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Particle-scale modeling of the drying characteristics of colloidal suspensions

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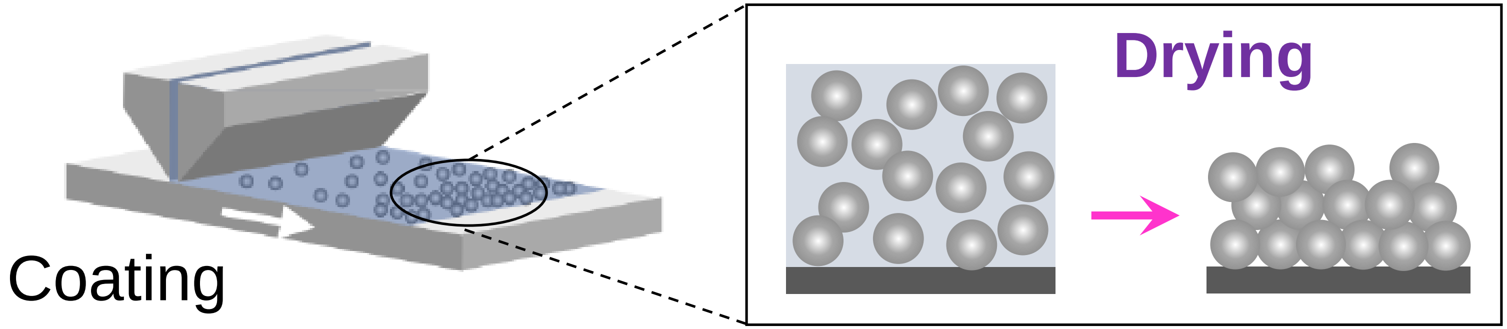
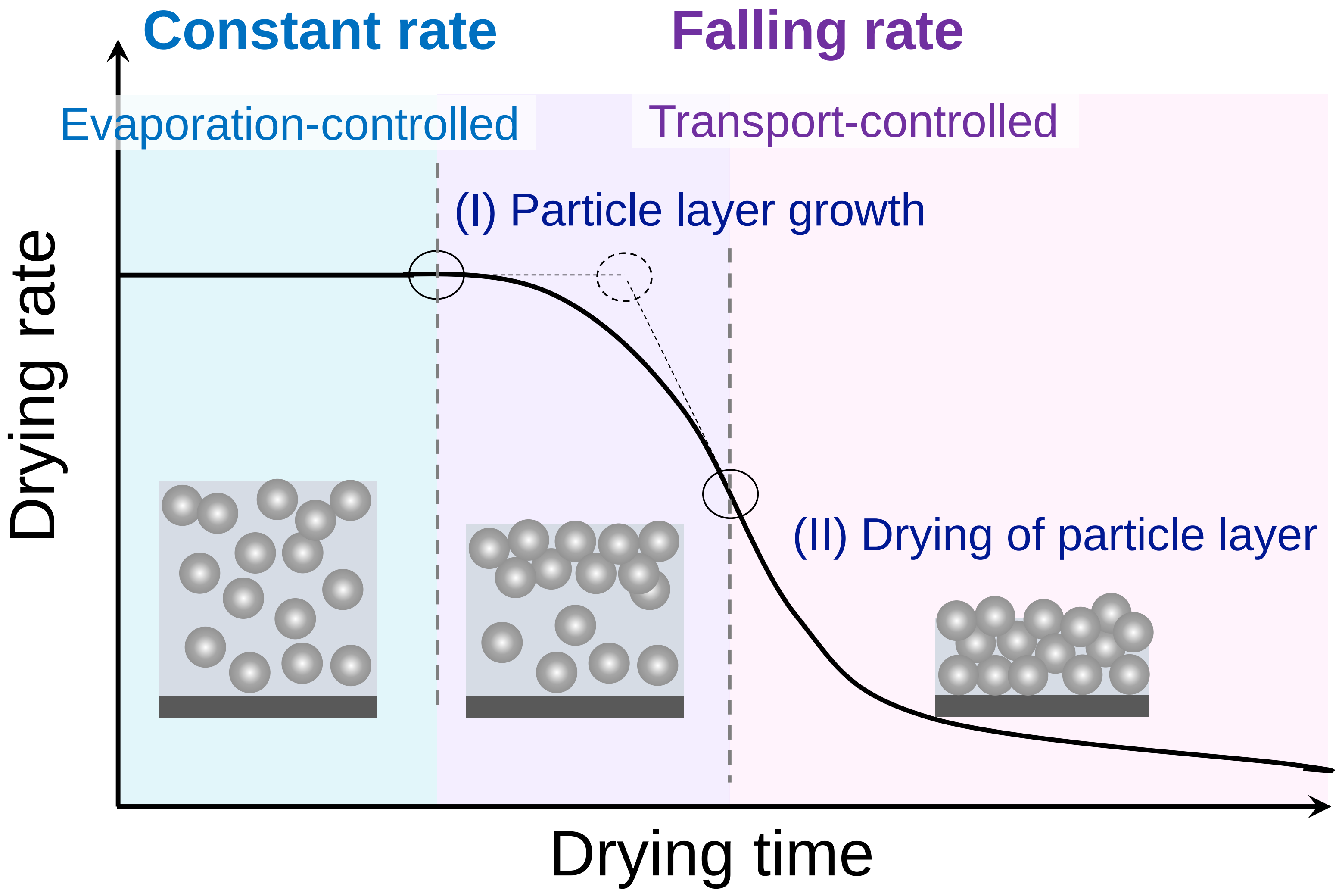


