9th Asian Coating Workshop
May 17, 2017, TUAT, Toyko

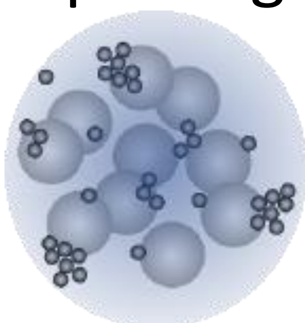
Numerical simulation of segregation in drying bimodal colloidal suspensions

Rei Tatsumi[1], Takuya Iwao[1], Osamu Koike[2], Yoshiko Tsuji[1], Yukio Yamaguchi[2]

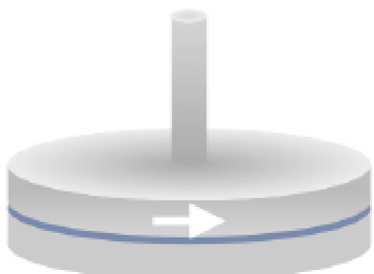
[1]The University of Tokyo
[2]Products Innovation Association (PIA)

Colloidal Suspensions in Industrial Use

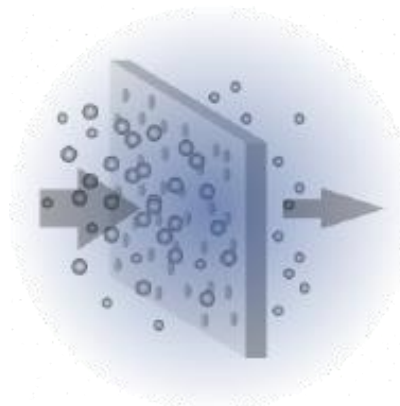
Kneading
Dispersing



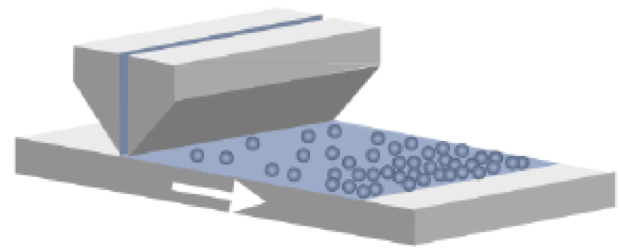
Polishing



Filtration



Coating



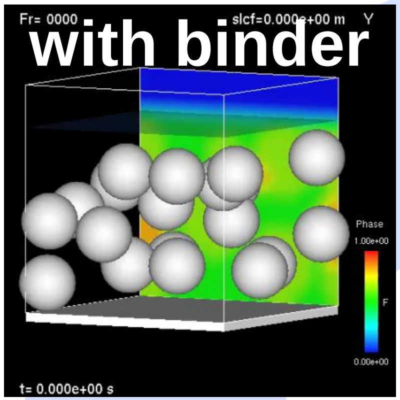
Structure formation of particles

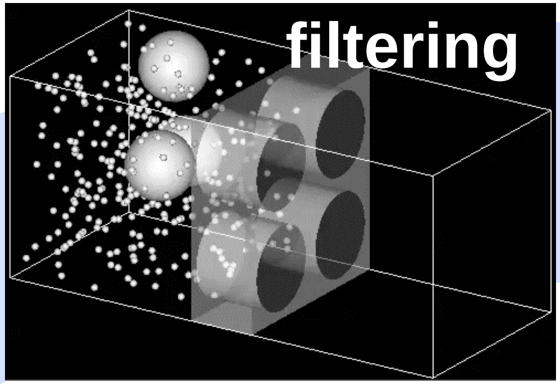
- Process efficiency
- Physical properties of products

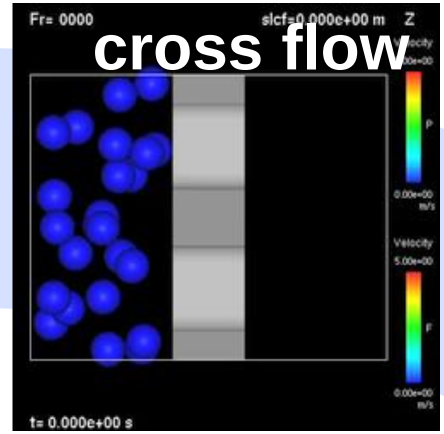
Mechanism

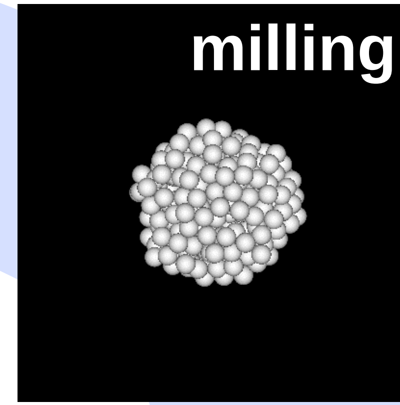
Numerical simulator: **SNAP** (Structure of NAno Particles)

