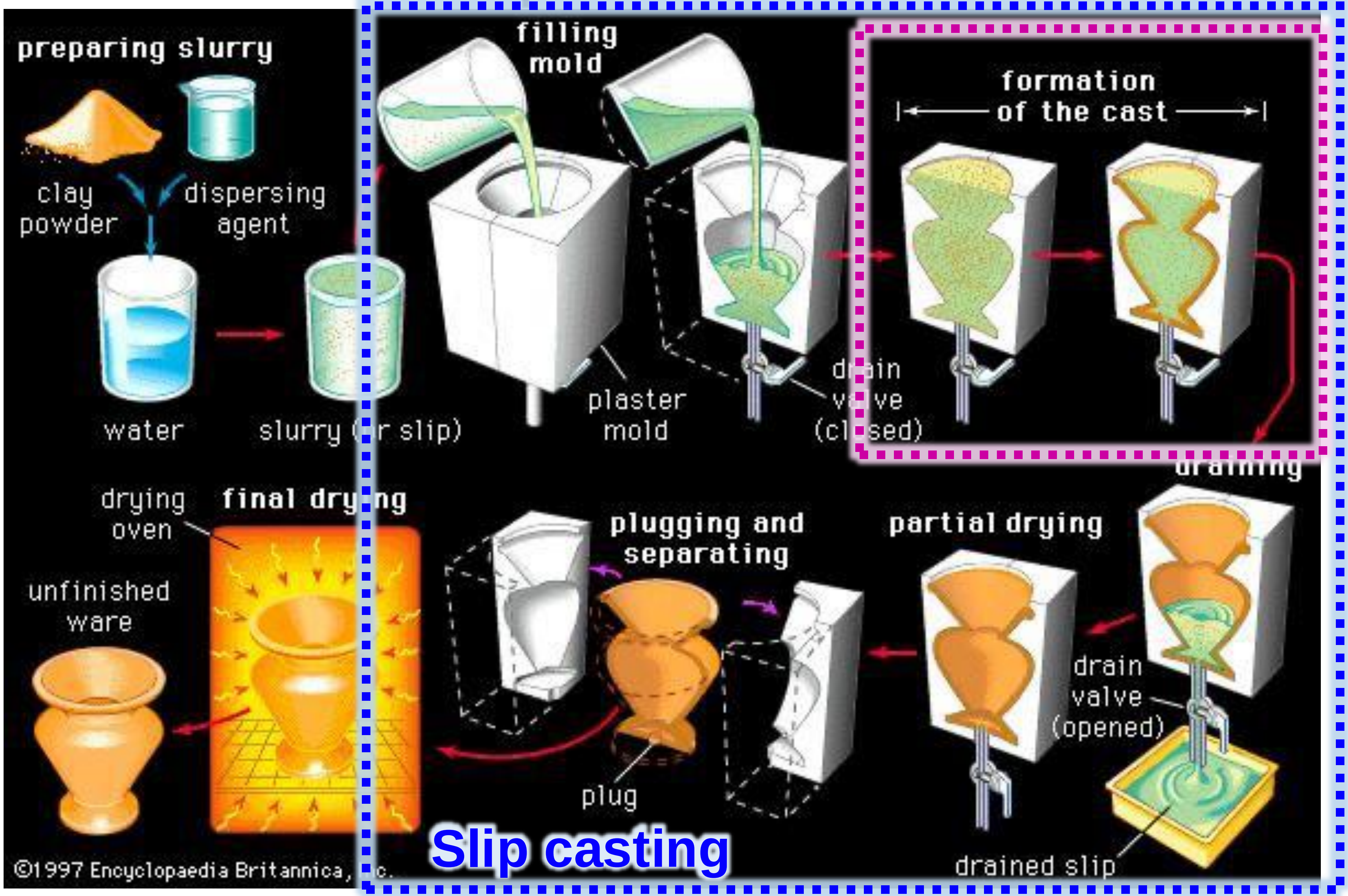
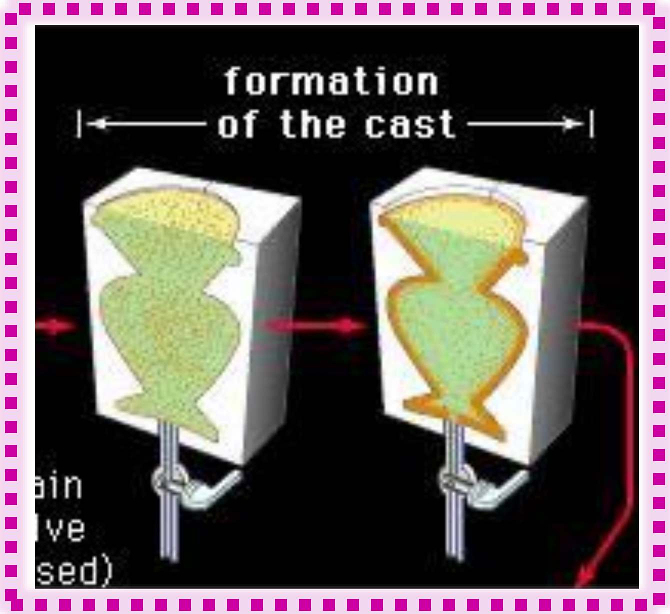
Fabrication process of ceramics



https://www.britannica.com/technology/traditional-ceramics

Objective & Method

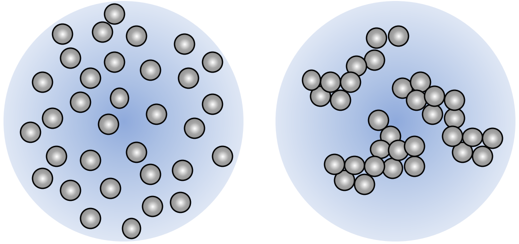
Meso-macro modeling of slip casting



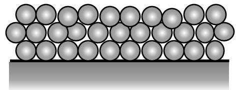
Slurry
- Particles
- Solvent
- Additives

Operation
- Pressure

Aggregation / Dispersion



Cake structure
- Packing density
- Permeability



Slip casting behavior
- Cake growth rate
- Density distribution

Meso-scale (~1 μm, <1 ms)
Discrete model

Macro-scale (>1 mm, >1 s)
Continuum model

Macro-scale model

Ruth's filtration equation

- Mass balance

(Liquid) $\dot{L} = v$

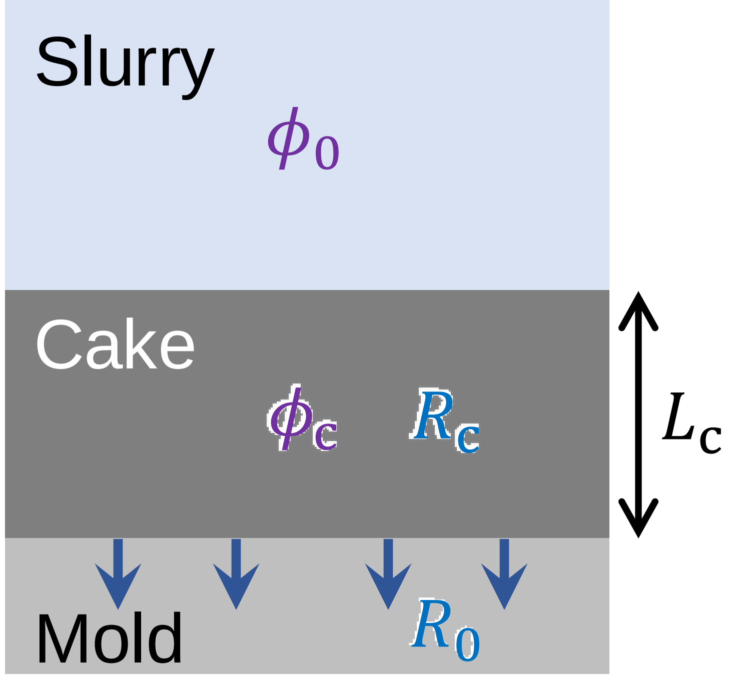
(Solid) $(\phi_c - \phi_0)L_c = \phi_0 L$