Drying Curve of Colloidal Suspensions

Drying rate ↔ Structure

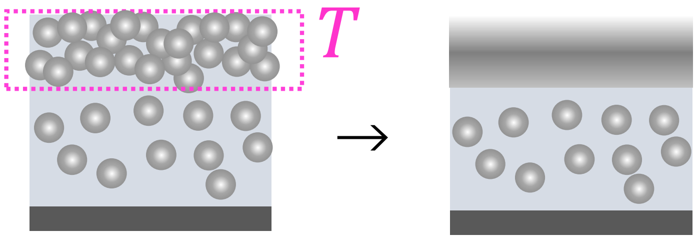


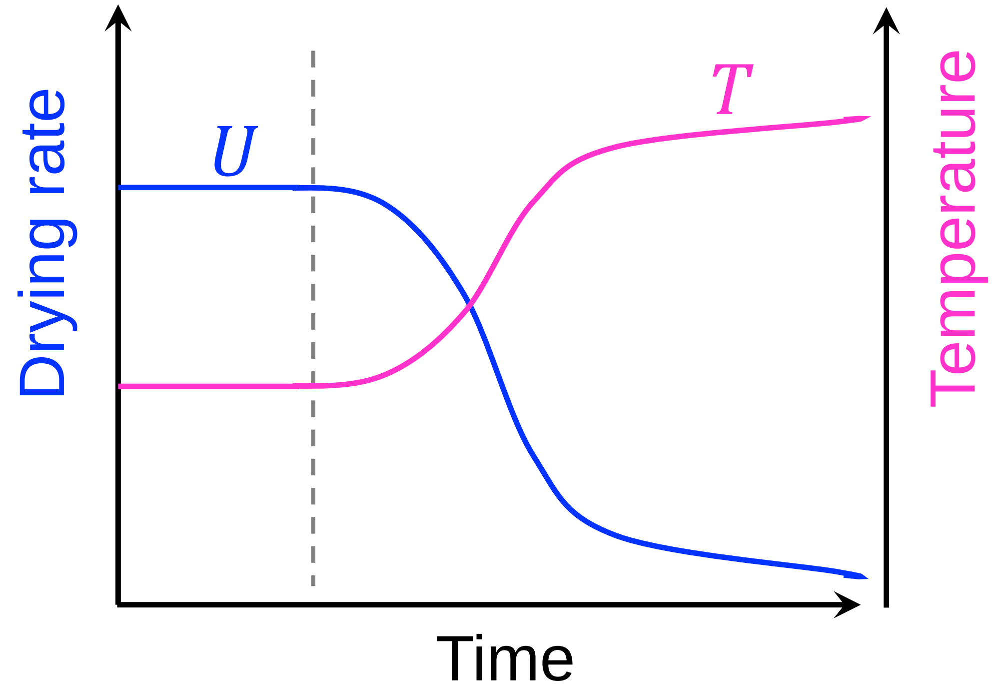
Skinning

Heat balance

$$\rho U \Delta H_{\mathrm{v}} = h(T - T_{\mathrm{ex}})$$

Liquid density: ρ
Latent heat: ΔH_{v}
Heat transfer coefficient: h
Drying temperature: T_{ex}





Drying rate falling → Temperature rising
→ Skinning (Thermal degradation at surface)

To avoid skinning:

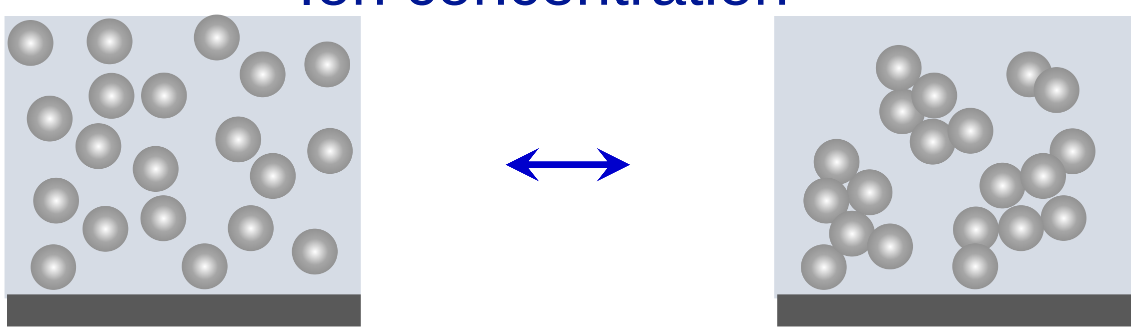
- Control of drying temperature according to drying rate
- Prevention of drying rate falling