Structure Formation Simulated by SNAP

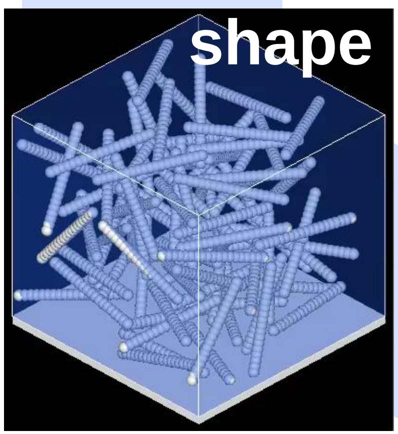


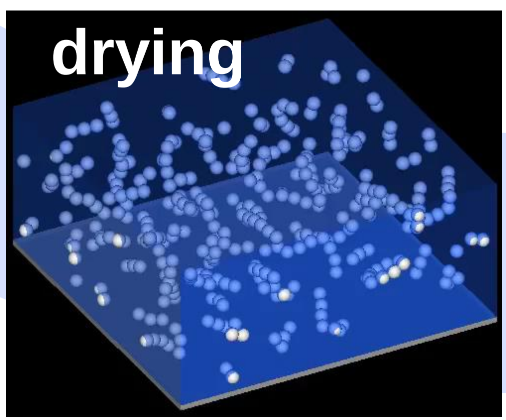


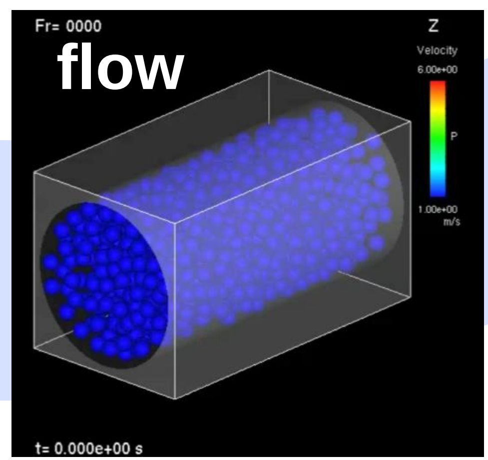


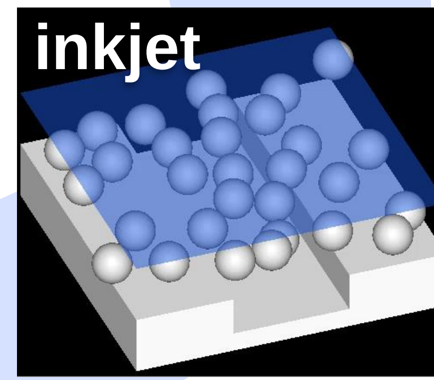


Toward colloid technology from colloid science





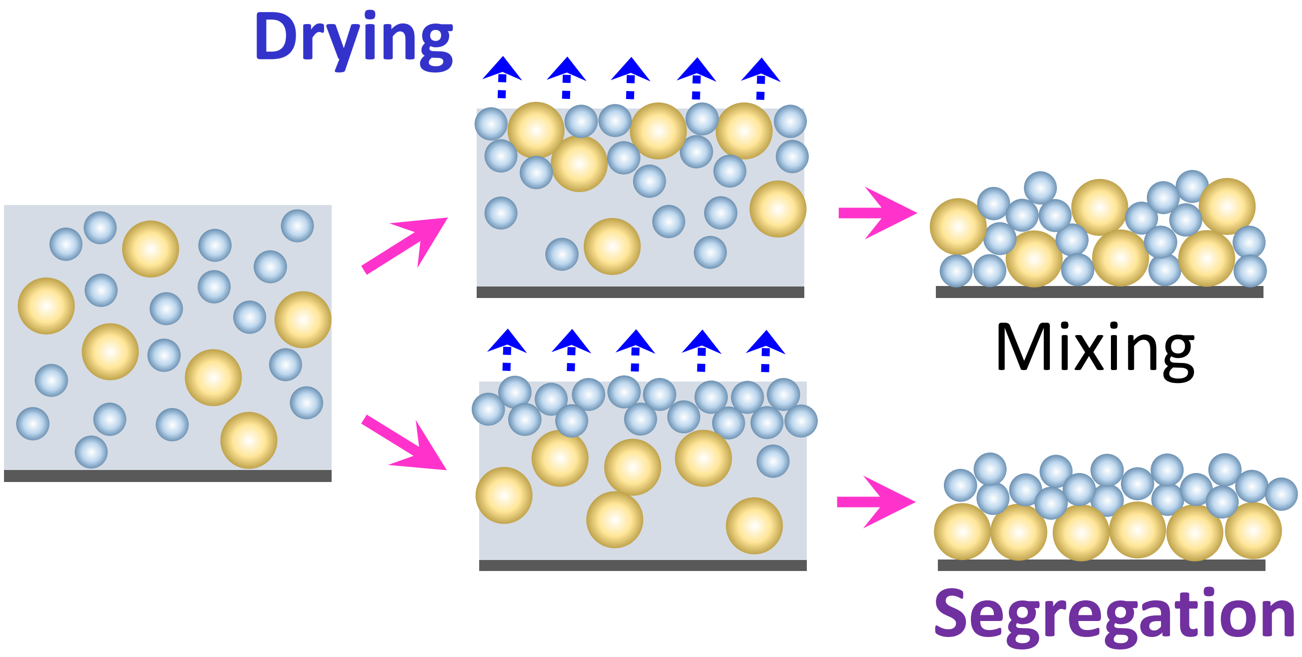


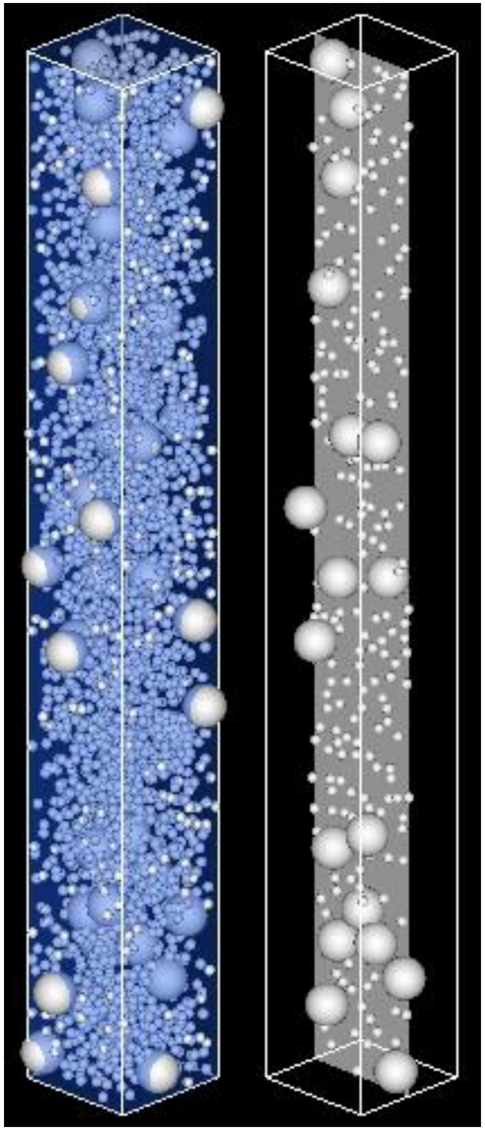


SNAP研究会

Today's Topic

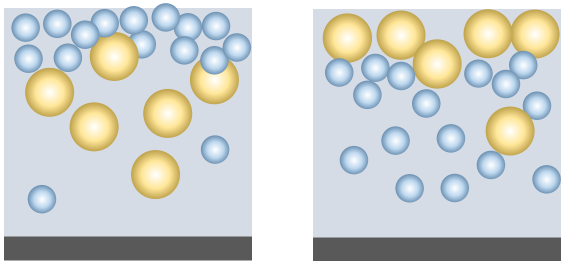