- Momentum balance

$P = \eta v(R_0 + R_c) \approx \eta v R_c \quad (R_c \gg R_0)$

$R_c = L_c/k_c$ (Incompressible cake)

Particle volume fraction



Permeation resistance

Cake thickness: $L_c = (Kt)^{1/2} \quad K = \frac{2\phi_0}{\phi_c - \phi_0}\frac{k_c P}{\eta}$

Filtrate volume per area: $L = \frac{\phi_c - \phi_0}{\phi_0}(Kt)^{1/2}$

Pressure: P

Liquid viscosity: η

Cake permeability: k_c

Meso-scale model

Particles

Inter-particle force

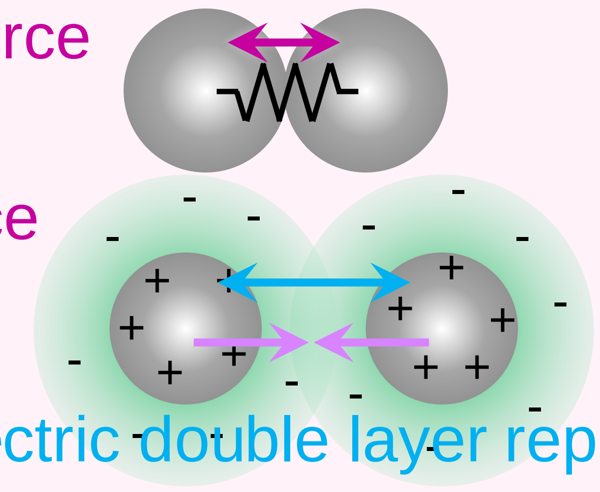
$$M\dot{\boldsymbol{V}} = \boldsymbol{F}^{\mathrm{H}} + \boldsymbol{F}^{\mathrm{P}}$$

$$I\dot{\boldsymbol{\Omega}} = \boldsymbol{N}^{\mathrm{H}}$$

Hydrodynamic force/torque

Contact force

DLVO force



Electric double layer repulsion

Van der Waals attraction

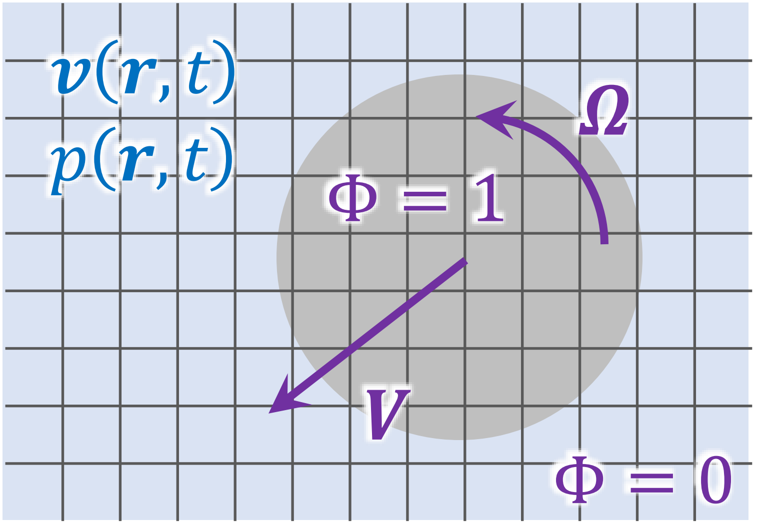
Fluid flow: Navier–Stokes equations

Imposition of velocity in particle domains

$$\nabla \cdot \boldsymbol{v} = 0$$

$$\rho(\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}) = \nabla \cdot \boldsymbol{\sigma} + \Phi \boldsymbol{f}_{\mathrm{P}}$$

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \eta[\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\mathrm{T}}]$$



Indicator function : $\Phi(\boldsymbol{r},t)$

Meso-scale model

- Additional terms for slip casting in Navier–Stokes equations

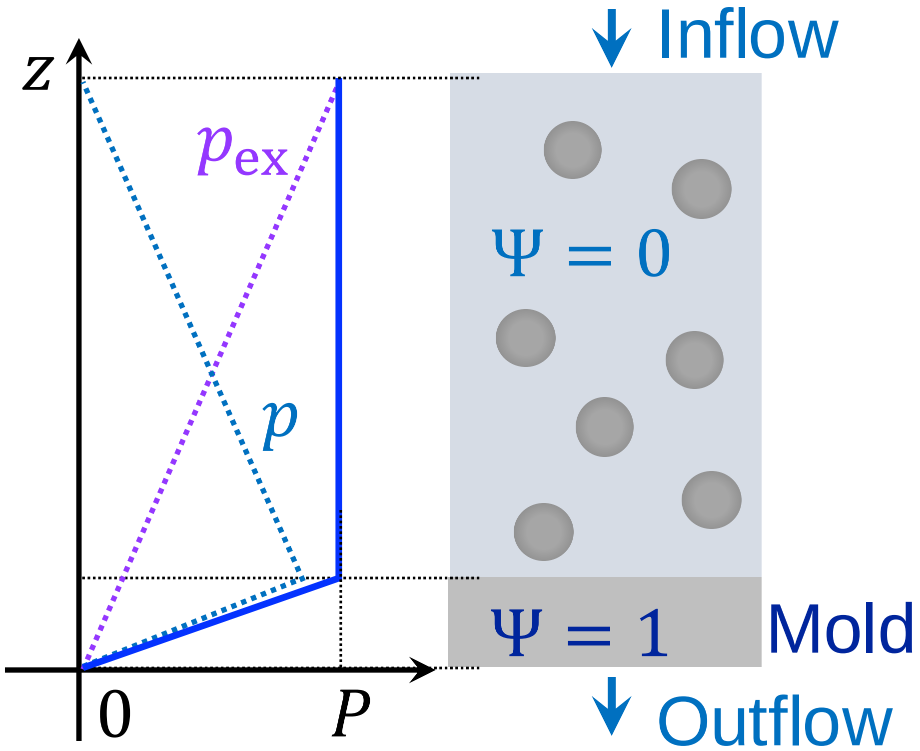
$$\rho(\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}) = \nabla \cdot \boldsymbol{\sigma} + \Phi \boldsymbol{f}_{\mathrm{P}} + \boldsymbol{D} - \frac{\eta}{k_0} \Psi \boldsymbol{v}$$