Objective

- Construction of a model to calculate the drying curve of colloidal suspensions

- Control of drying curves by dispersion/aggregation

Ion concentration

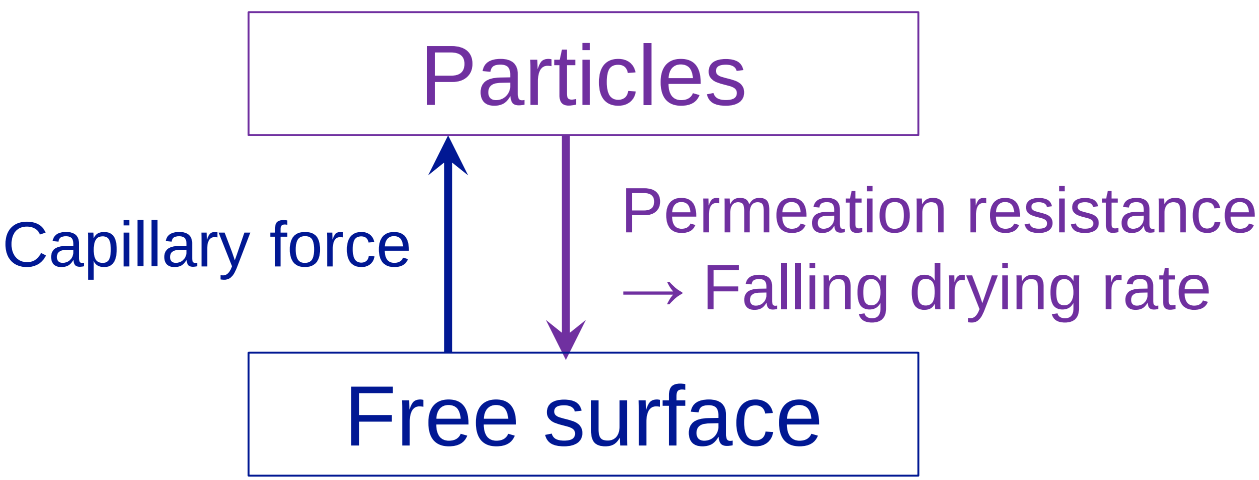


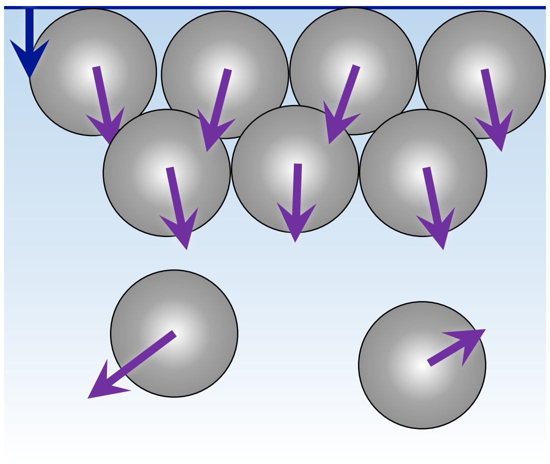
Dispersion　　　　　　Aggregation

Drying curves ↔ Structure

Model

- **Particles**: Equation of motion (Langevin eq.)
- **Free surface**: Recession with a varying rate





Particles' Brownian Motion

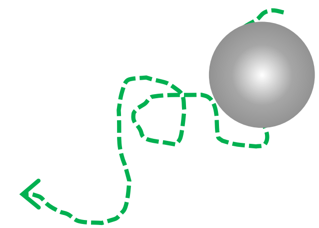
Langevin equation

$$M\dot{\boldsymbol{V}} = -\xi \boldsymbol{V} + \boldsymbol{F}^{\mathrm{R}} + \boldsymbol{F}^{\mathrm{cpl}} + \boldsymbol{F}^{\mathrm{cnt}} + \boldsymbol{F}^{\mathrm{DLVO}}$$

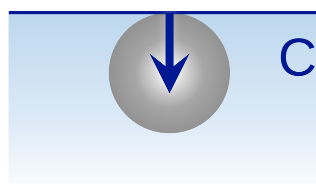
Liquid Free surface Interparticle

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

→ **Brownian Diffusion** (Diffusion coefficient: $D = \frac{k_{\mathrm{B}}T}{3\pi\eta d}$)