Analysis of segregation by SNAP

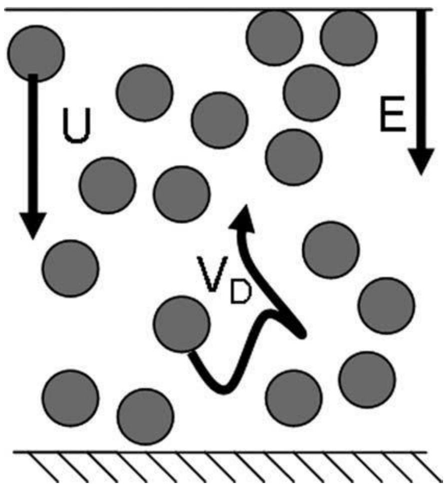


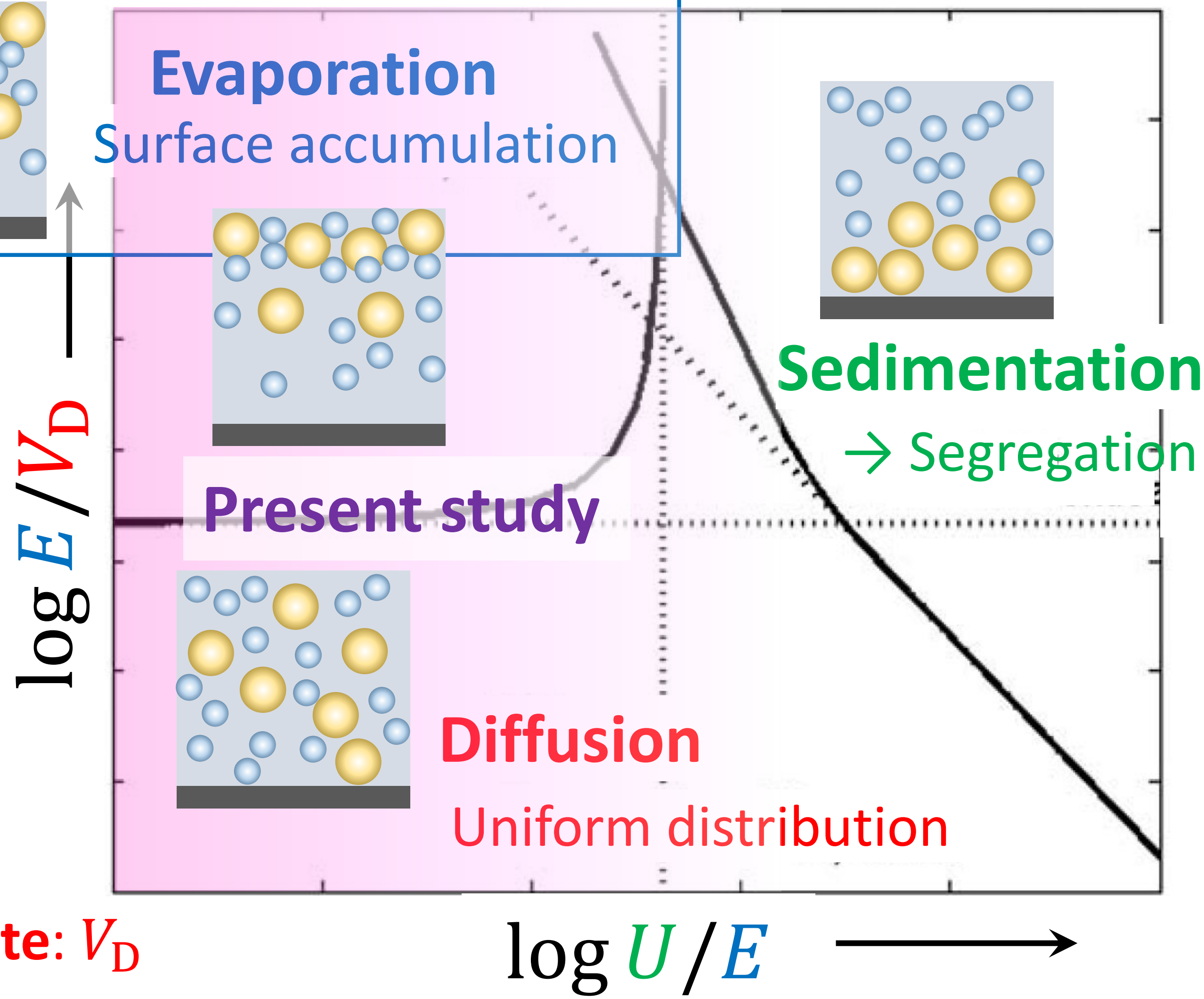


Particle distribution during Drying

How does segregation occur?







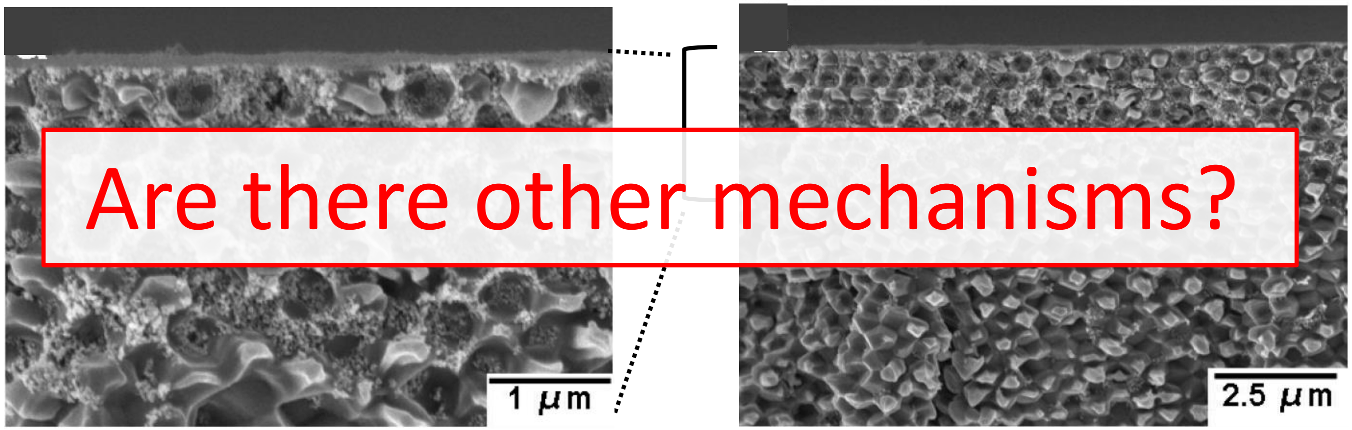
Evaporation rate: E

Brownian diffusion rate: V_D

Sedimentation velocity: U

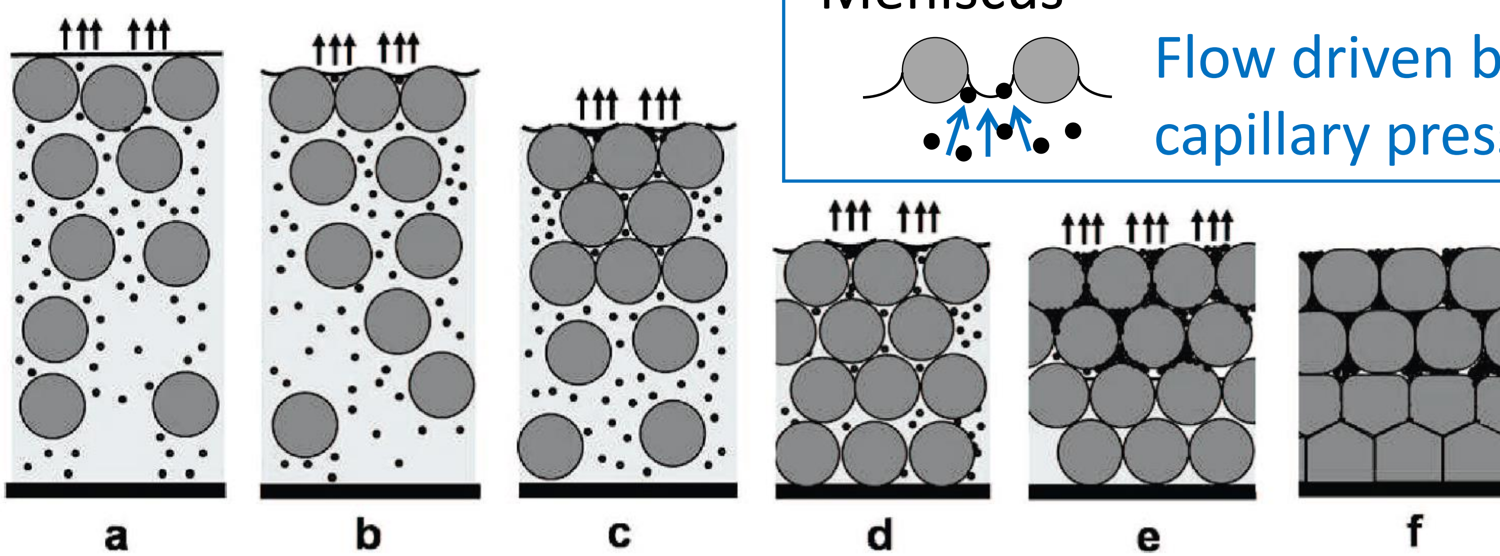
Cardinal et al., AIChE J. (2010).