External pressure gradient: $\boldsymbol{D} = -\nabla p_{\mathrm{ex}}$

Permeability of mold: k_0

- Generation of particles on inflow plane

Volume generation rate per area: $\phi_0 v$



Simulation conditions

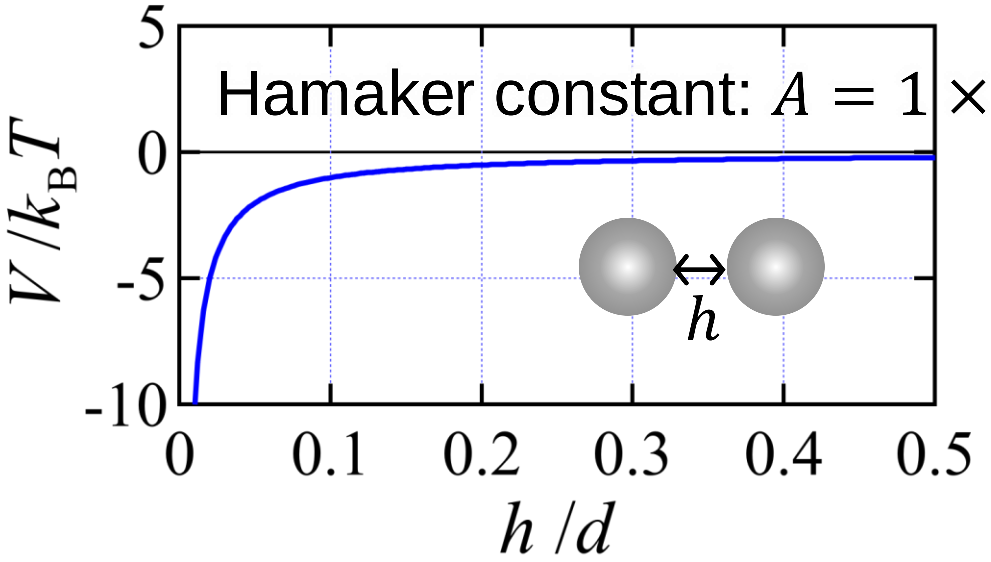
Particles

- Diameter: $d = 1\ \mu\mathrm{m}$
- Concentration: $40\ \mathrm{vol\%}$
- Zeta potential: $0\ \mathrm{mV}$