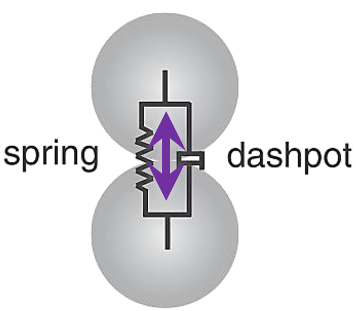


- **Vertical capillary force**: $\boldsymbol{F}^{\mathrm{cpl}}$

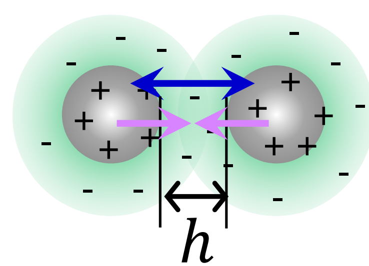


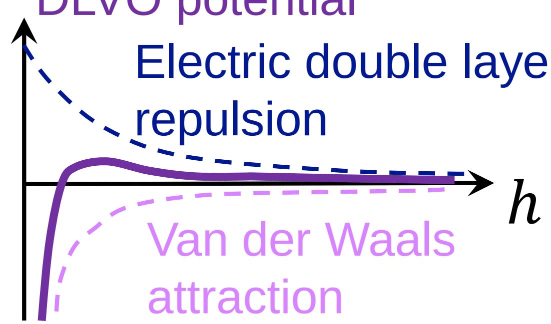
Contact angle $\alpha = 0$

- **Contact force**: $\boldsymbol{F}^{\mathrm{cnt}}$



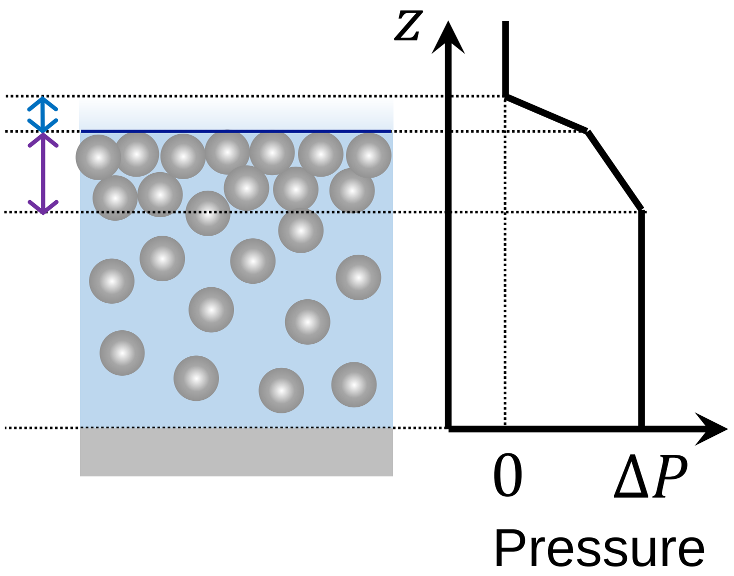
- **DLVO force**: $\boldsymbol{F}^{\mathrm{DLVO}}$





→ **Dispersion / Aggregation**

Drying Rate



Darcy's law

Drying rate: $$U = \frac{\Delta P}{\eta(R_0 + R_\mathrm{p})}$$

Resistance of evaporation: R_0

Resistance of particle layer: R_p

Viscosity of liquid: η

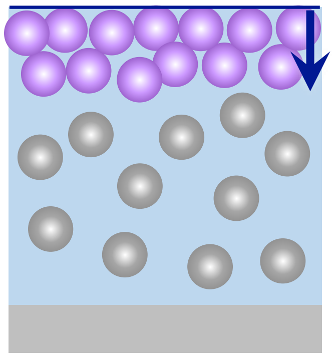
$$\rightarrow \quad \frac{U}{U_0} = \frac{R_0}{R_0 + R_\mathrm{p}}$$

Initial drying rate: $$U_0 = \frac{\Delta P}{\eta R_0}$$

(Constant drying period)

Resistance of Particle Layer

Drying rate: $\dfrac{U}{U_0} = \dfrac{R_0}{R_0 + R_\mathrm{p}}$



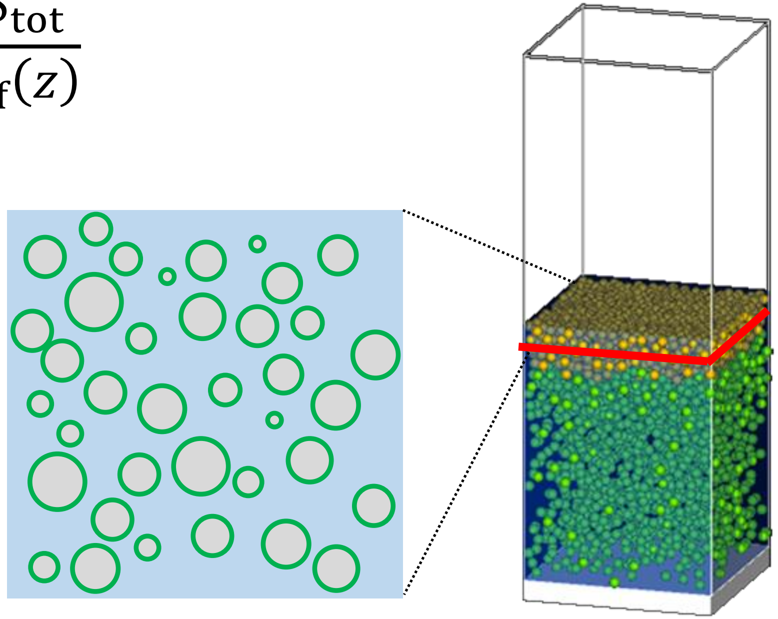
Particle layer = Aggregation moving with free surface

$$R_\mathrm{p} = \int_P r(z)\mathrm{d}z \qquad r(z) = \frac{80}{[D_\mathrm{H}(z)]^2}\frac{S_\mathrm{tot}}{S_\mathrm{f}(z)}$$

