二峰性微粒子分散液の乾燥における偏析現象のメカニズム

Mechanism of Segregation in Drying Bimodal Colloidal Suspensions

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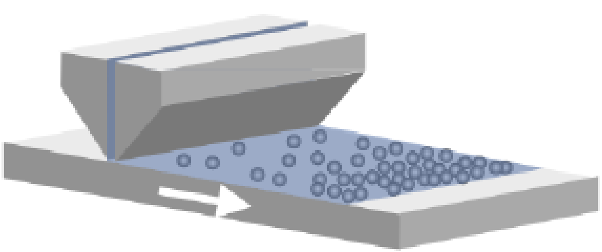
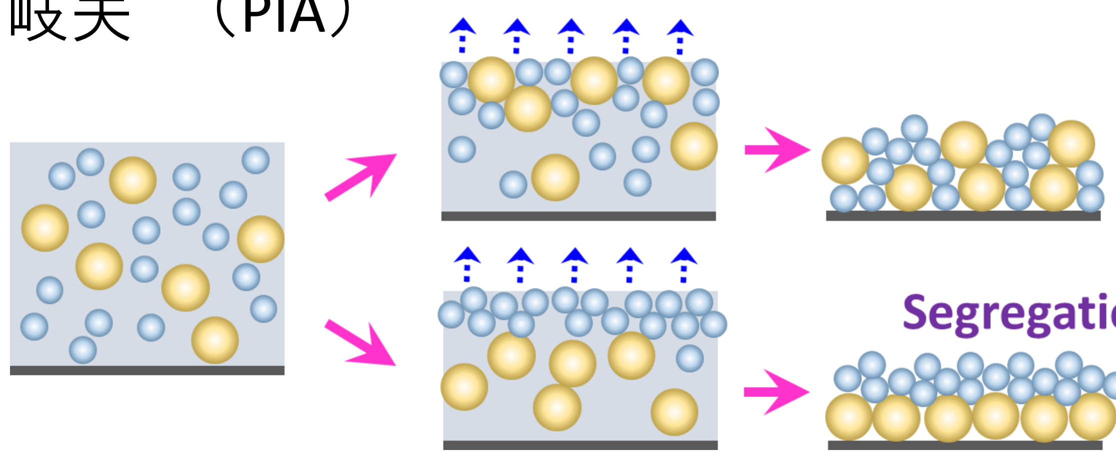
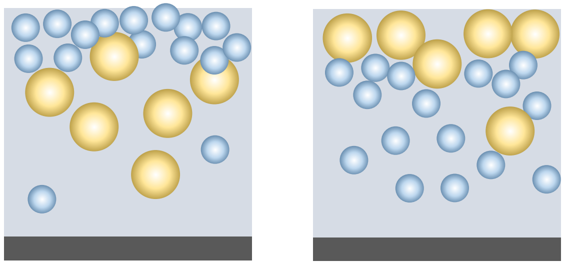


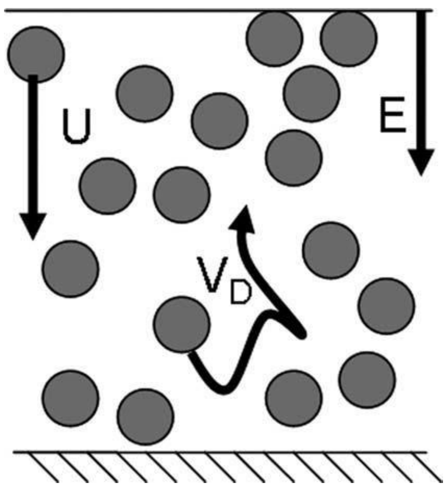
Coating, **Drying**

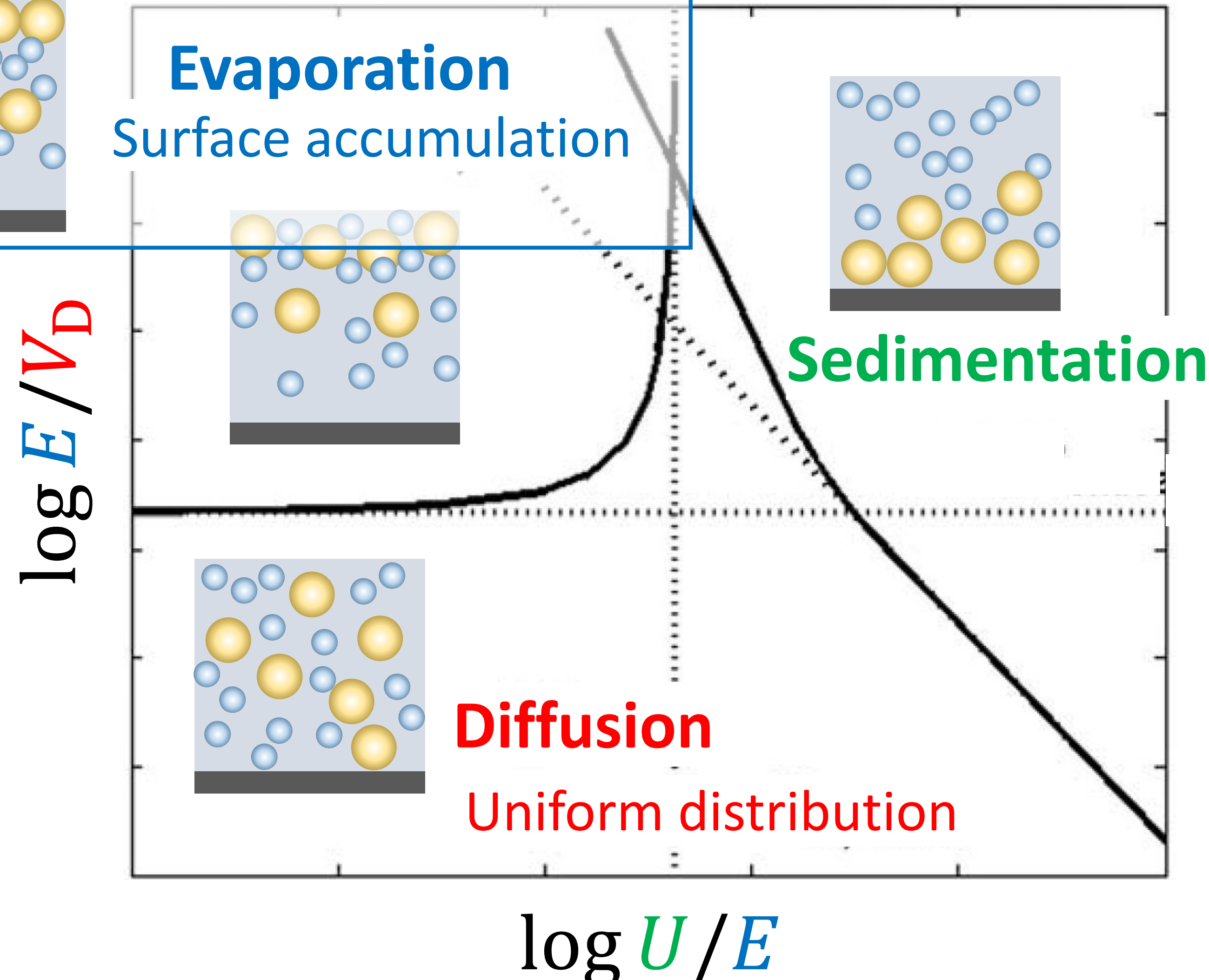


Particle Distribution during Drying

Segregation?