Fluid: Water

DLVO potential

Hamaker constant: $A = 1 \times 10^{-20}\ \mathrm{J}$

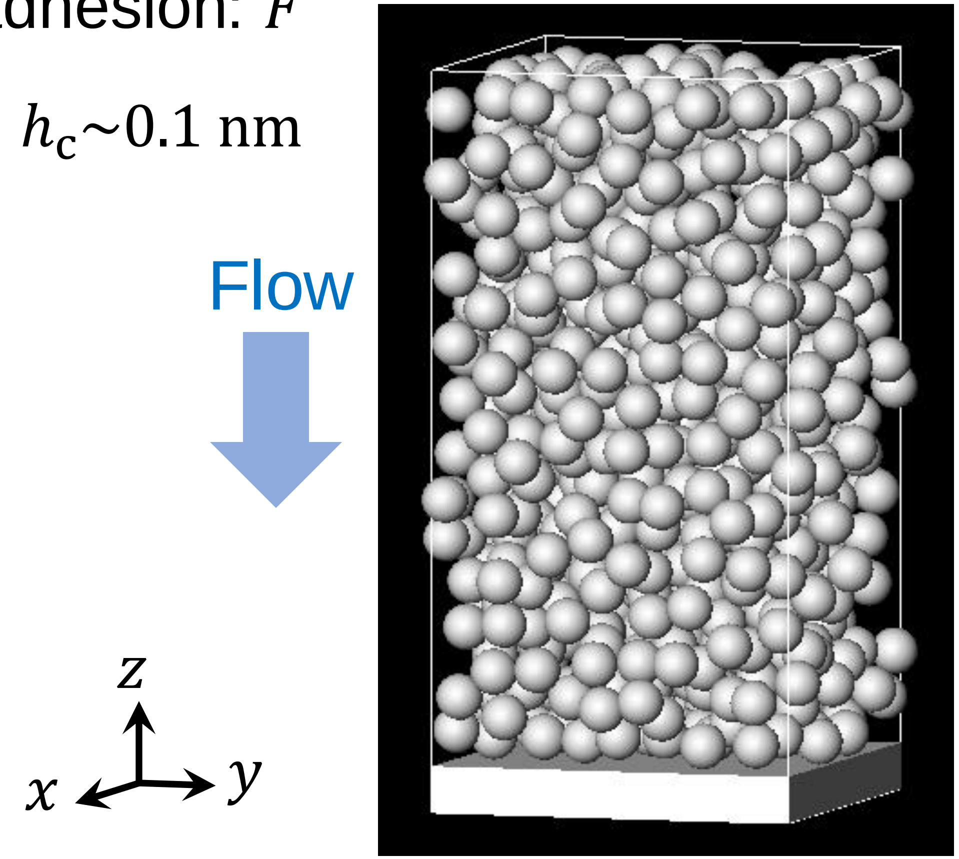


Varied parameters

- Pressure: $P^* \equiv Pd^2/F = 10^{-1} - 10^1$

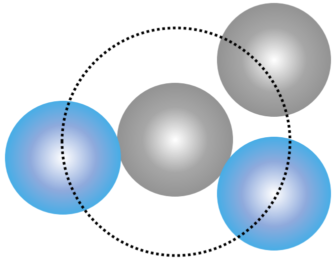
Interparticle adhesion: F

$$F = \frac{Ad}{24h_c^2} \qquad h_c \sim 0.1\ \mathrm{nm}$$