Hydraulic diameter: $D_\mathrm{H} = \dfrac{4S_\mathrm{f}}{L_\mathrm{f}}$

Cross-sectional area of the flow: S_f

Wetted perimeter: L_f



Simulation Conditions

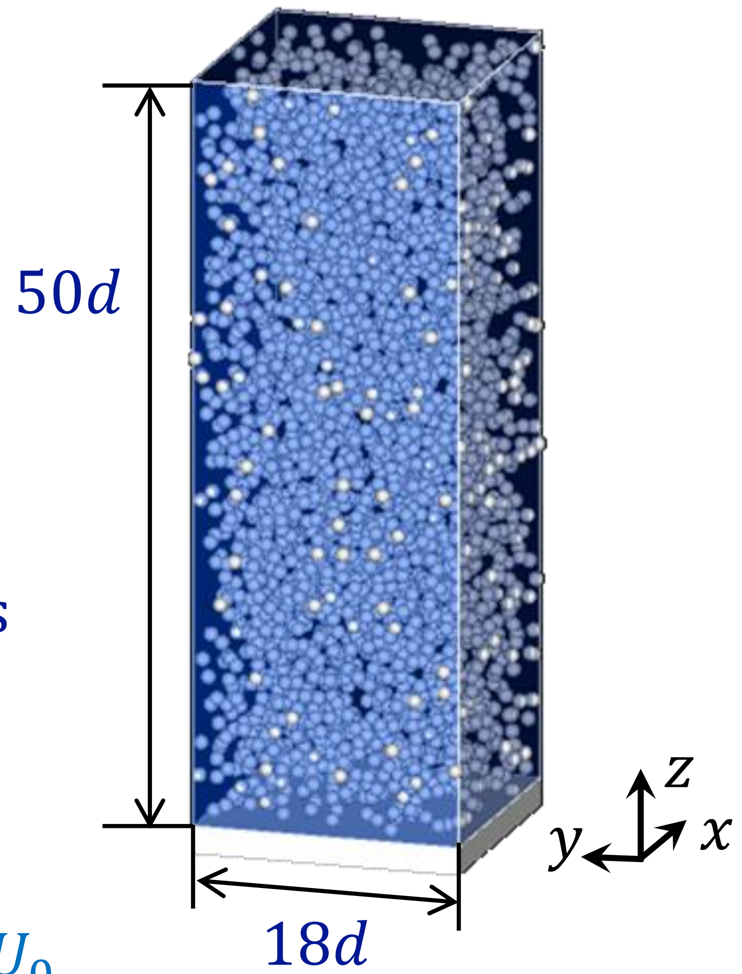
<u>Particles</u>

- Diameter $d = 100\ \mathrm{nm}$
- Initial volume fraction $10\ \mathrm{vol.\%}$
- Zeta potential $30\ \mathrm{mV}$

<u>Liquid</u>

- Water
- Initial drying rate $U_0 = 5 \times 10^{-3}\ \mathrm{m/s}$
- Ion concentration

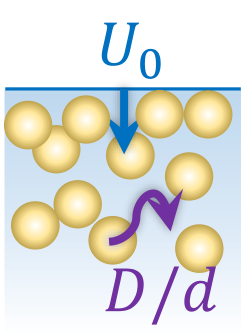
  $5 \times 10^{-4} - 1 \times 10^{-2}\ \mathrm{M}$