<u>Velocity</u>

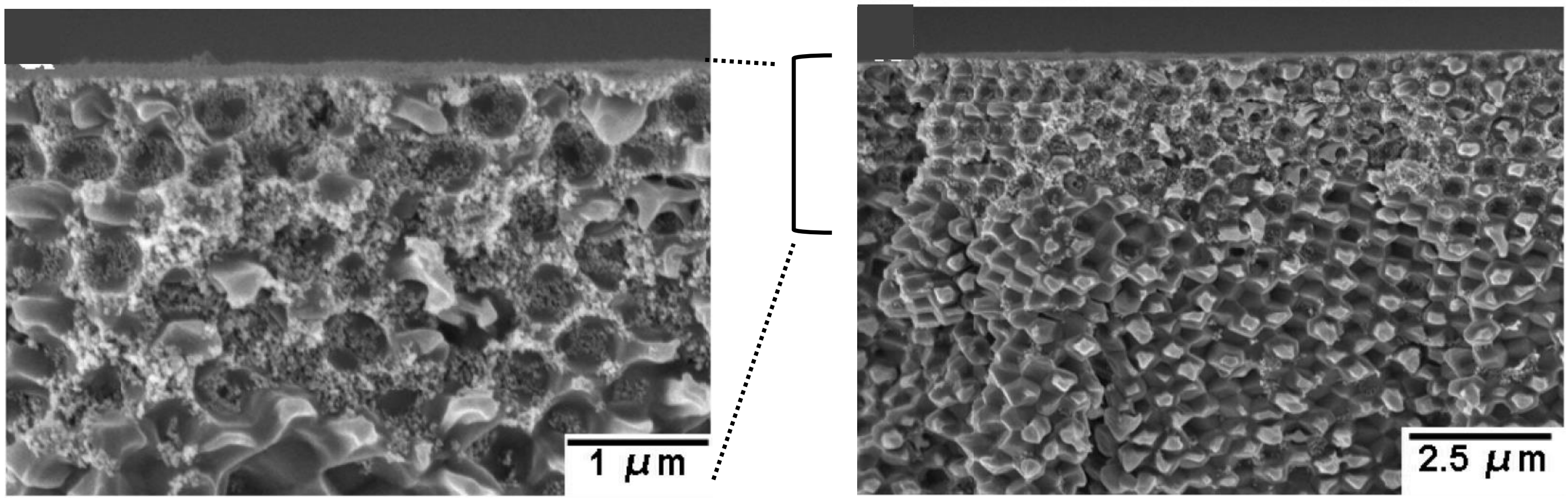
Sedimentation: U

Evaporation: E

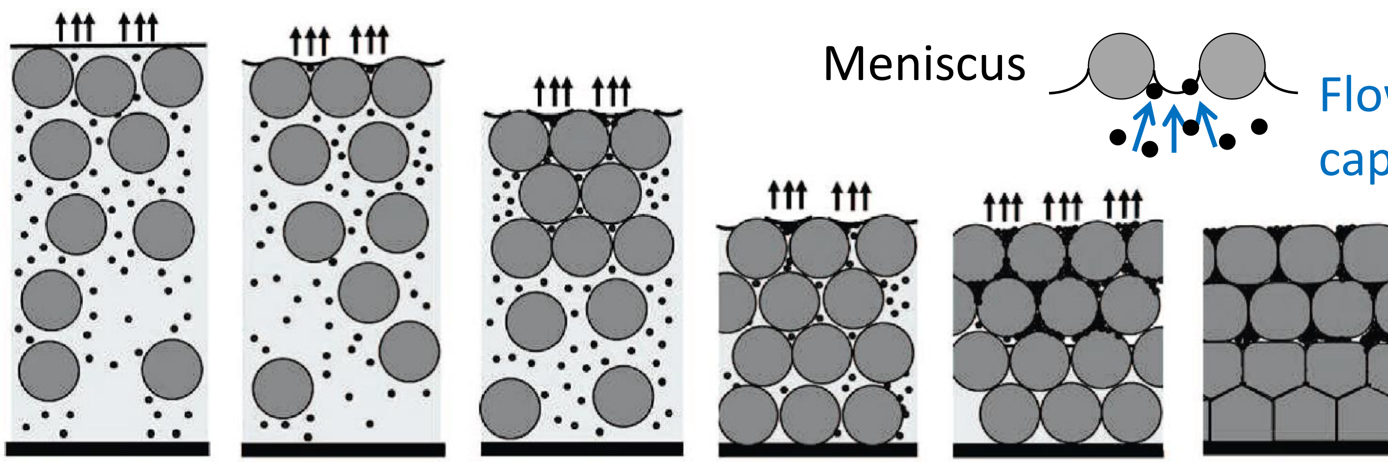
Brownian diffusion: V_{D}

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

A Proposed Mechanism



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



Luo et al., Langmuir (2008).

Drying Curve of Colloidal Suspensions

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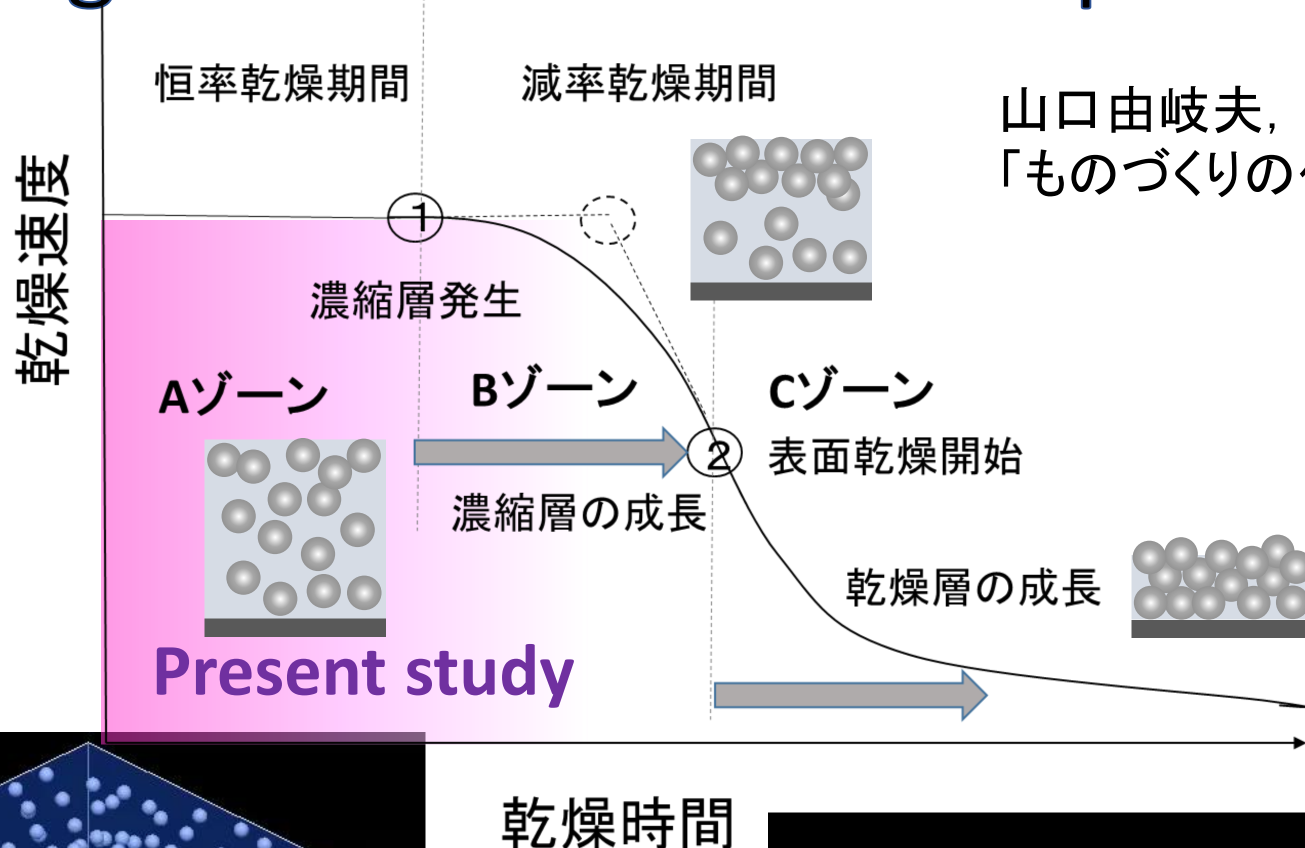
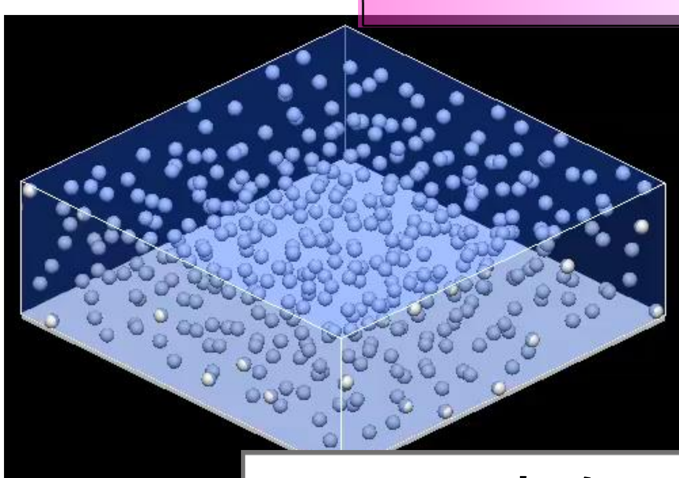
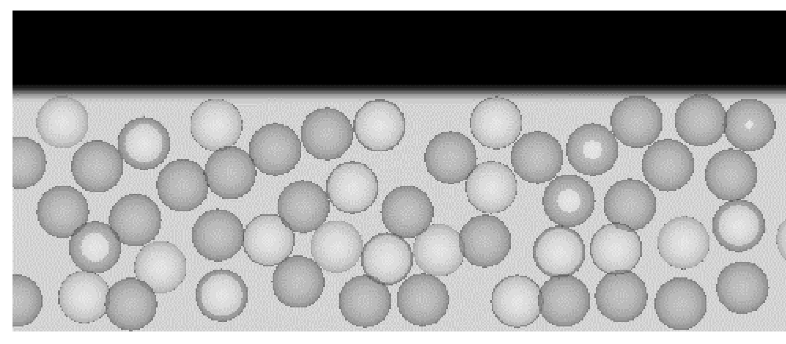
「ものづくりの化学工学」