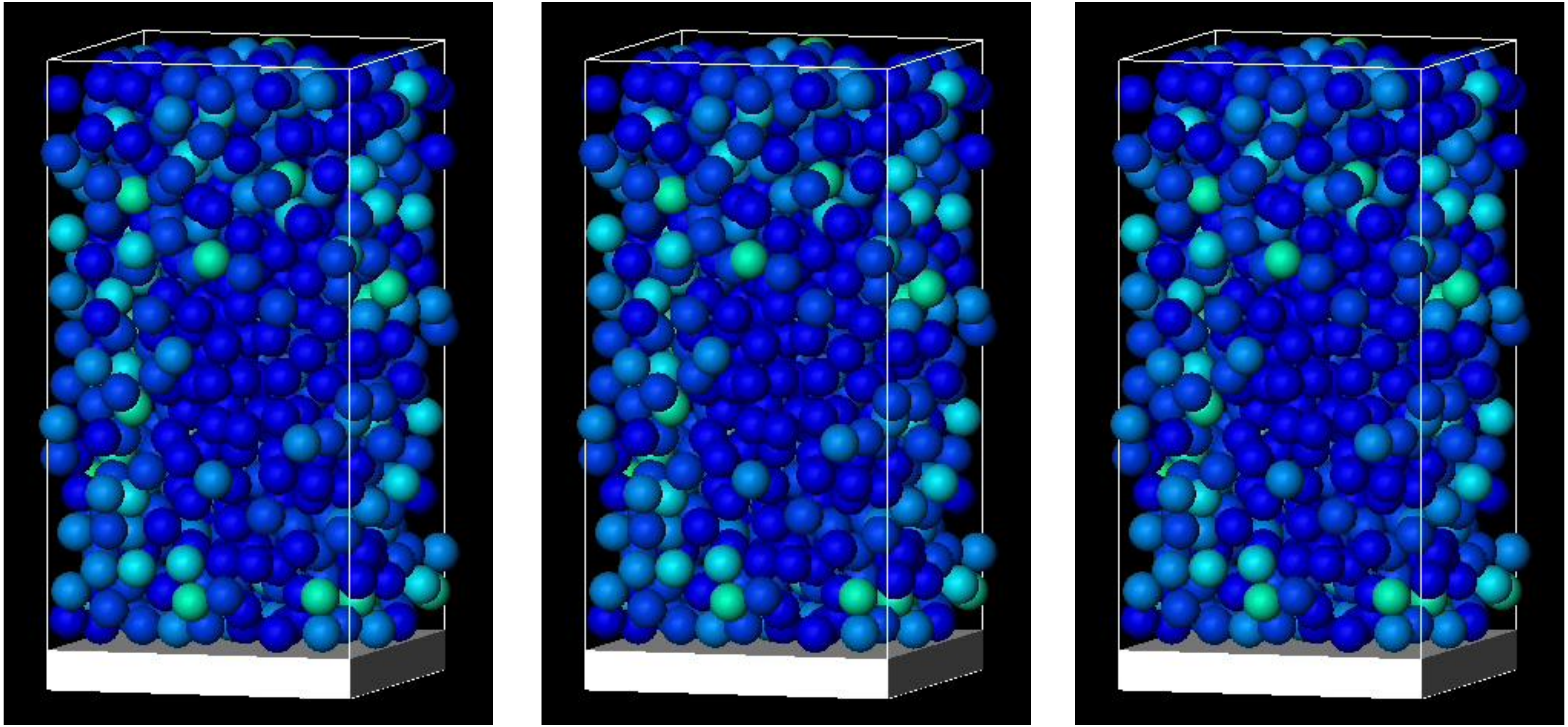


System size: $8d \times 8d \times 16d$

Simulation results



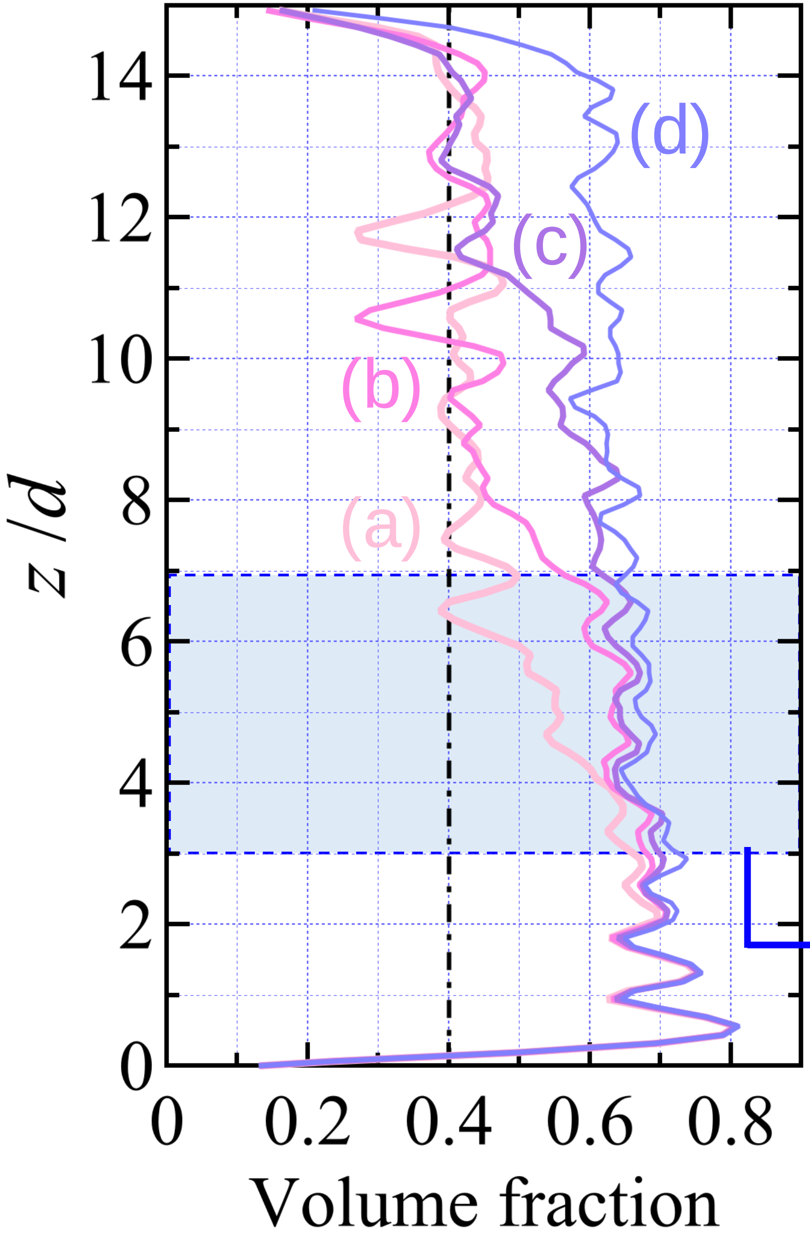
Contact number 0 12

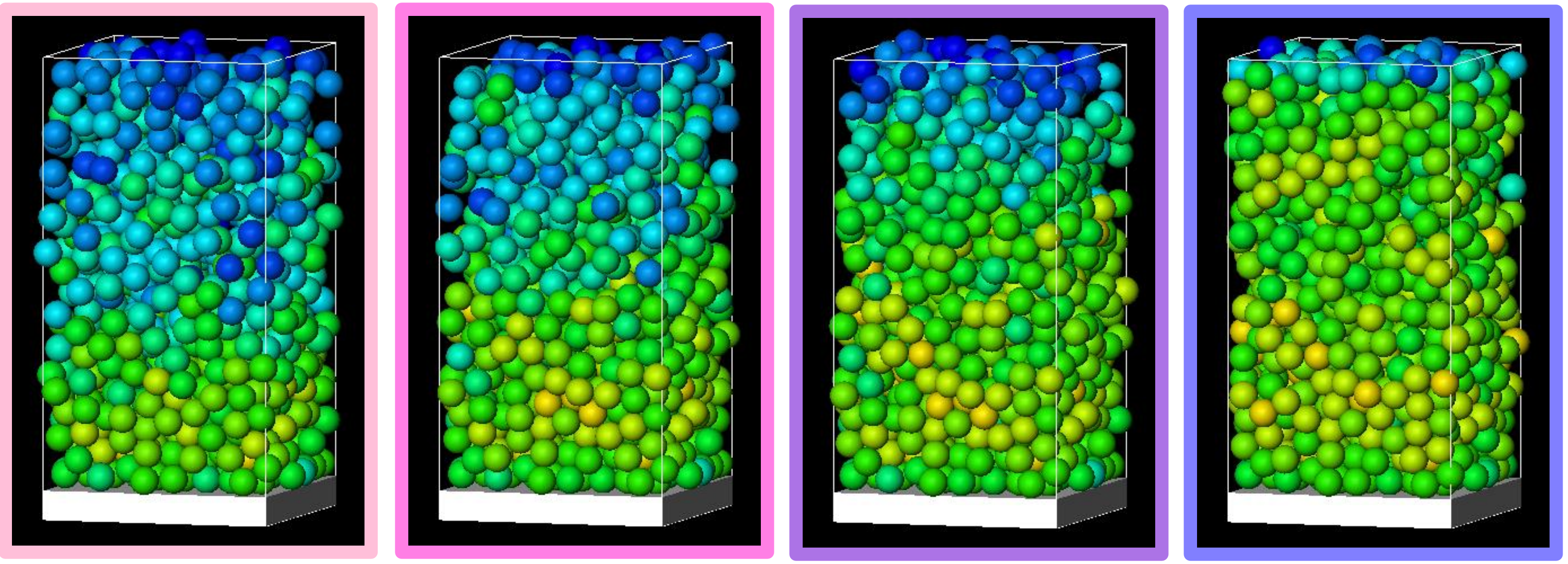


$P^* = 0.1$ $P^* = 1$ $P^* = 10$

$P^* = 1$

Cake growth (Meso-scale)