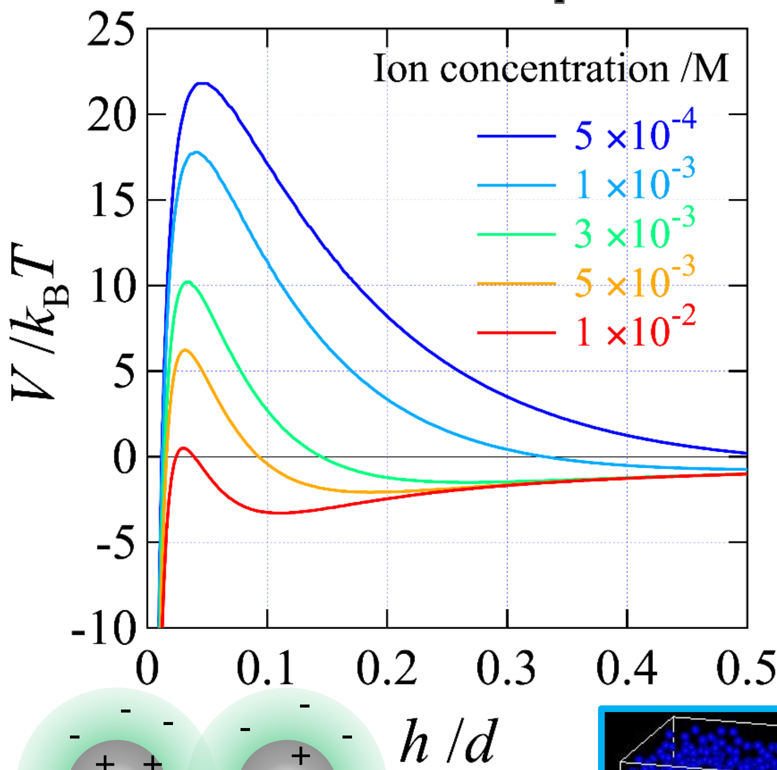
Periodic boundaries x, y

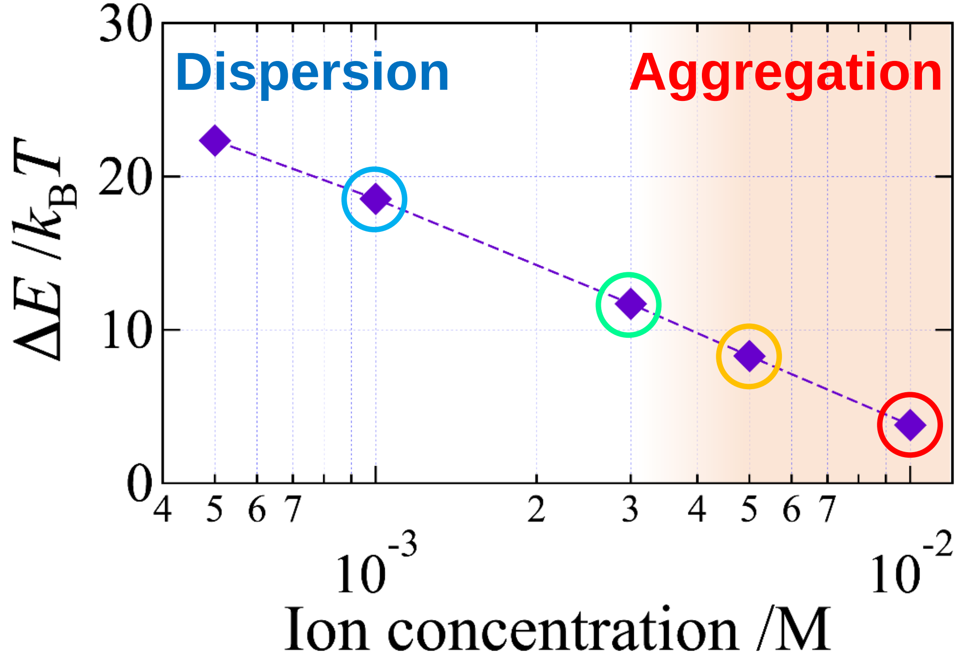
Initial particle drying Péclet number

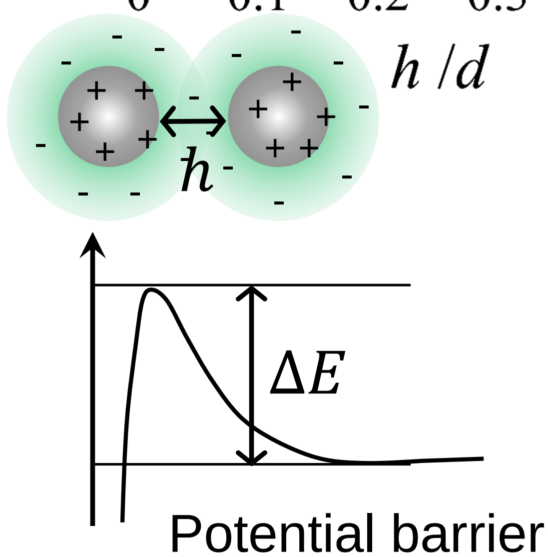
$$\mathrm{Pe}_0 = \frac{(\text{Drying rate})}{(\text{Diffusion rate})} = \frac{U_0}{D/d} = 100$$