SNAP研究会 to get detailed information

Objective

- Elucidation of the mechanism of segregation

- Analysis using a simple model
  - Brownian motion of particles
  - Free surface moving at constant rate
  - No consideration of gravity and fluid flow

Langevin Equation

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

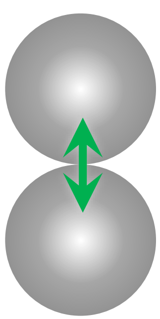
Position $\dot{\boldsymbol{R}}_i = \boldsymbol{V}_i$

Random force: Sotchastic variables obeying the Gaussian distribution

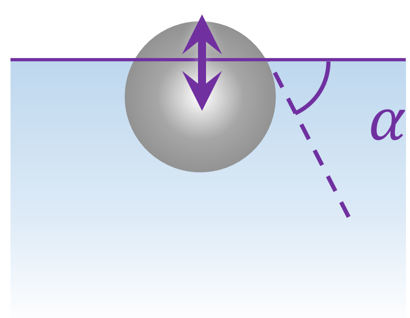
$$\langle F_{i\alpha}^{\mathrm{R}}(t)\rangle = 0$$

$$\langle F_{i\alpha}^{\mathrm{R}}(0)F_{i\beta}^{\mathrm{R}}(t)\rangle = 2\xi k_{\mathrm{B}}T\delta_{\alpha\beta}\delta(t) \qquad \xi = 3\pi\eta d$$

Contact force



Vertical capillary force

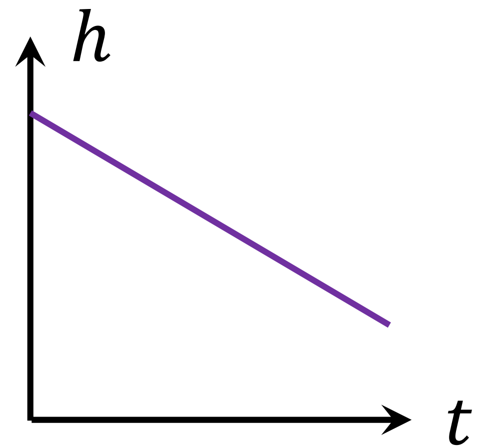


α : Contact angle

Gravity and **fluid flow** are not considered.

Particle Drying Péclet Number

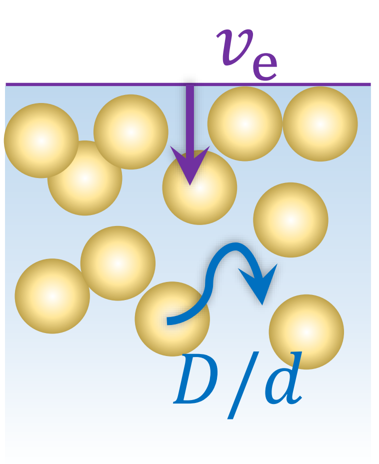
Film height $h(t) = h_0 - v_e t$



- Constant evaporation rate v_e

- Diffusion coefficient (Stokes-Einstein relation)

$$D = \frac{k_B T}{3\pi\eta d}$$



Particle drying Péclet number

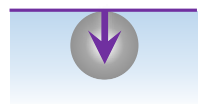
$$\mathrm{Pe} = \frac{(\text{Evaporation rate})}{(\text{Diffusion rate})} = \frac{v_e}{D/d} = \frac{v_e d}{D}$$

Simulation Conditions

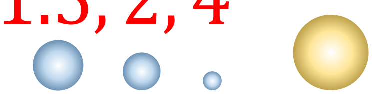
- Particle diameter **L**: d **S**: $\kappa^{-1}d$

- Initial volume fraction
  L: 0.05 **S**: 0.05 (Total : 0.1)

- Contact angle $\alpha = 0$

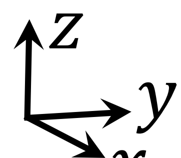


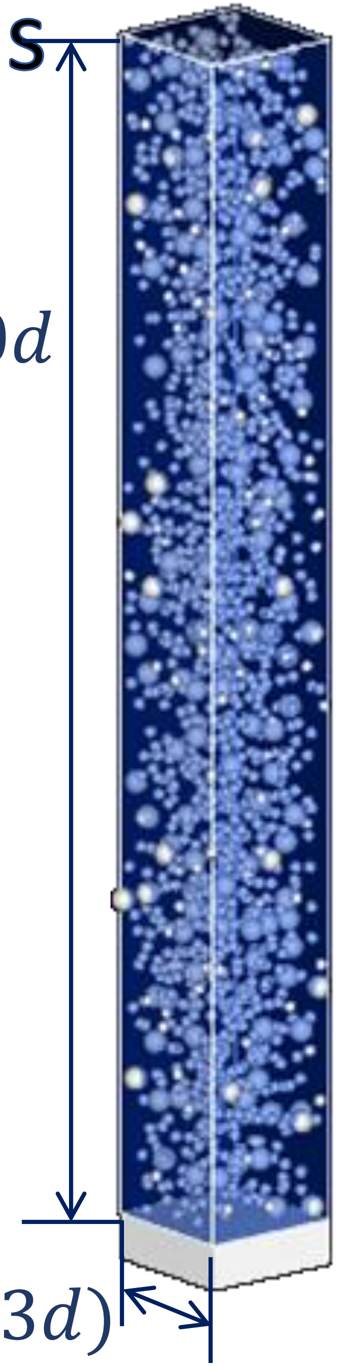
- Diameter ratio (**L**/**S**) $\kappa = 1.5, 2, 4$



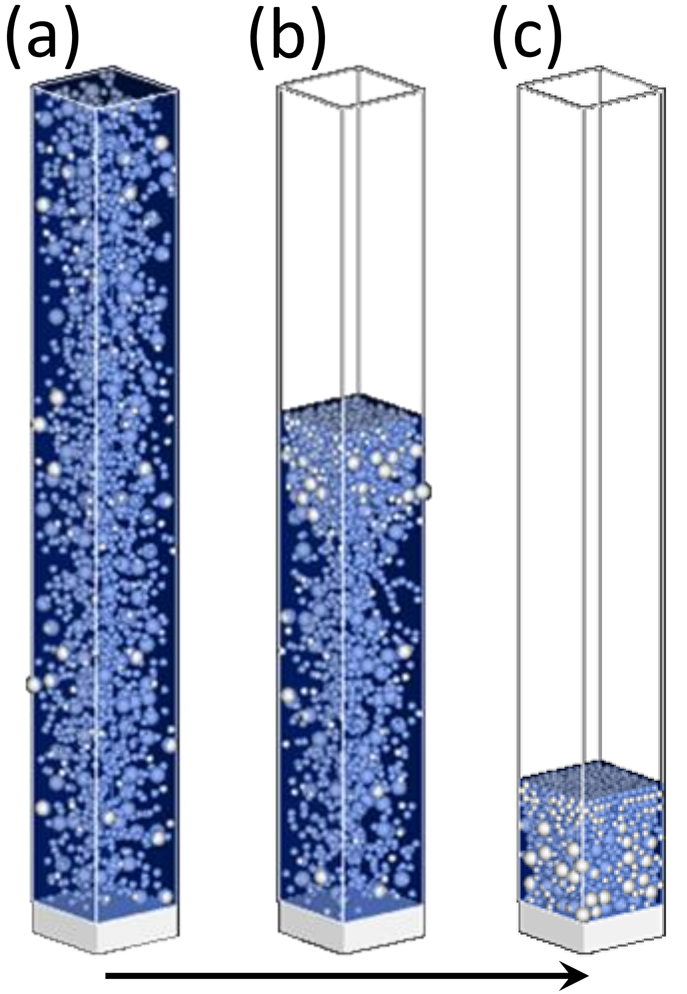
- Particle drying Péclet number (**L**)
  $\mathrm{Pe} = 0.3 \sim 1000$