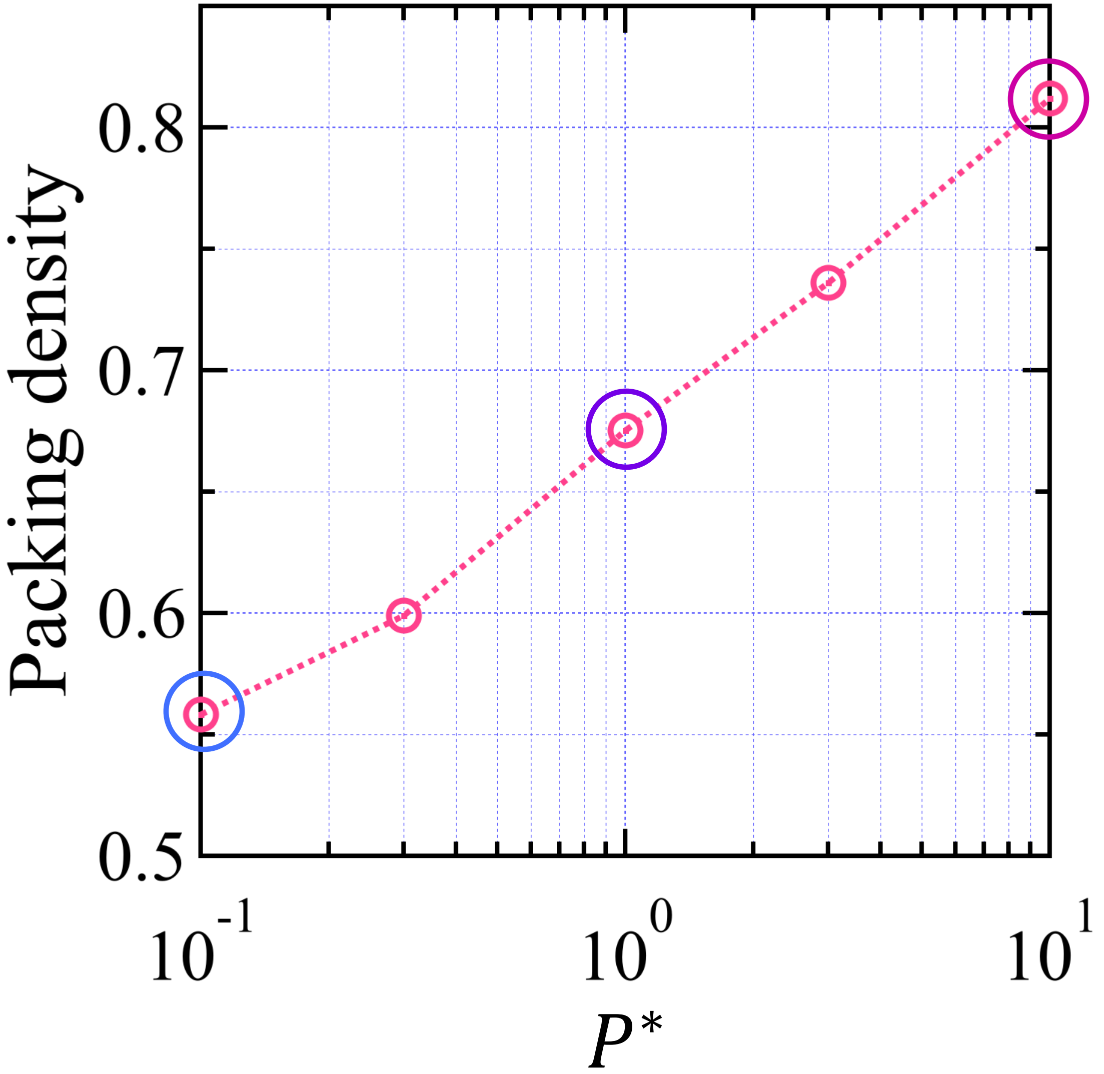


(a) 0.46 (b) 0.93 (c) 1.86 (d) 3.71

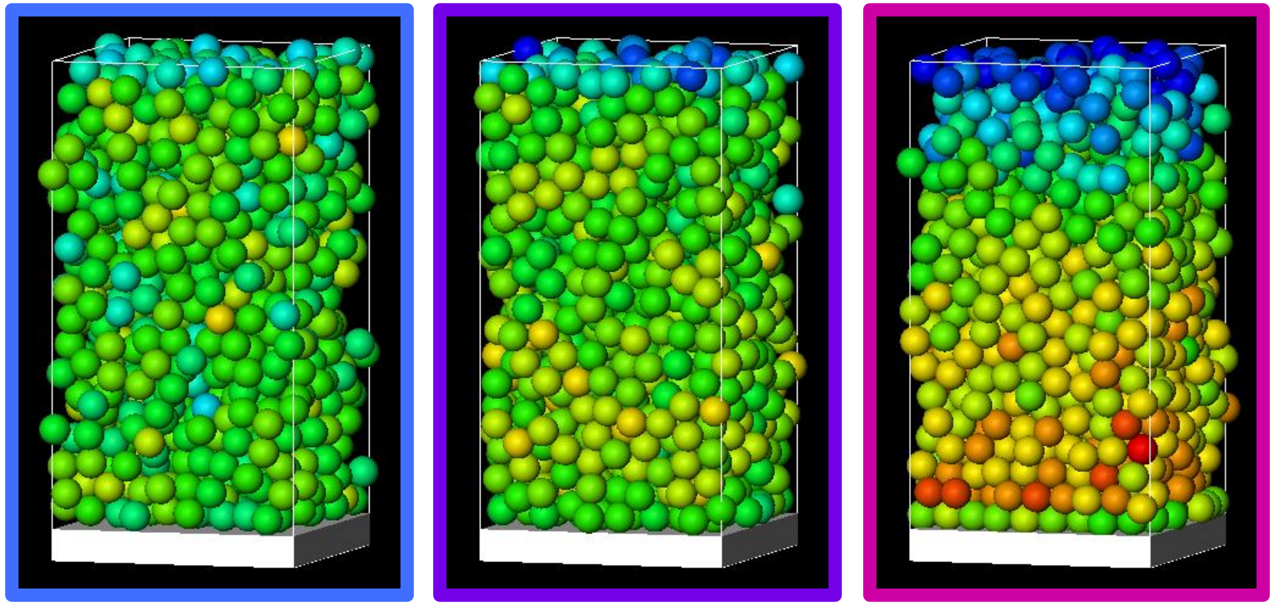
Time: $Pt/\eta \times 10^{-3}$

Average → Packing density

Packing density



$P^* = Pd^2/F$



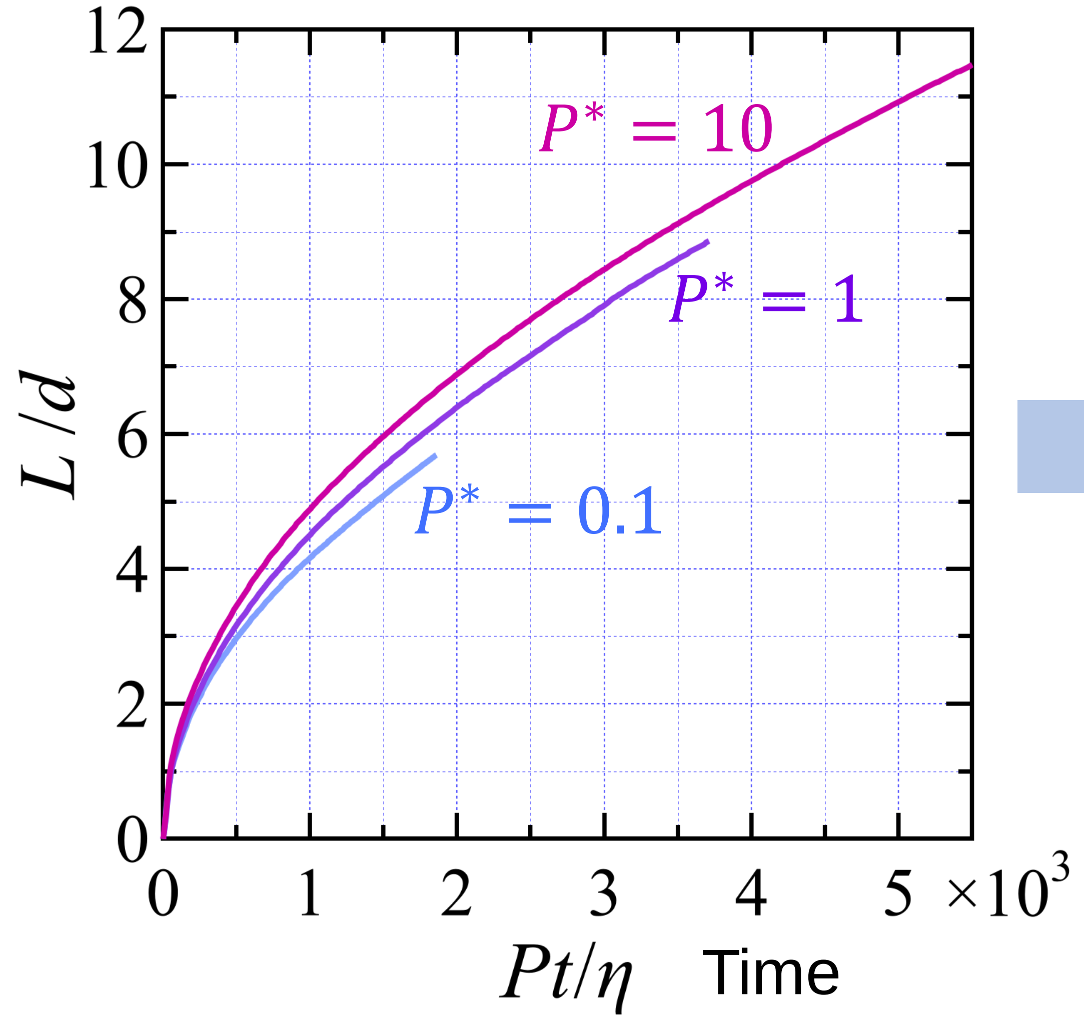
$P^* = 0.1$ | $P^* = 1$ | $P^* = 10$