A Proposed Mechanism



Are there other mechanisms?

SEM images of the cross section of a dried silica (20 nm) /latex (550 nm) coating

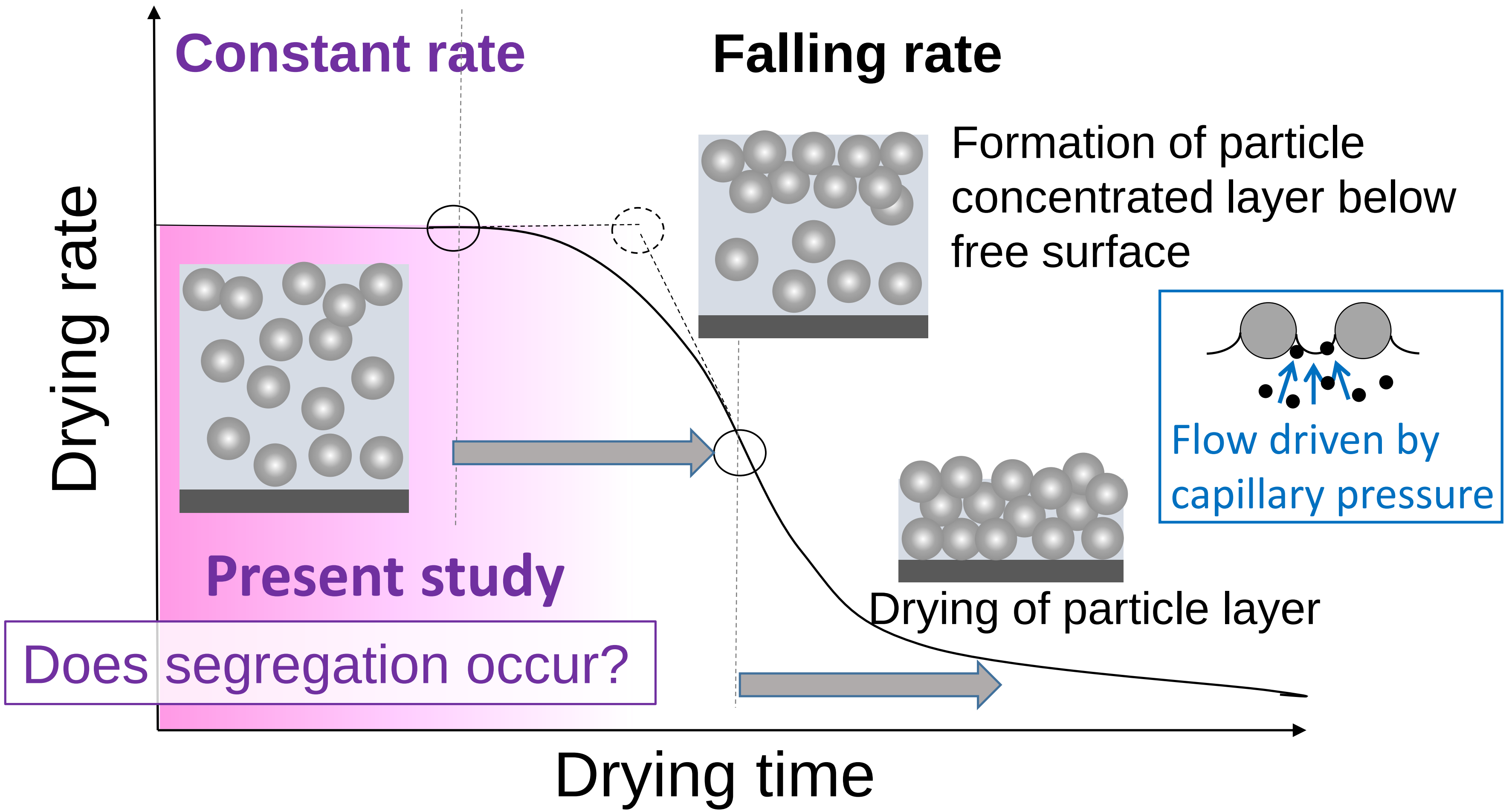


Meniscus

Flow driven by capillary pressure

Luo et al., Langmuir (2008).

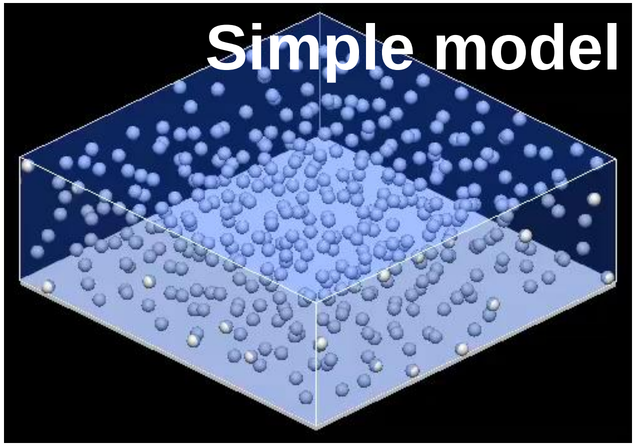
Drying Curve of Colloidal Suspensions



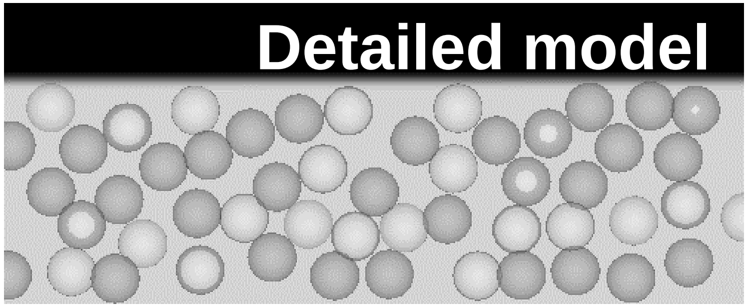
Objective

- Investigation of the segregation in the constant drying rate period

- Analysis using a simple model
  - Brownian motion of particles
  - Free surface moving at constant rate
  - Not included:
    gravity, fluid flow, free-surface deformation



Models of SNAP



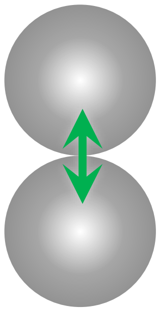
Equation of Particles' Brownian Motion

Langevin equation $M_i \dot{\boldsymbol{V}}_i = -\xi \boldsymbol{V}_i + \boldsymbol{F}_i^{\mathrm{R}} + \boldsymbol{F}_i^{\mathrm{contact}} + \boldsymbol{F}_i^{\mathrm{capillary}}$

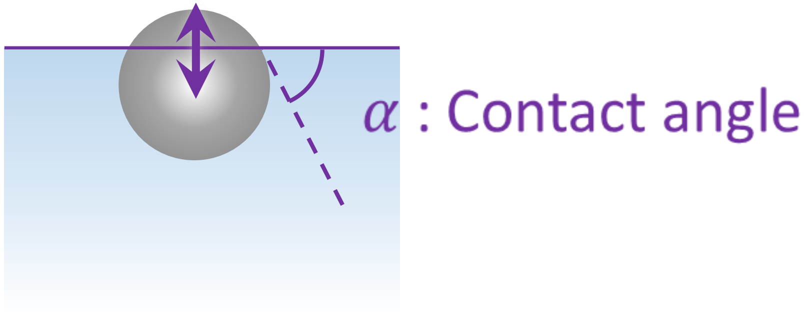
- **Drag force**: $-\xi \boldsymbol{V}_i$ Stokes' law: $\xi = 3\pi\eta d$
- **Random force**: $F_{i\alpha}^{\mathrm{R}}(t) \sim N(0, 2\xi k_{\mathrm{B}} T)$ Stochastic variables obeying the Gaussian dist.