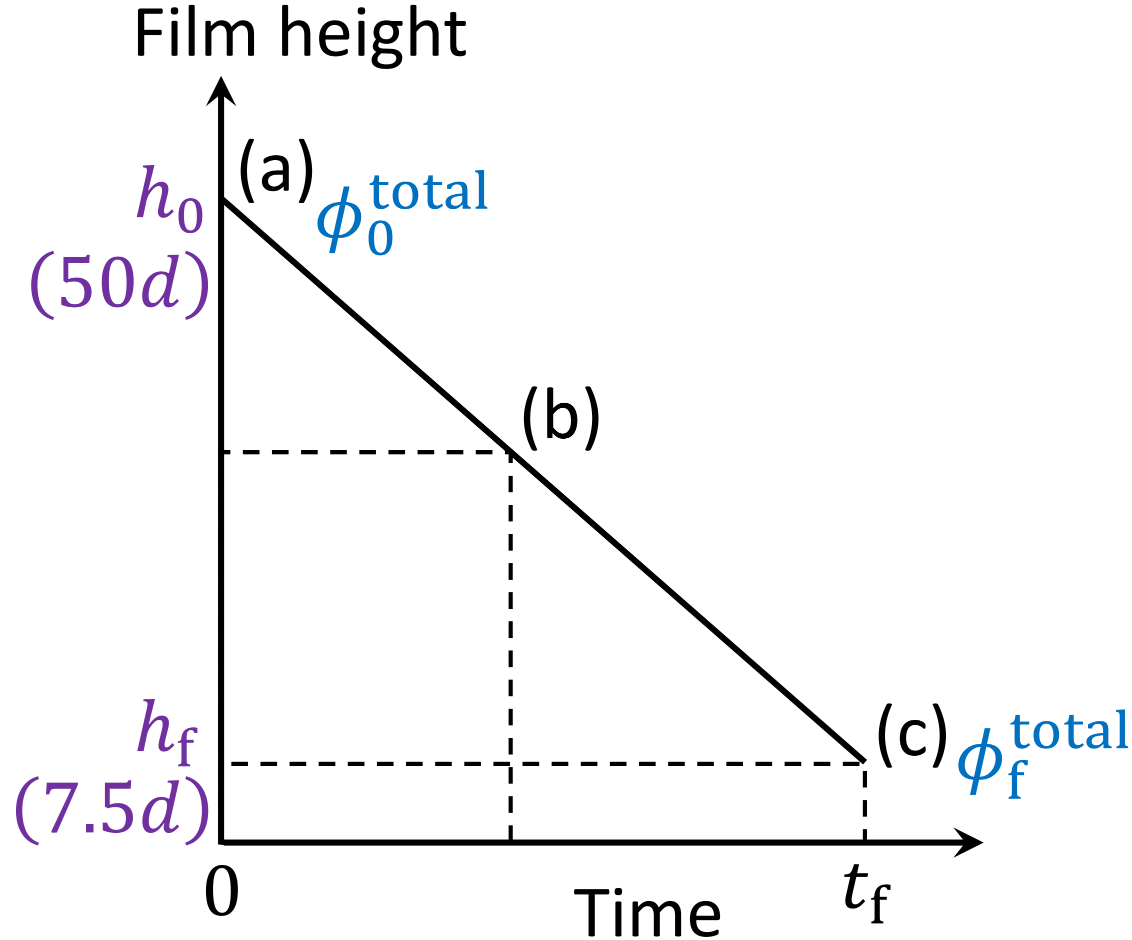
Periodic boundaries: x, y





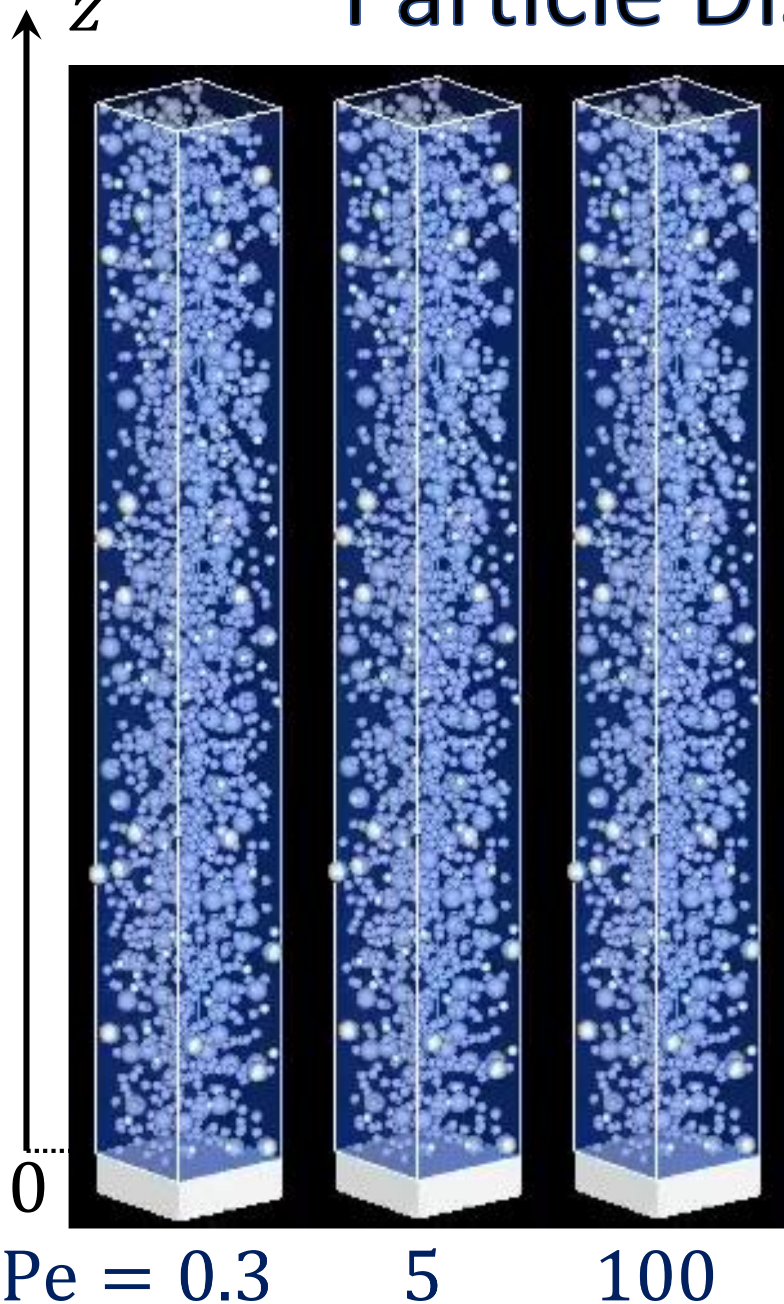
Simulation Conditions

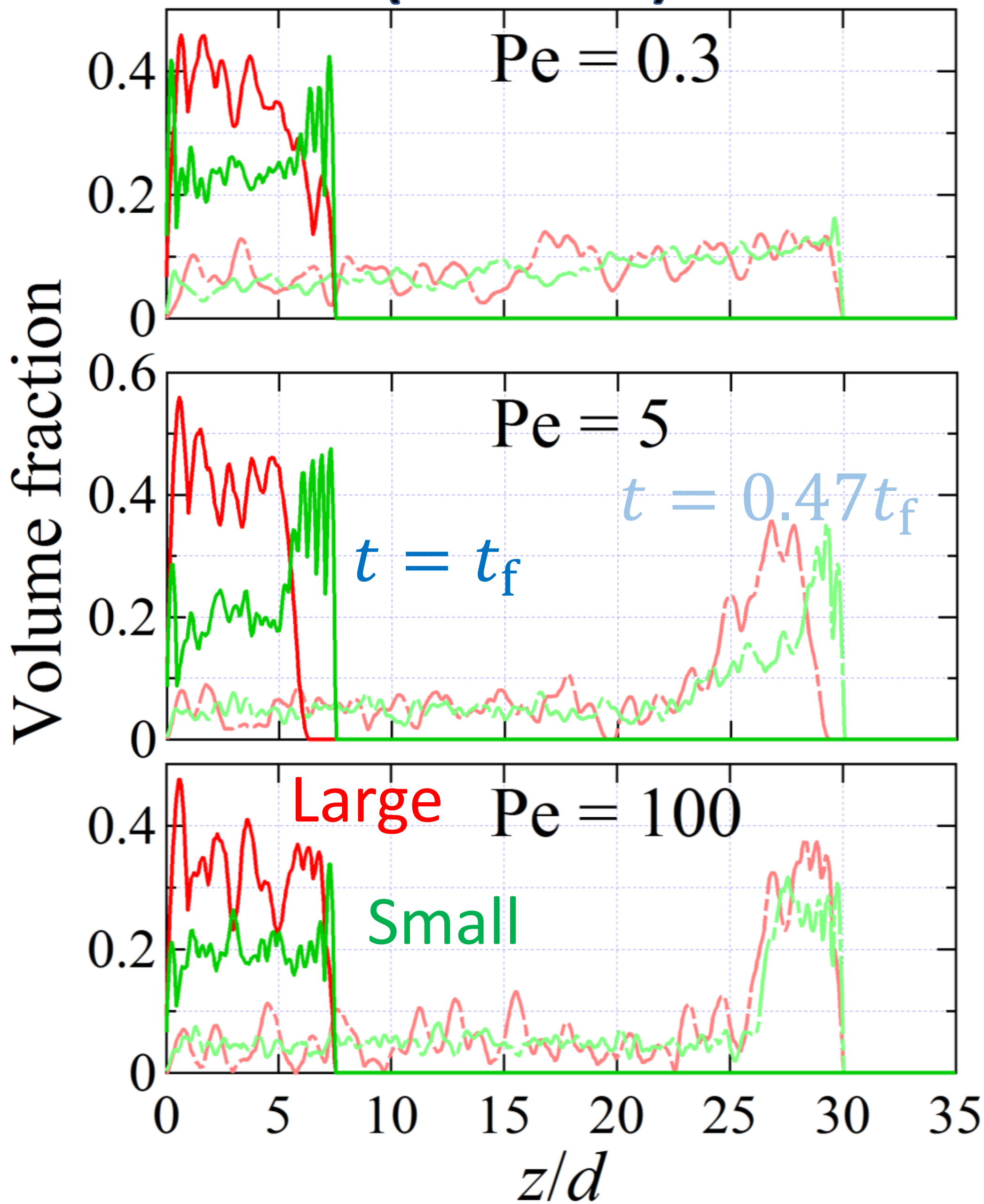




Final state $h_\mathrm{f} = \frac{3}{20} h_0 = 7.5d \quad \phi_\mathrm{f}^{\mathrm{total}} = \frac{20}{3} \phi_0^{\mathrm{total}} \approx 0.67$

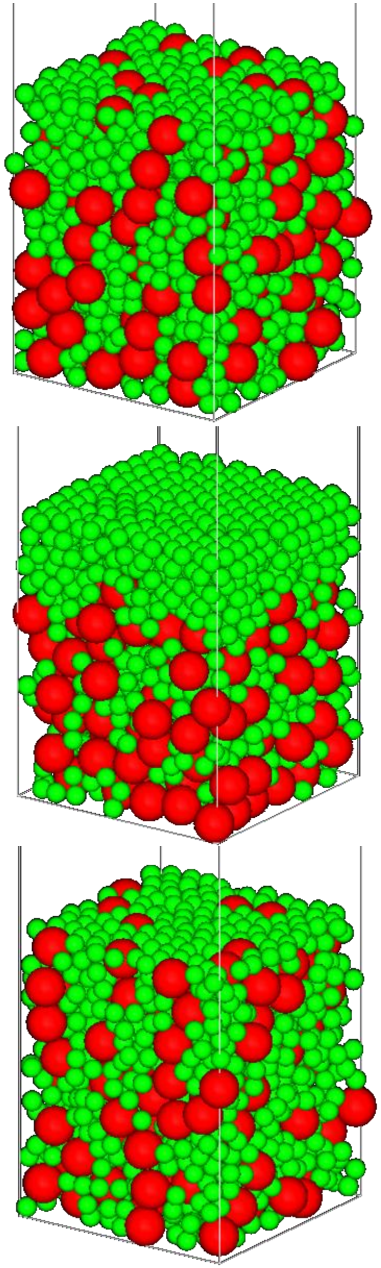
Particle Distribution ($\kappa = 2$)

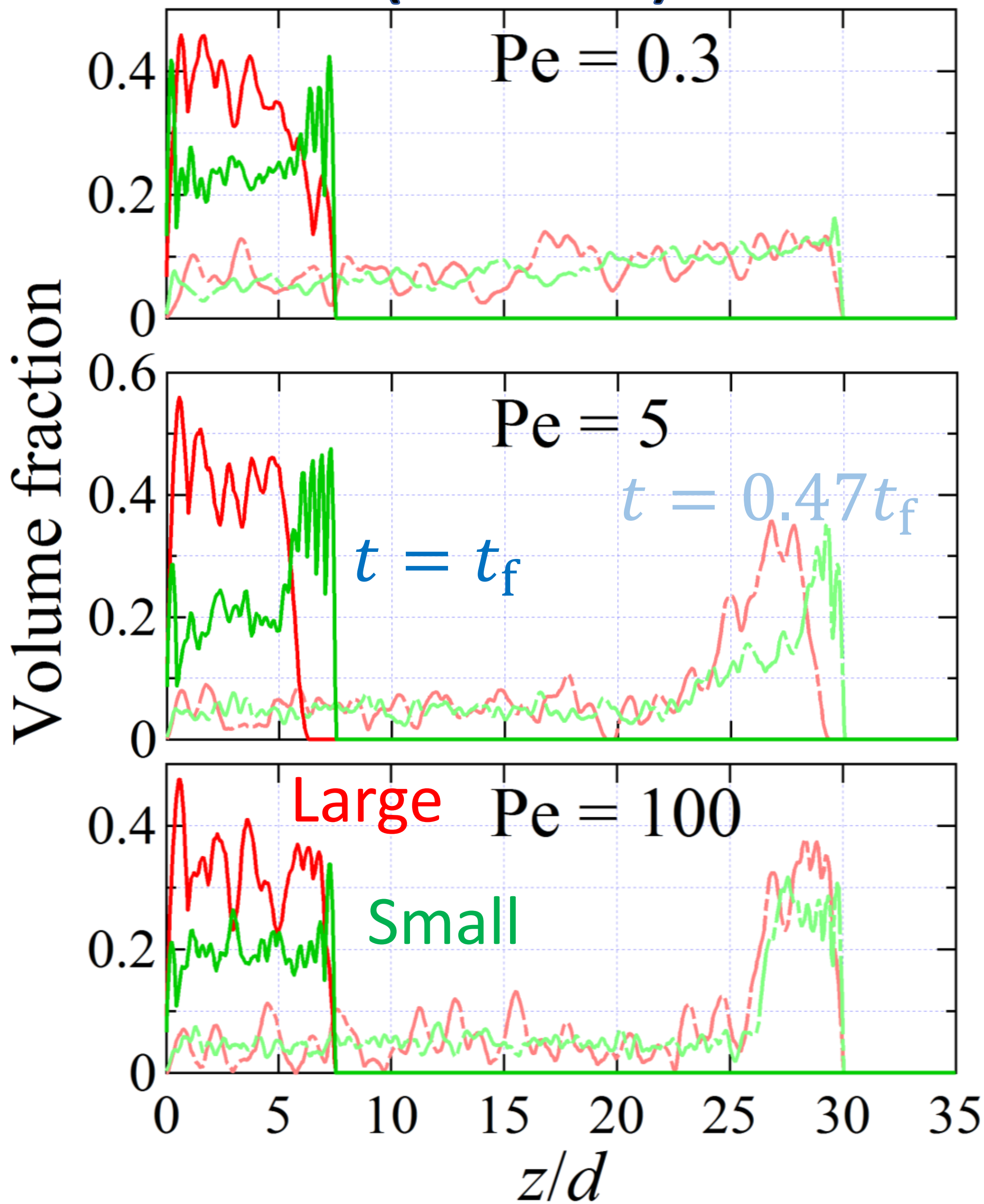




Particle Distribution ($\kappa = 2$)