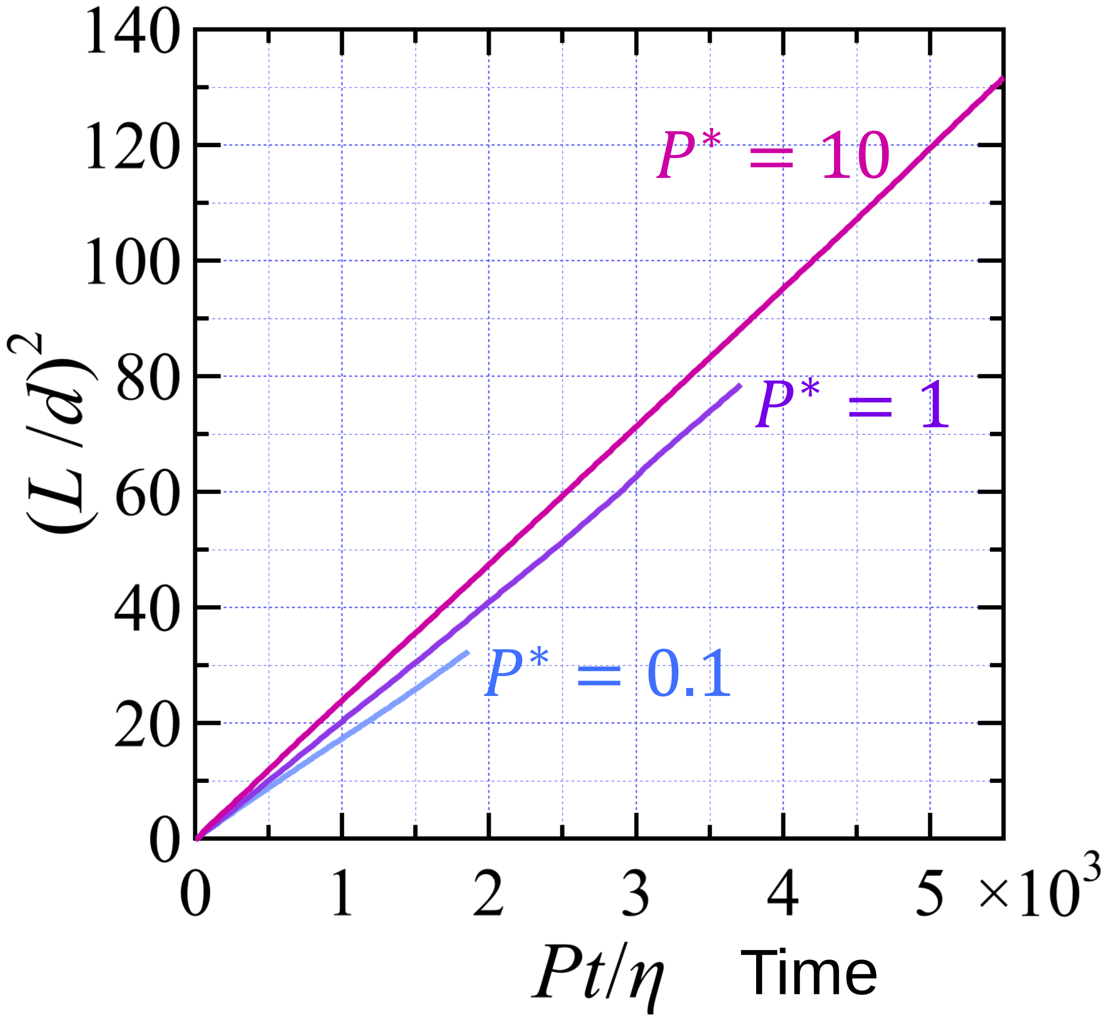
1.86 | 3.71 | 5.57

Time: $Pt/\eta\ \times 10^{-3}$

Dehydration curve

Filtrate volume per area: L

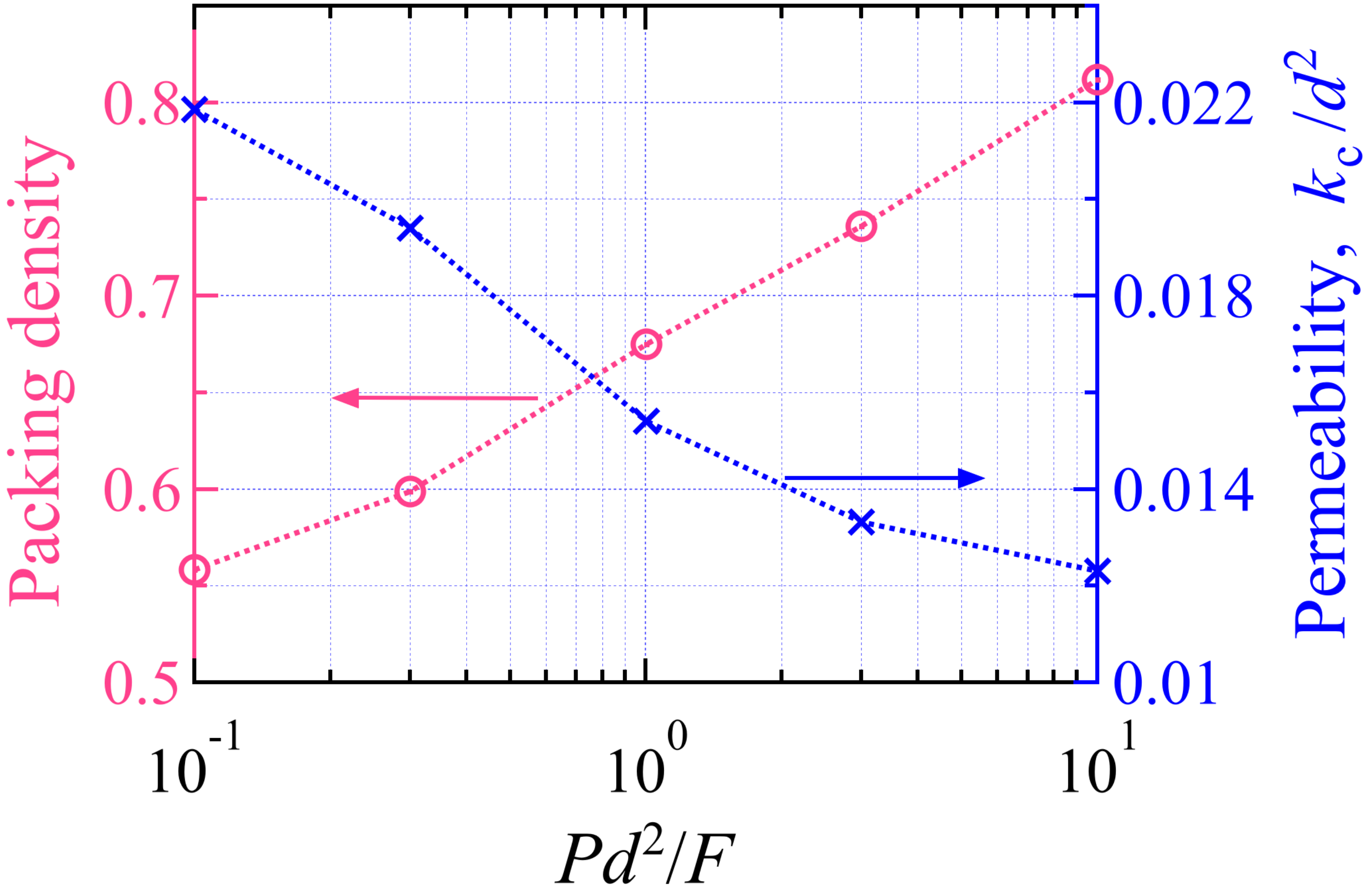




$$\frac{L}{d} = \left[\frac{2(\phi_c - \phi_0)}{\phi_0}\frac{k_c}{d^2}\frac{Pt}{\eta}\right]^{1/2}$$