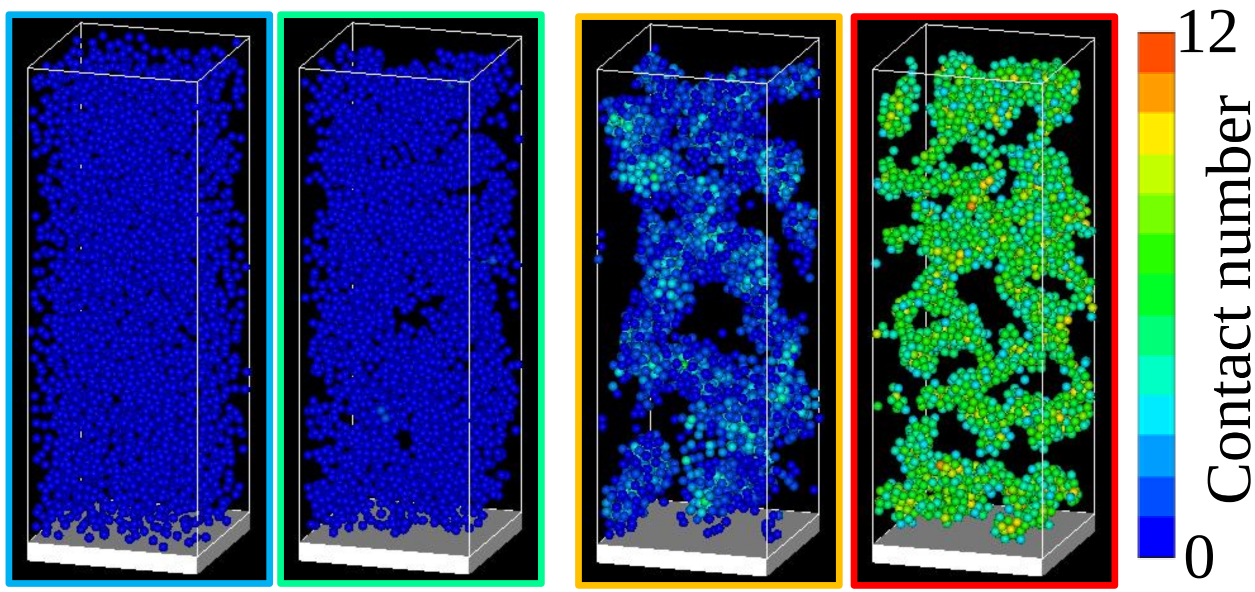


Interparticle DLVO potential

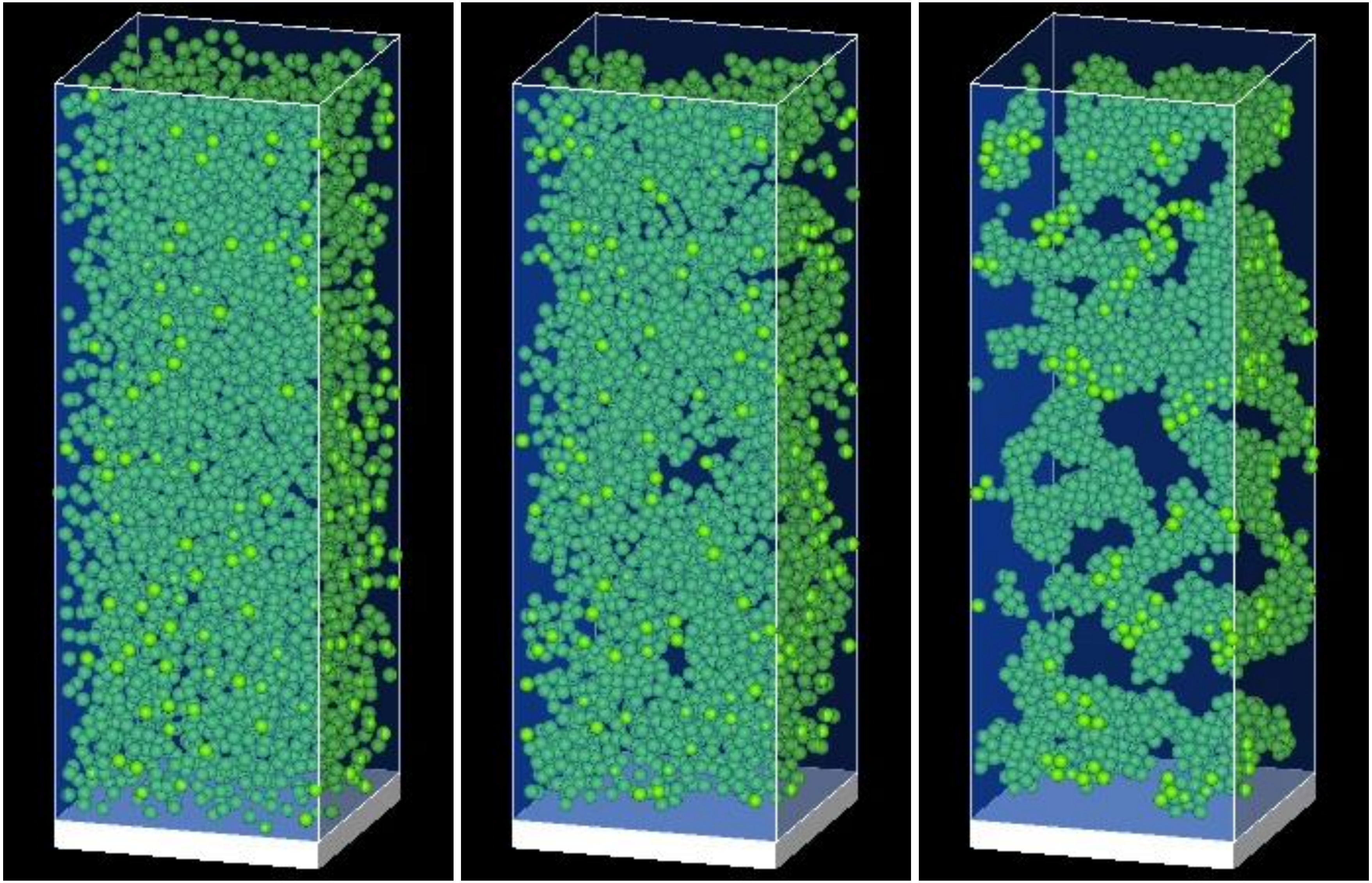






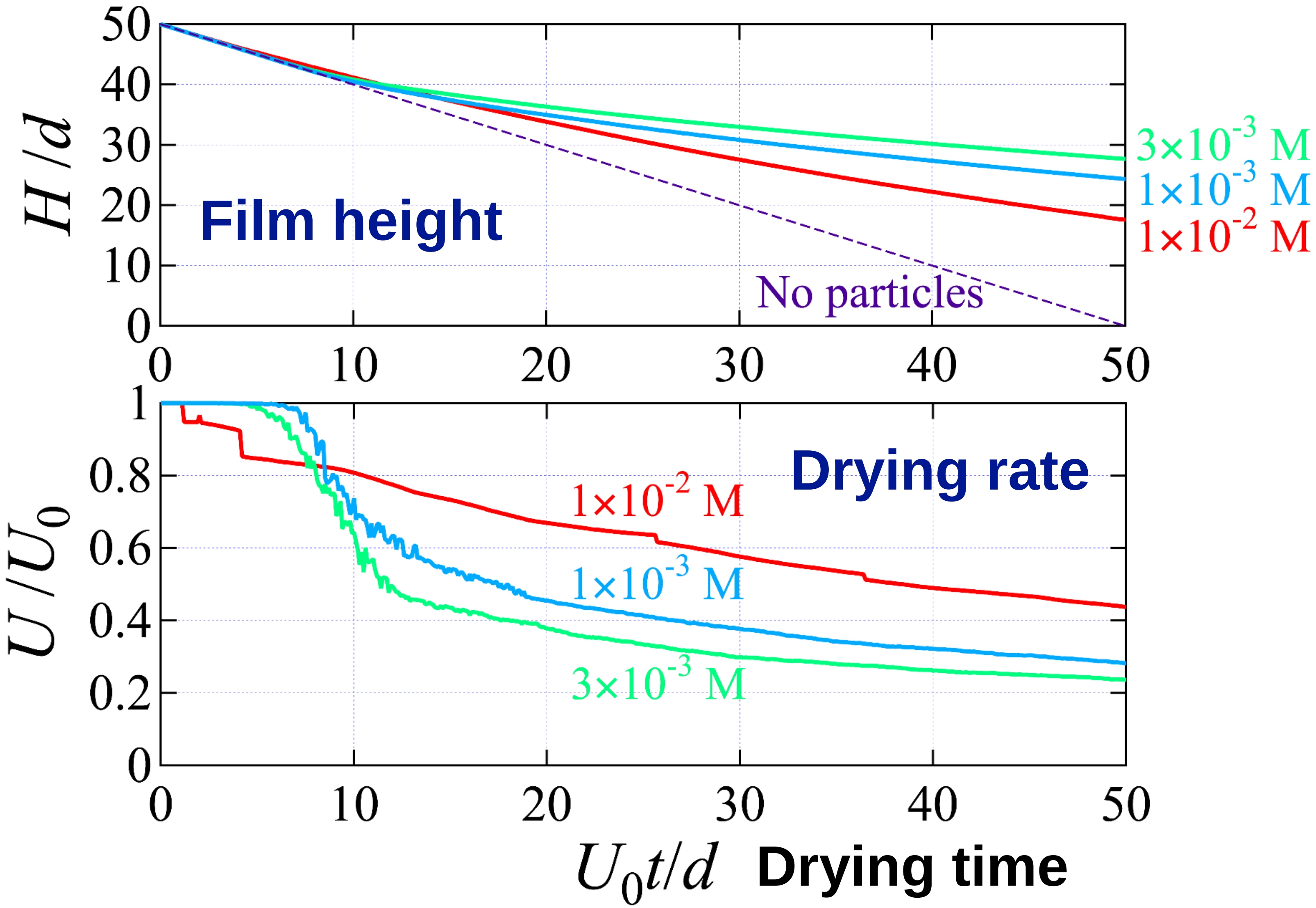