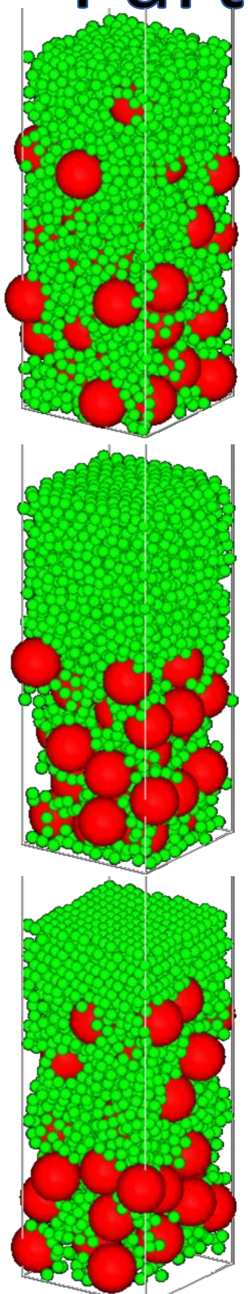
$t = t_f$

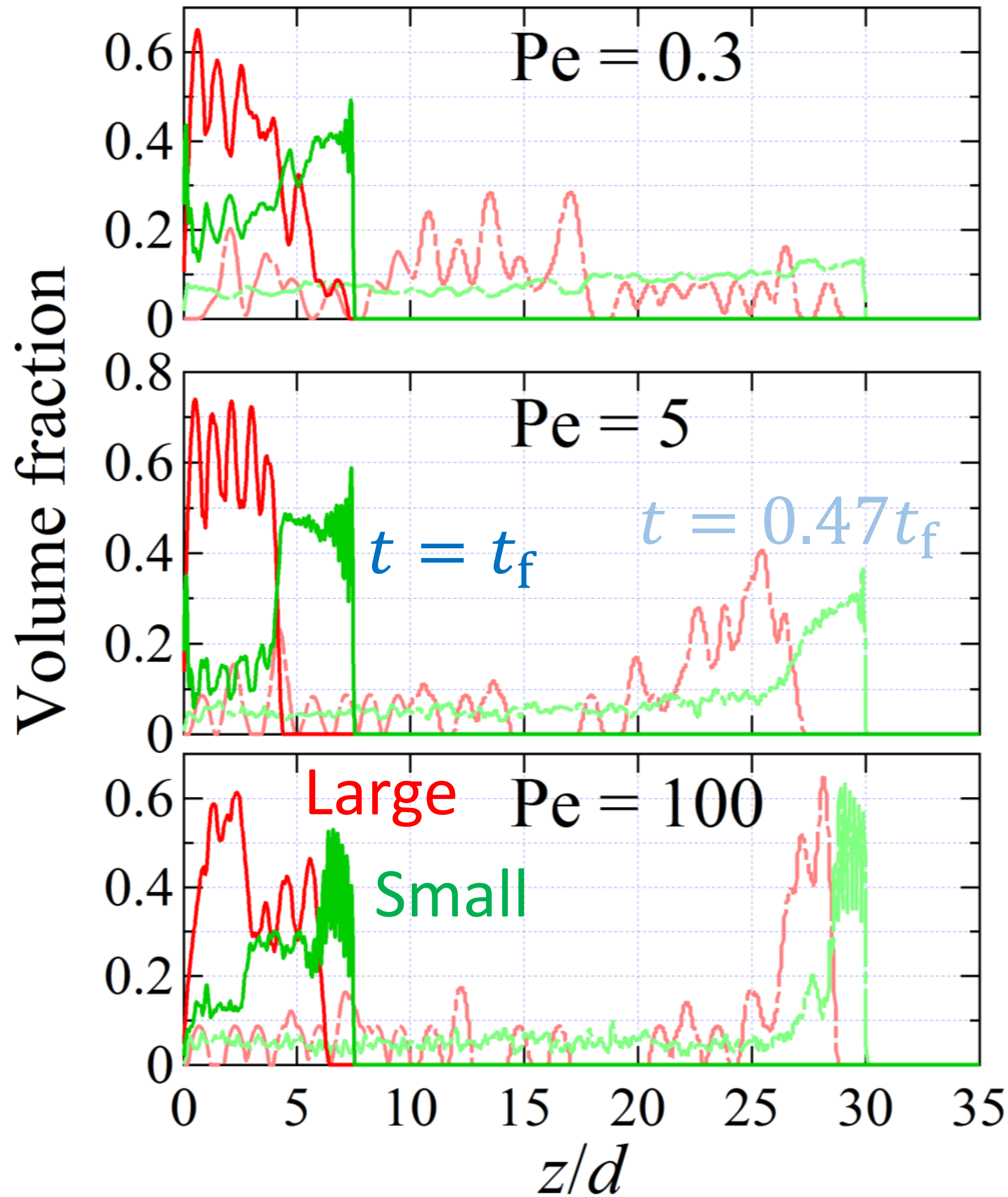




Particle Distribution ($\kappa = 4$)