→ **Brownian Diffusion**: $D = \dfrac{k_{\mathrm{B}} T}{3\pi\eta d}$ Diffusion coefficient in infinite dilution

Contact force



Vertical capillary force



Not included: Gravity, Transport by fluid flow

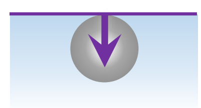
Simulation Conditions

- Particle diameter **L**: d **S**: $\kappa^{-1}d$

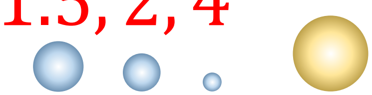
- Initial volume fraction

  L: 0.05 **S**: 0.05 (Total : 0.1)

- Contact angle $\alpha = 0$

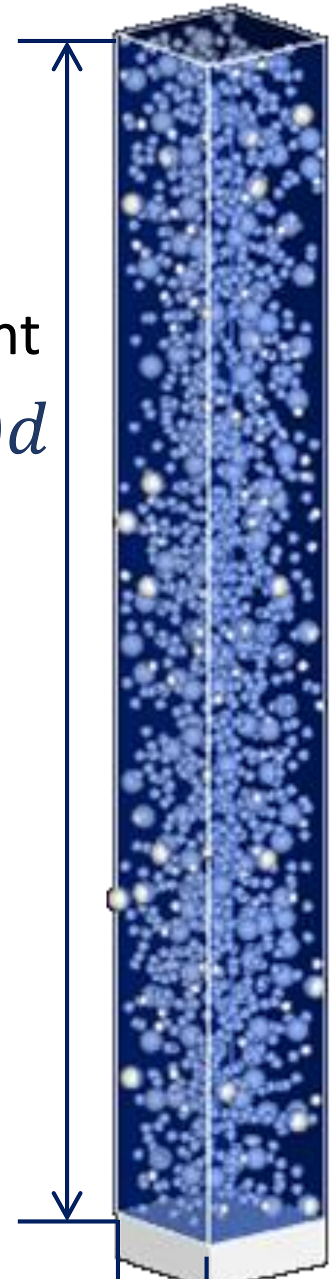


- Diameter ratio (**L**/**S**) $\kappa = 1.5, 2, 4$