Slope → Permeability

Packing density & Permeability

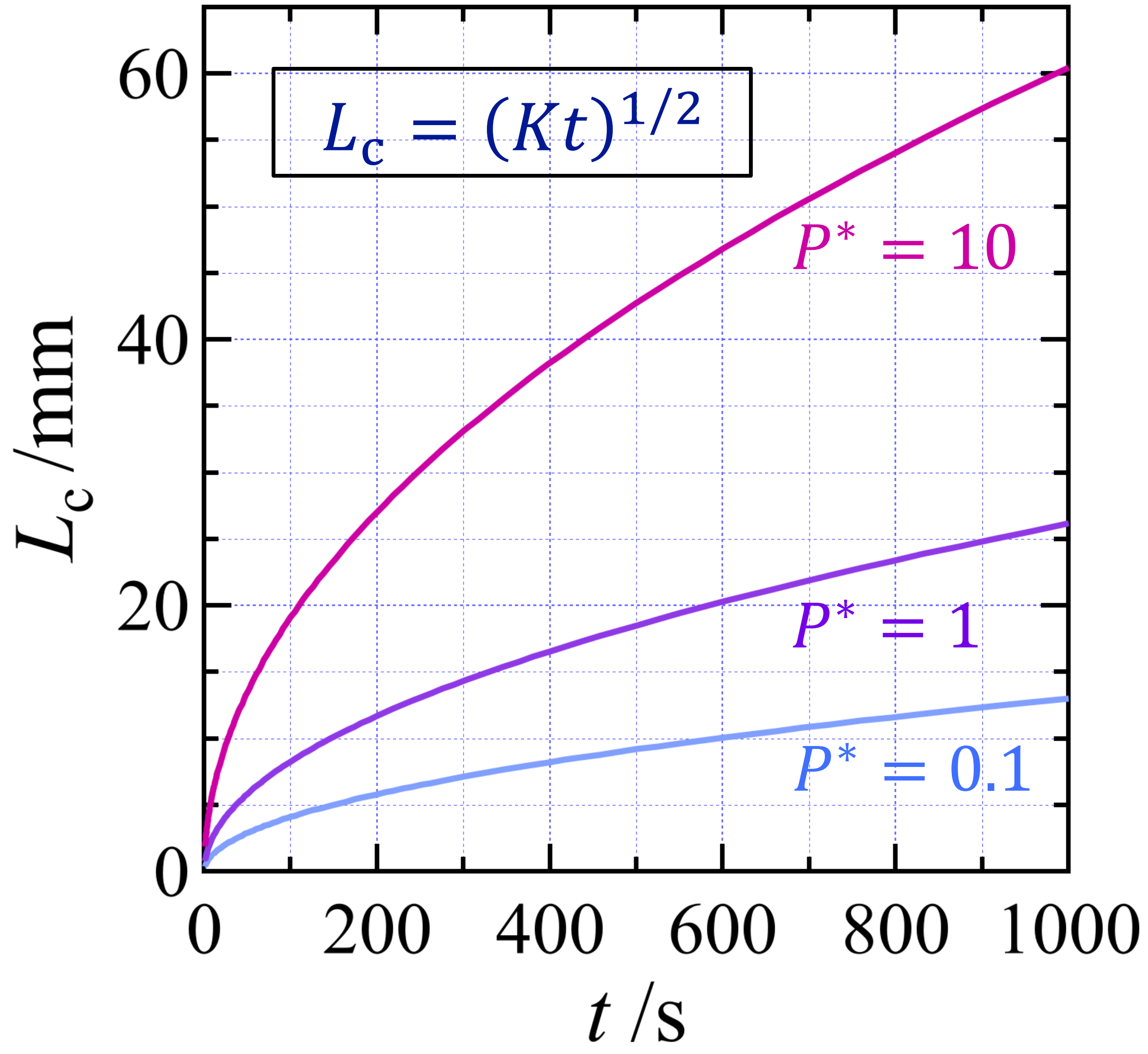


Increase in pressure P
Decrease in interparticle adhesion F

→

Increase in packing density
Decrease in permeability

Cake growth (Macro-scale)



$$K = \frac{2\phi_0}{\phi_c - \phi_0} \frac{k_c P}{\eta}$$

P^*	P /kPa	$K/(\mathrm{mm}^2/\mathrm{s})$
0.1	1.5	0.17
1	15	0.69
10	150	3.7

$$P^* = \frac{Pd^2}{F} \qquad F = \frac{Ad}{24h_c^2}$$

$$A = 1 \times 10^{-20}\ \mathrm{J}$$

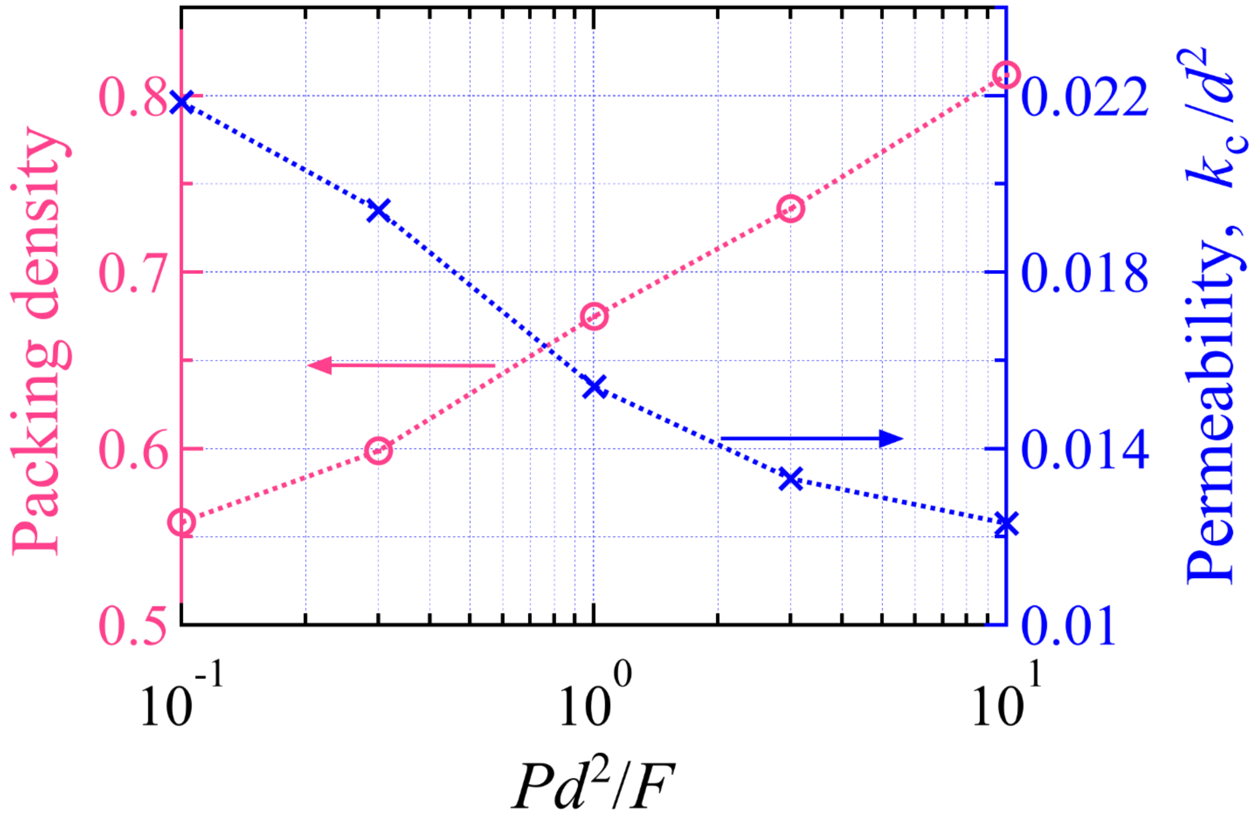
$$h_c = 0.165\ \mathrm{nm}$$

Summary

Particle interactions
Pressure

Meso-scale model **Macro-scale model**

Cake structure



Slip casting behavior