$t = t_\mathrm{f}$

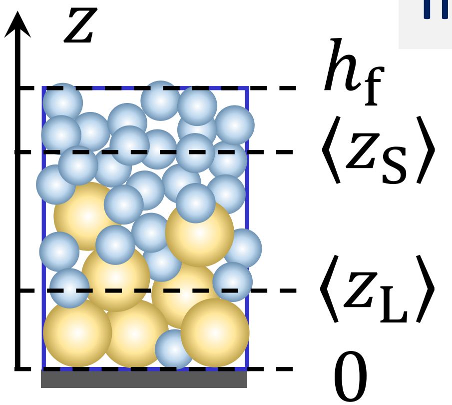


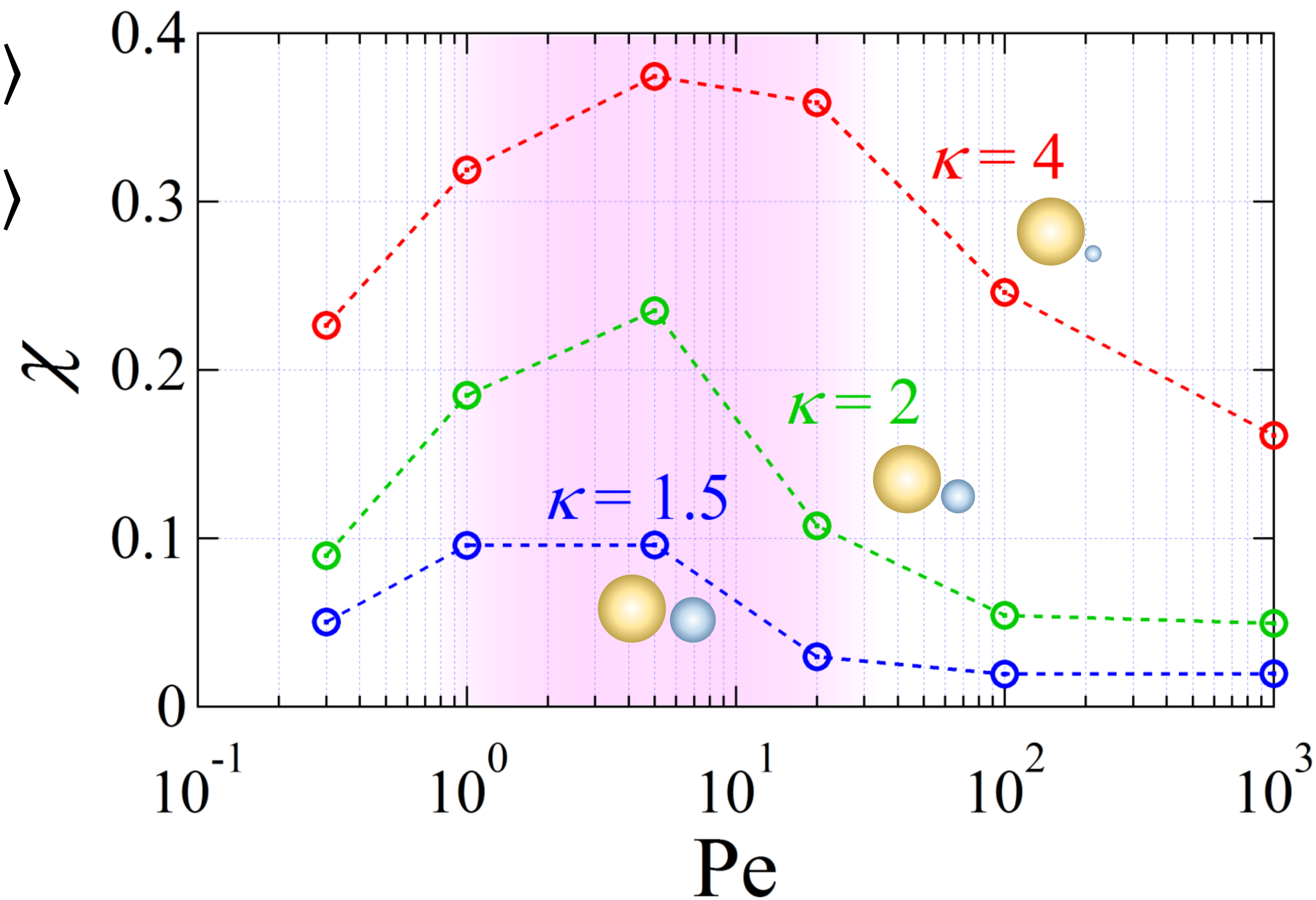


Segregation in Final State

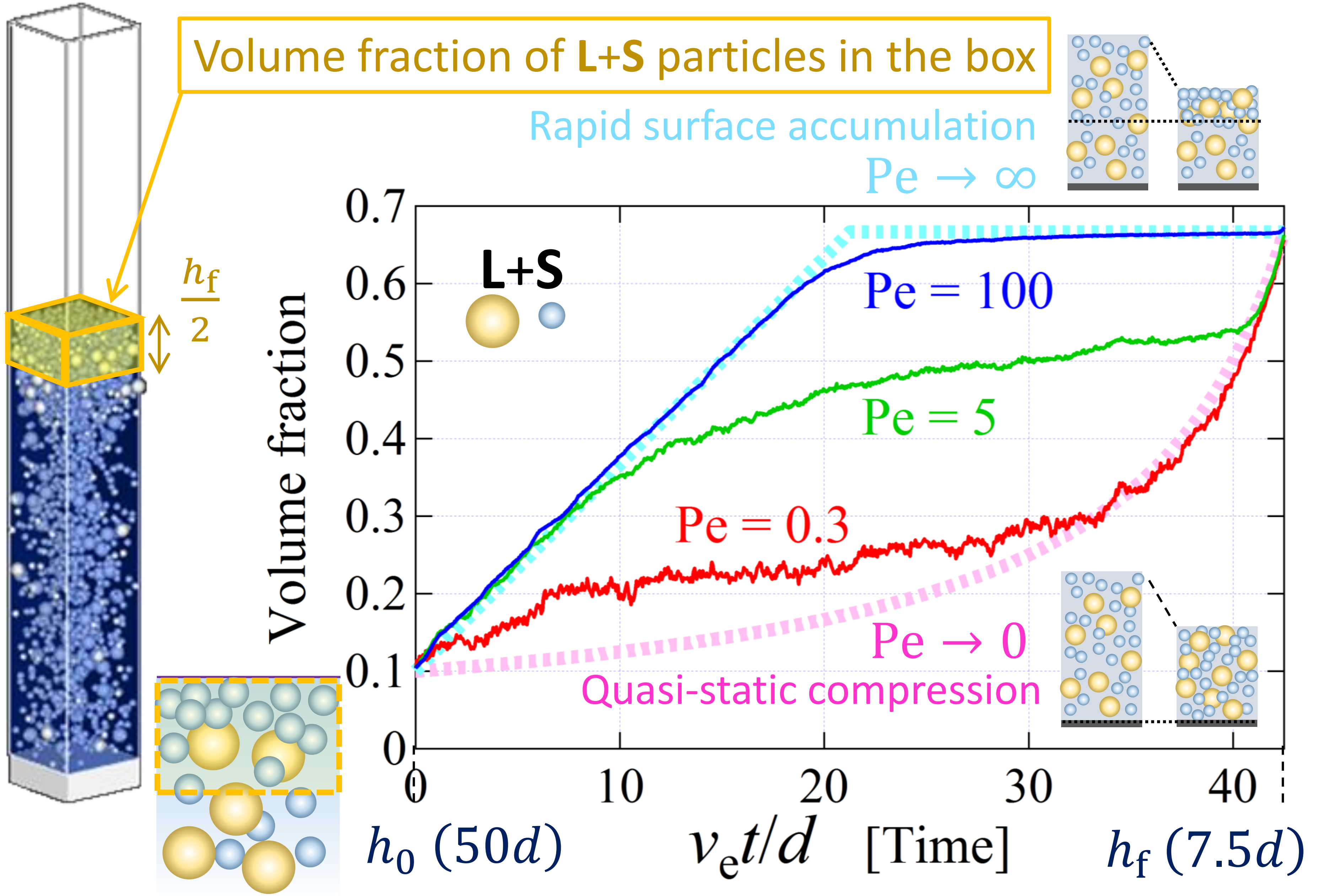
Average z-coordinate of the particles **L**: $\langle z_L \rangle$ **S**: $\langle z_S \rangle$

Indictor of segregation: $\chi \equiv (\langle z_S \rangle - \langle z_L \rangle)/h_f$



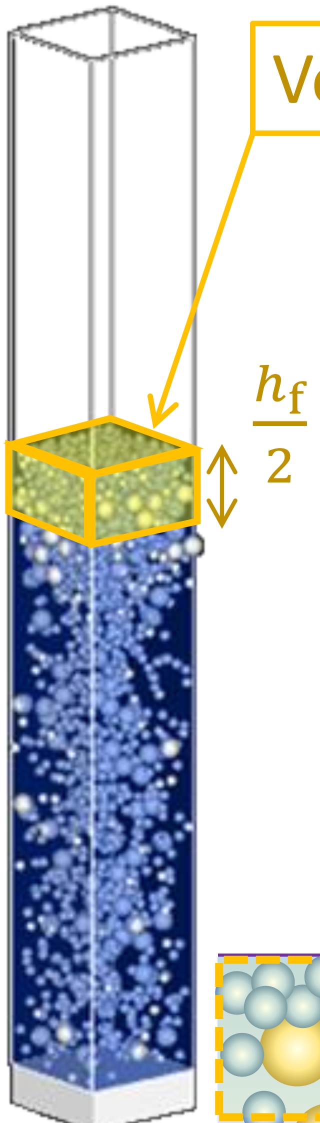


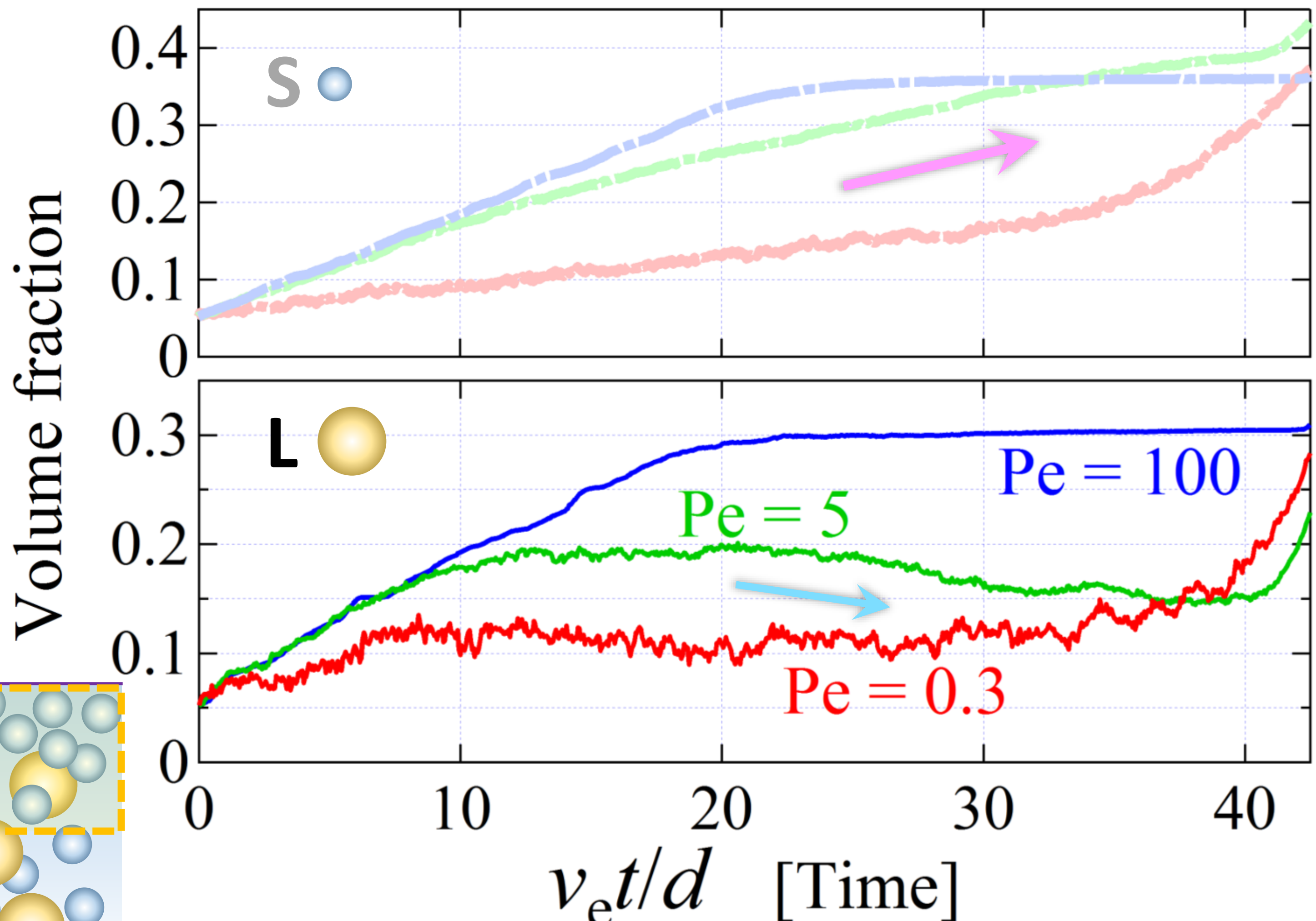
Surface Accumulation ($\kappa = 2$)