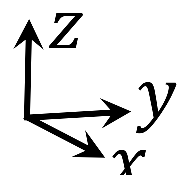


Initial height

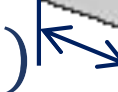
$h_0 = 50d$



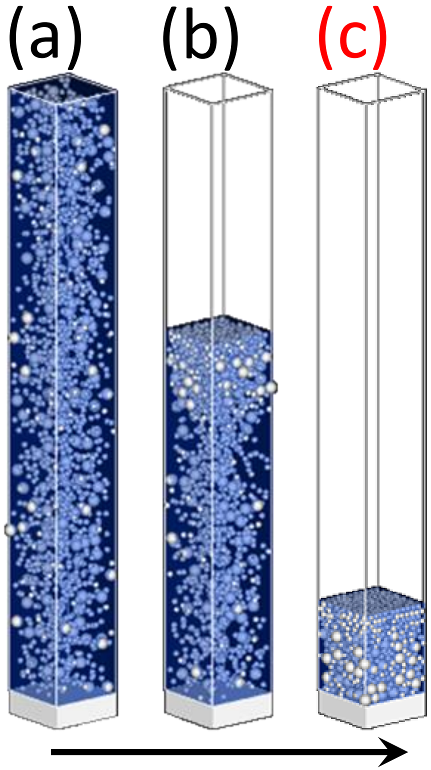
Periodic boundaries: x, y



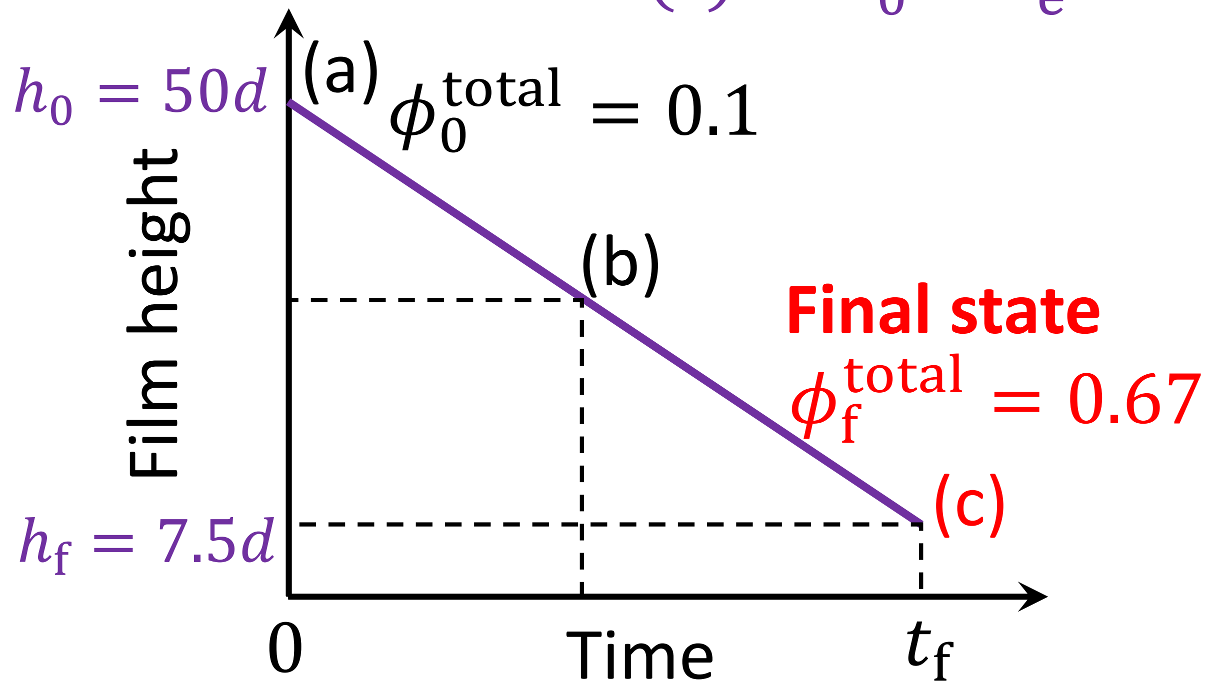
$6d\ (3d)$



Simulation Conditions

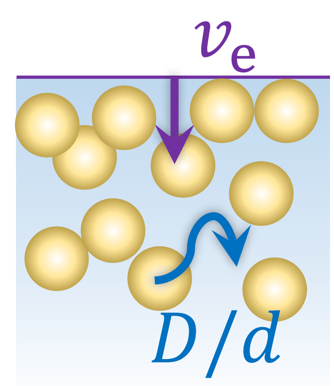


$$h(t) = h_0 - v_\mathrm{e} t$$



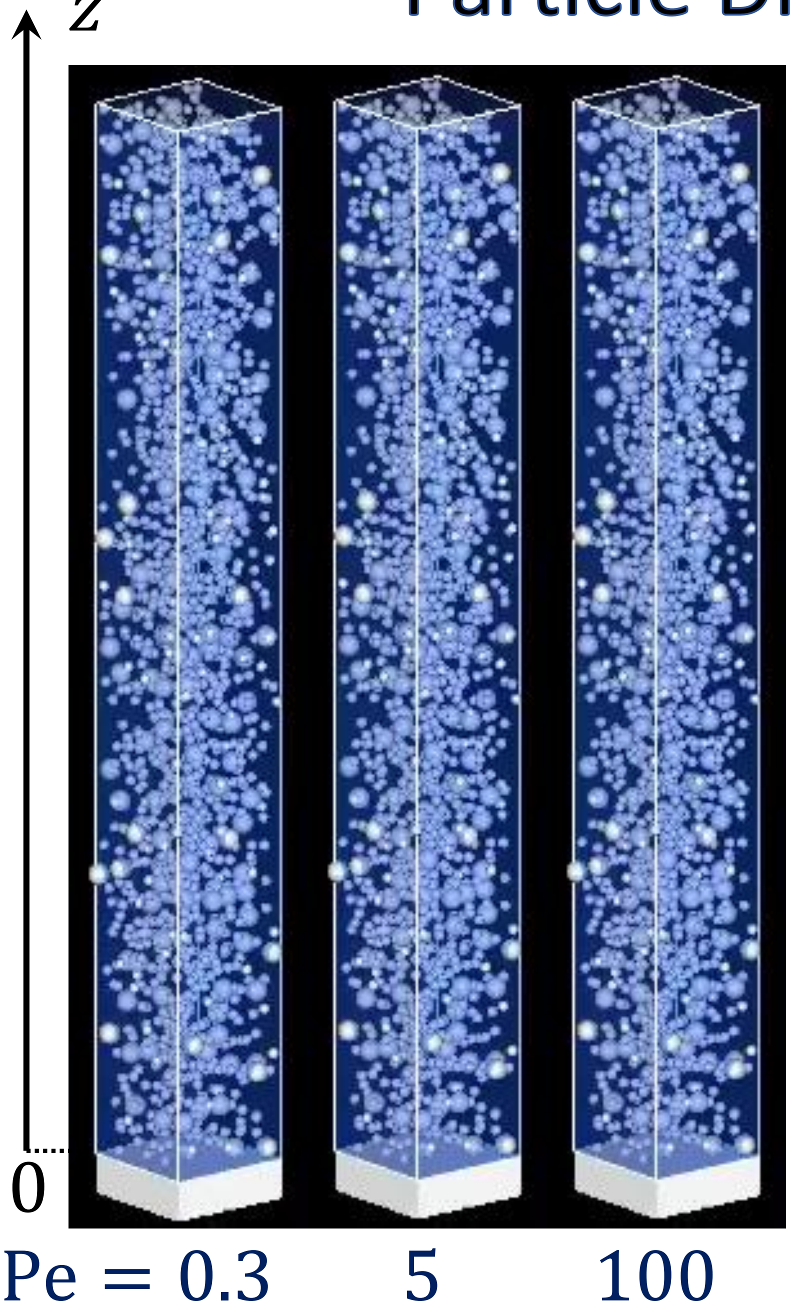
- Particle drying Péclet number (**L**)

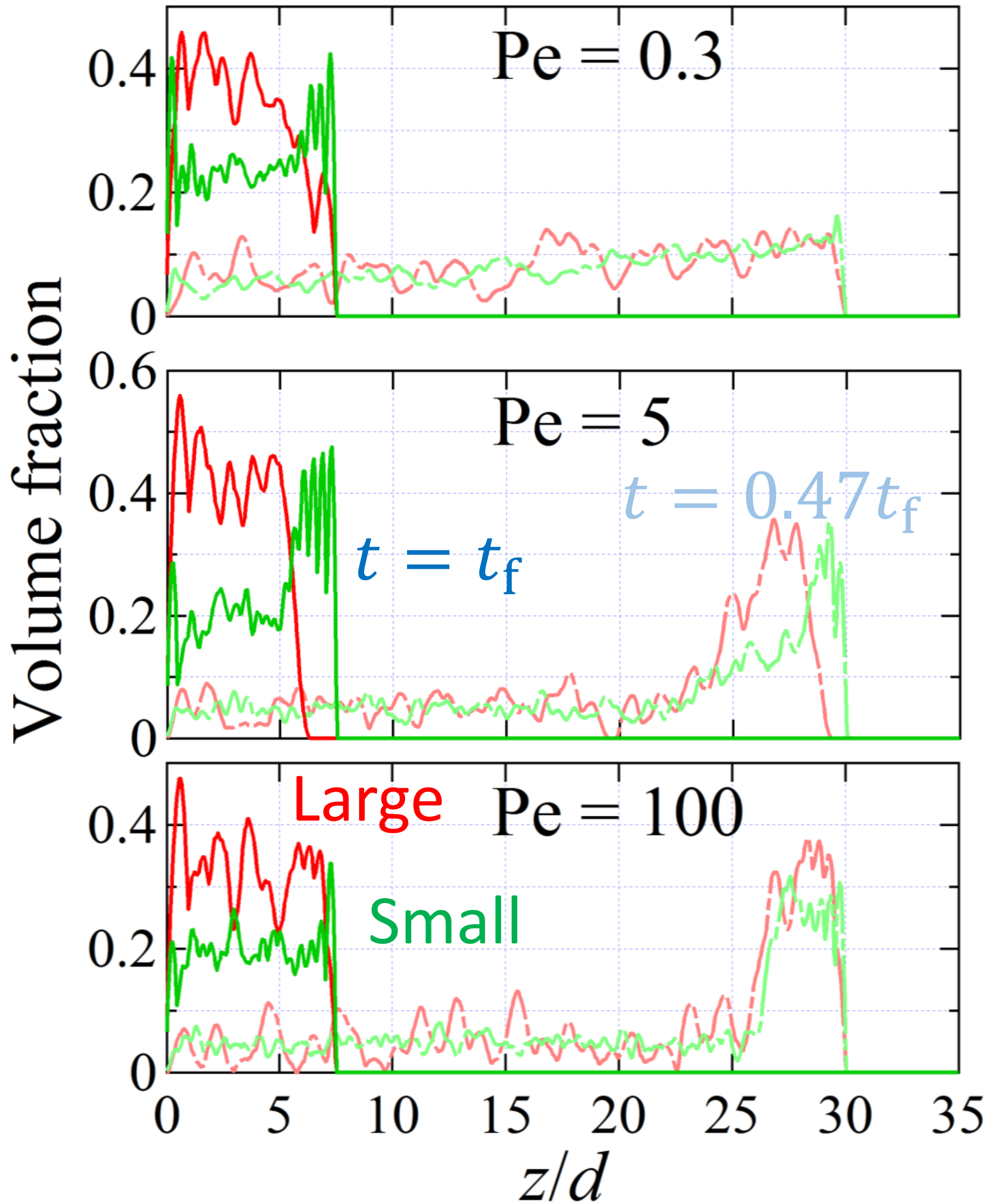
$$\mathrm{Pe} = \frac{(\text{Drying rate})}{(\text{Diffusion rate})} = \frac{v_\mathrm{e}}{D/d} = \frac{v_\mathrm{e} d}{D}$$



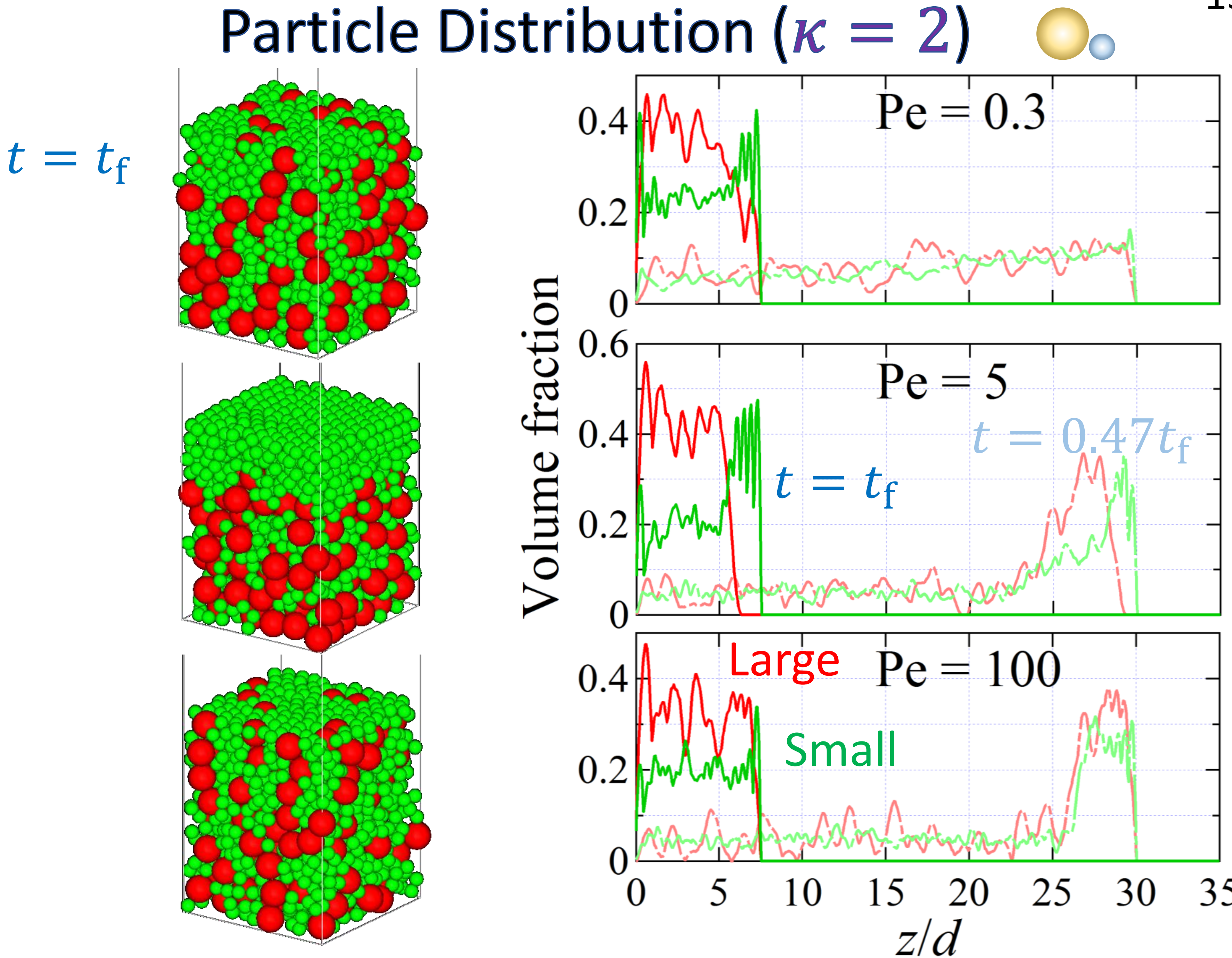
Simulation: $\mathrm{Pe} = 0.3 \sim 1000$

Particle Distribution ($\kappa = 2$)