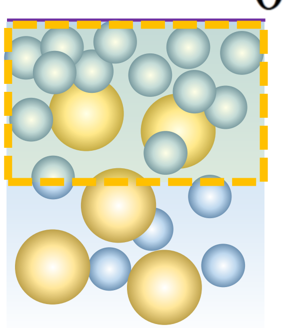


Surface Accumulation ($\kappa = 2$)

Volume fraction of **L** (**S**) particles in the box

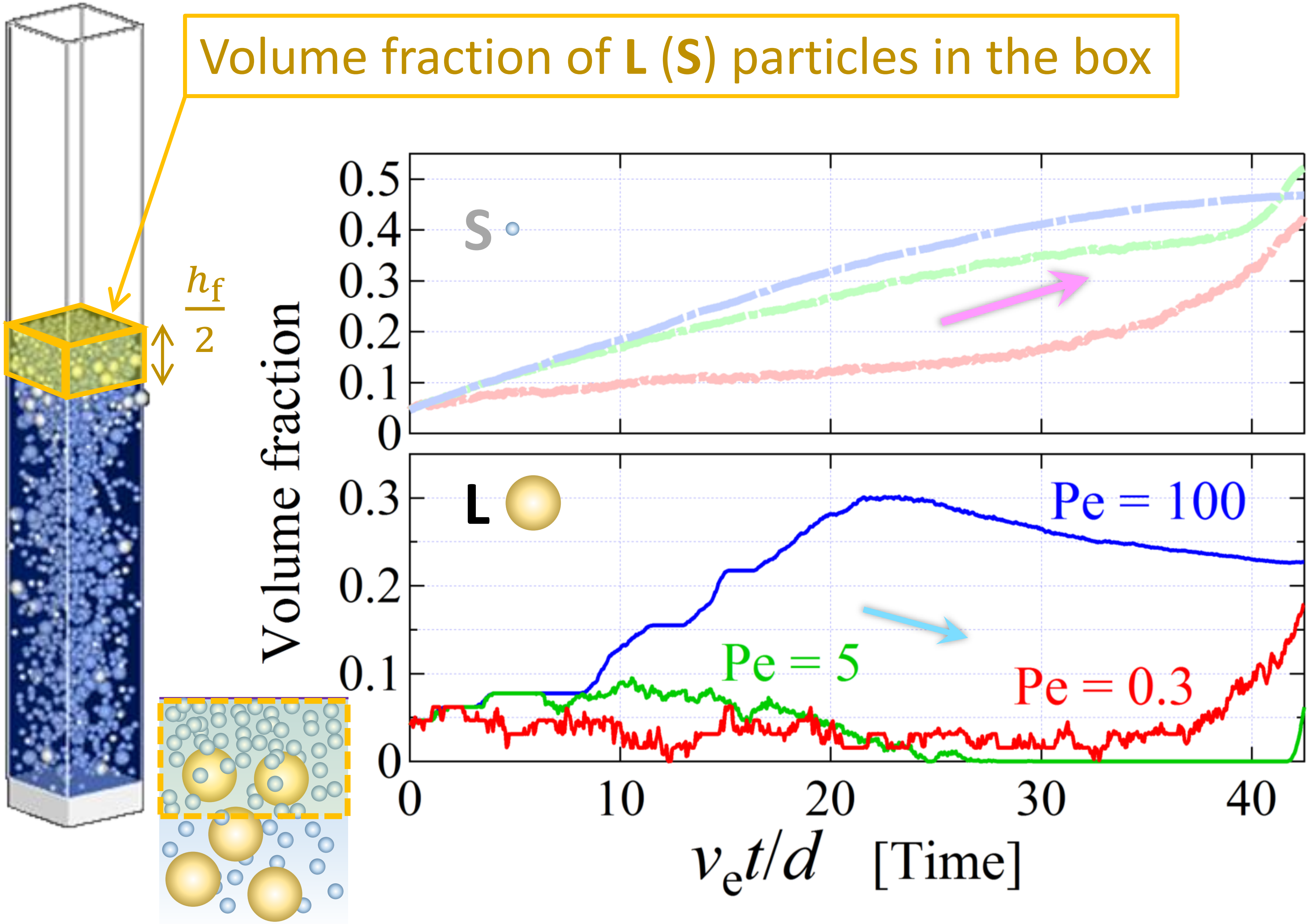






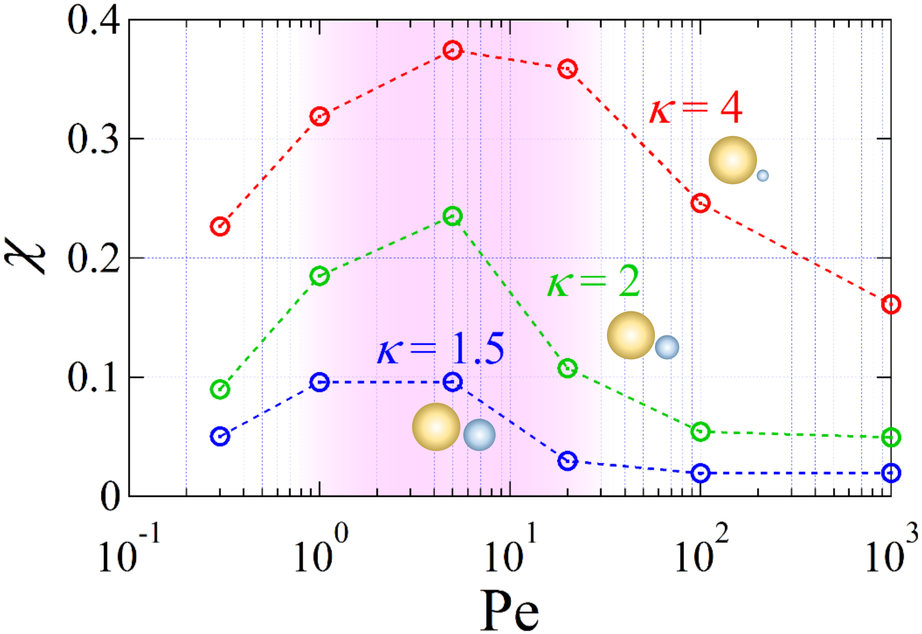
Surface Accumulation ($\kappa = 4$)

Volume fraction of **L** (**S**) particles in the box



Summary

- Segregation is reproduced by the simple model without gravity and fluid flow.
- The condition that segregation is enhanced is obtained as right figure.



- **L** particles are diffused by accumulated **S** particles. This diffusion is suppressed at low/high Péclet number.
  - ・Low Pe → Less particle accumulation
  - ・High Pe → Dense particle accumulation