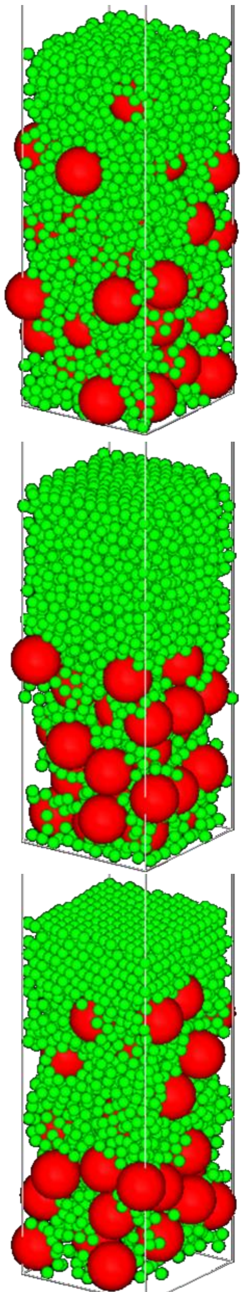


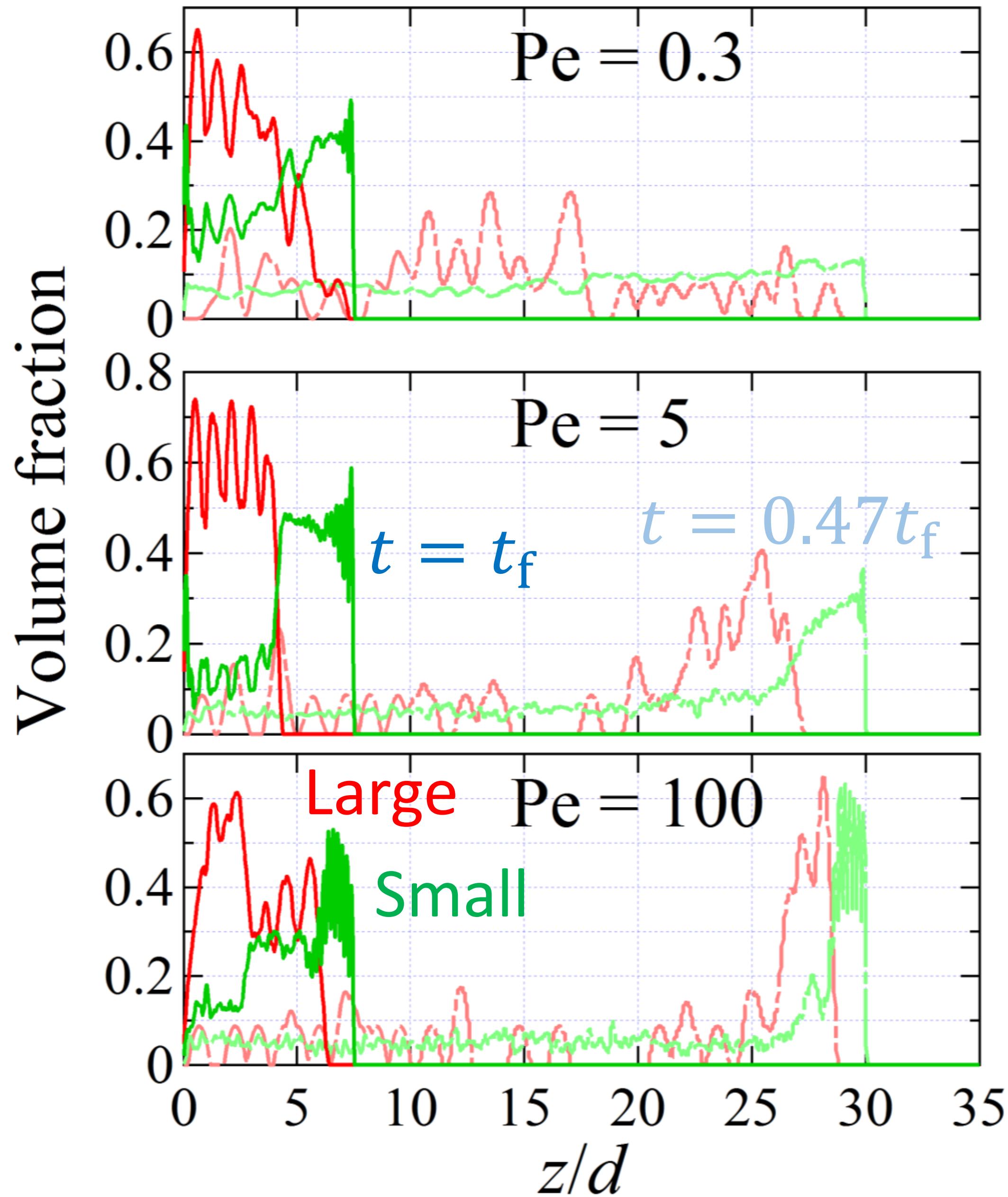
Particle Distribution ($\kappa = 2$)



Particle Distribution ($\kappa = 4$)

$t = t_{\mathrm{f}}$

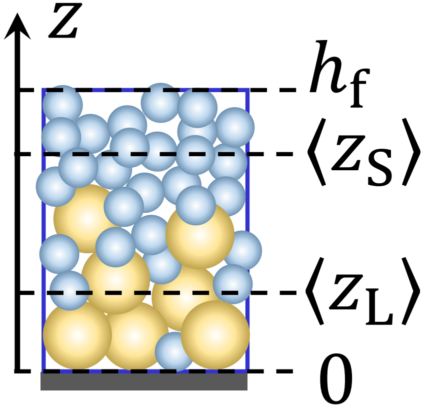


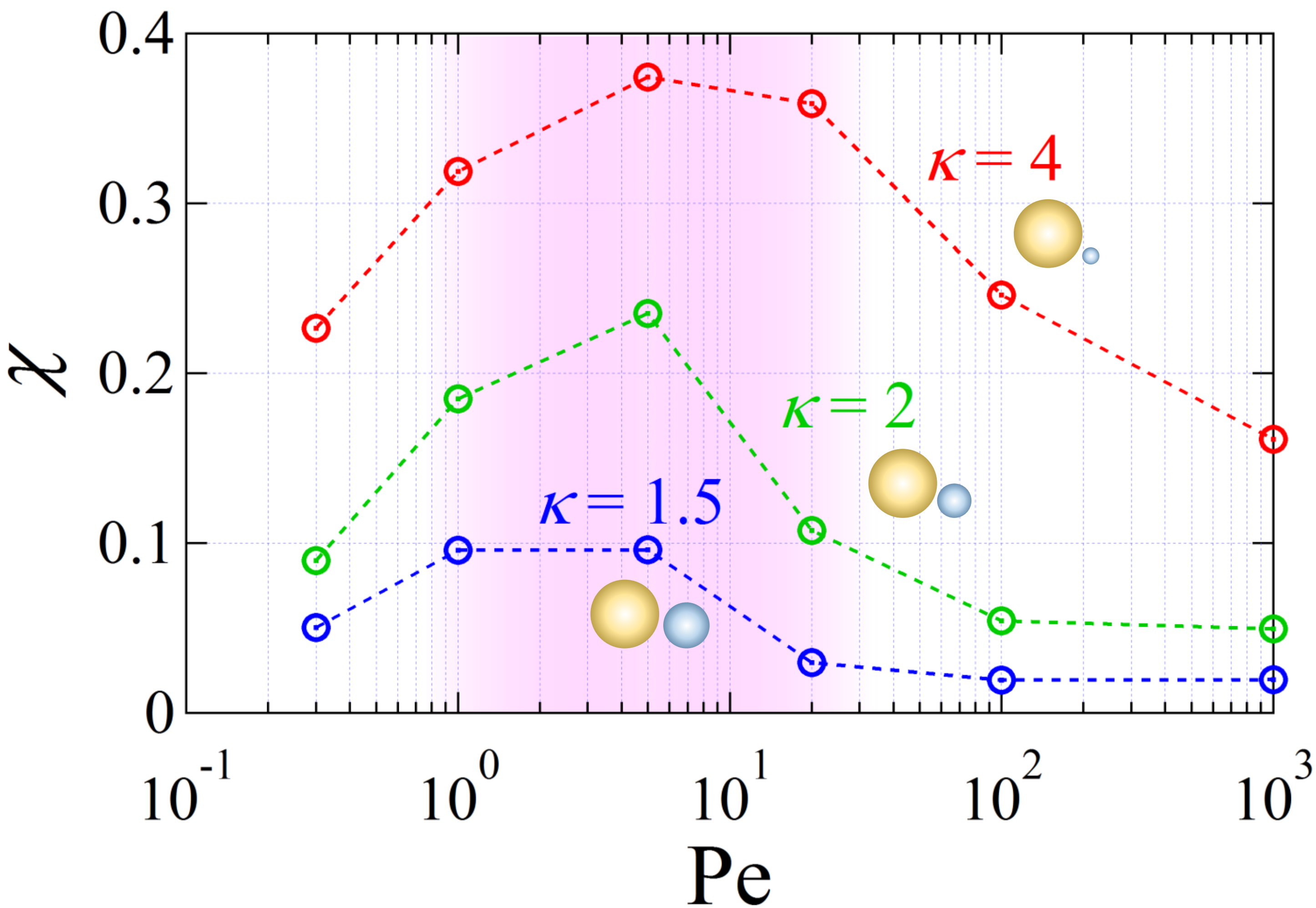


Segregation in Final State

Indicator of segregation: $\chi \equiv (\langle z_\mathrm{S}\rangle - \langle z_\mathrm{L}\rangle)/h_\mathrm{f}$

Average z-coordinate of the particles **L**: $\langle z_\mathrm{L}\rangle$ **S**: $\langle z_\mathrm{S}\rangle$





Summery

- SNAP enables us to visualize the structure formation of colloidal particles.

- The present analysis suggests that segregation can occur in the constant drying rate period.

- Segregation is enhanced by increasing particle size ratio.
- Segregation is maximized at Péclet number Pe = 1～10.