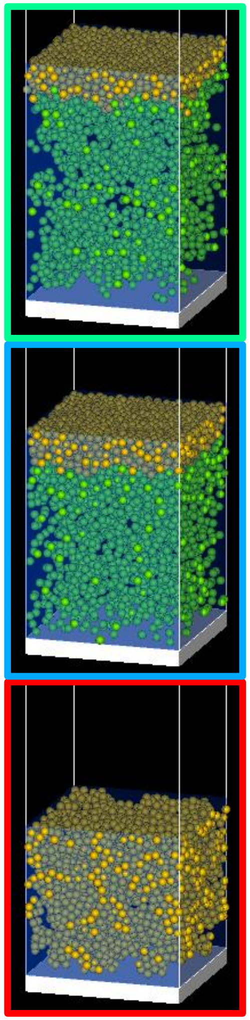
Particle Distribution



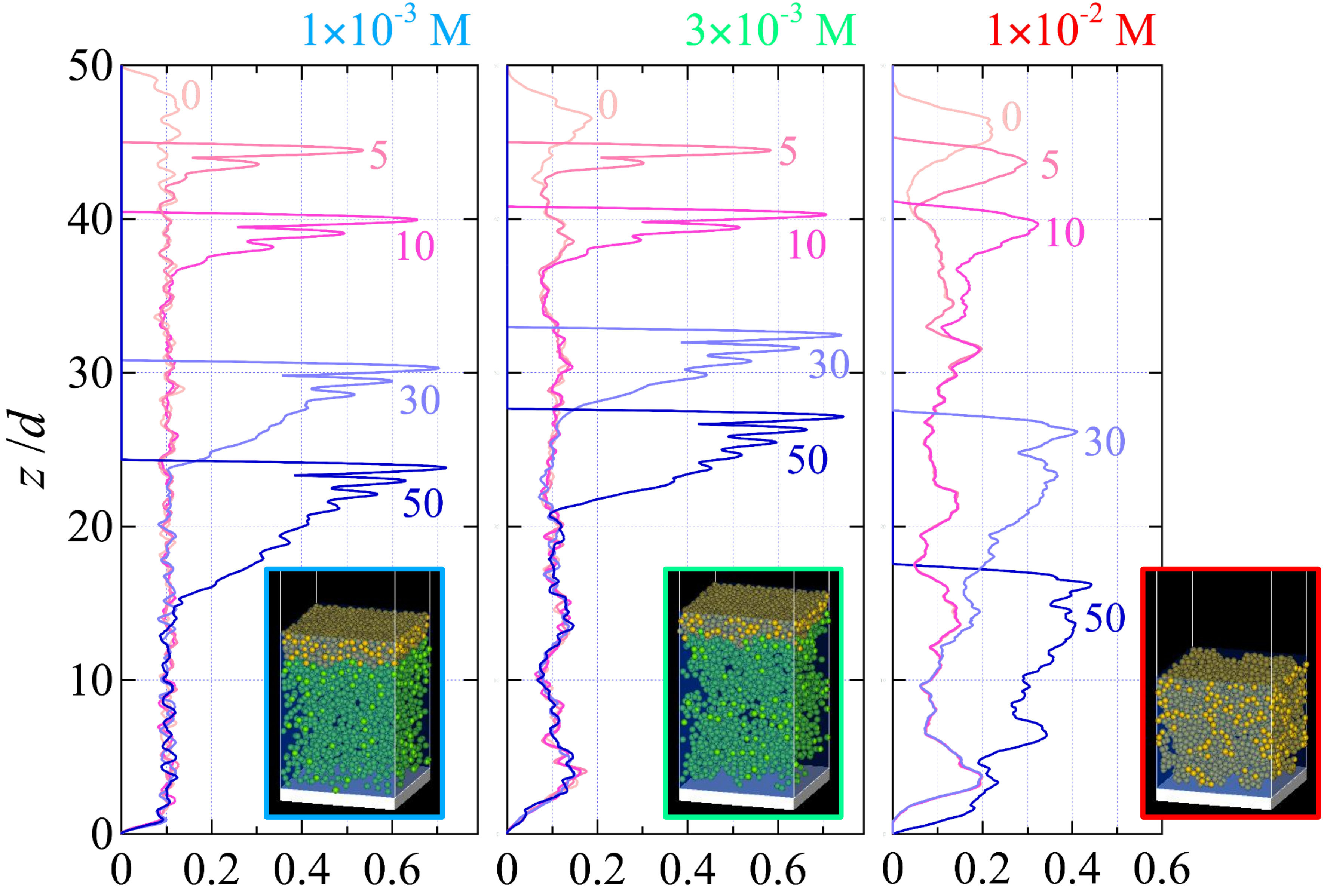
1×10^{-3} M　　3×10^{-3} M　　1×10^{-2} M

Drying Curves



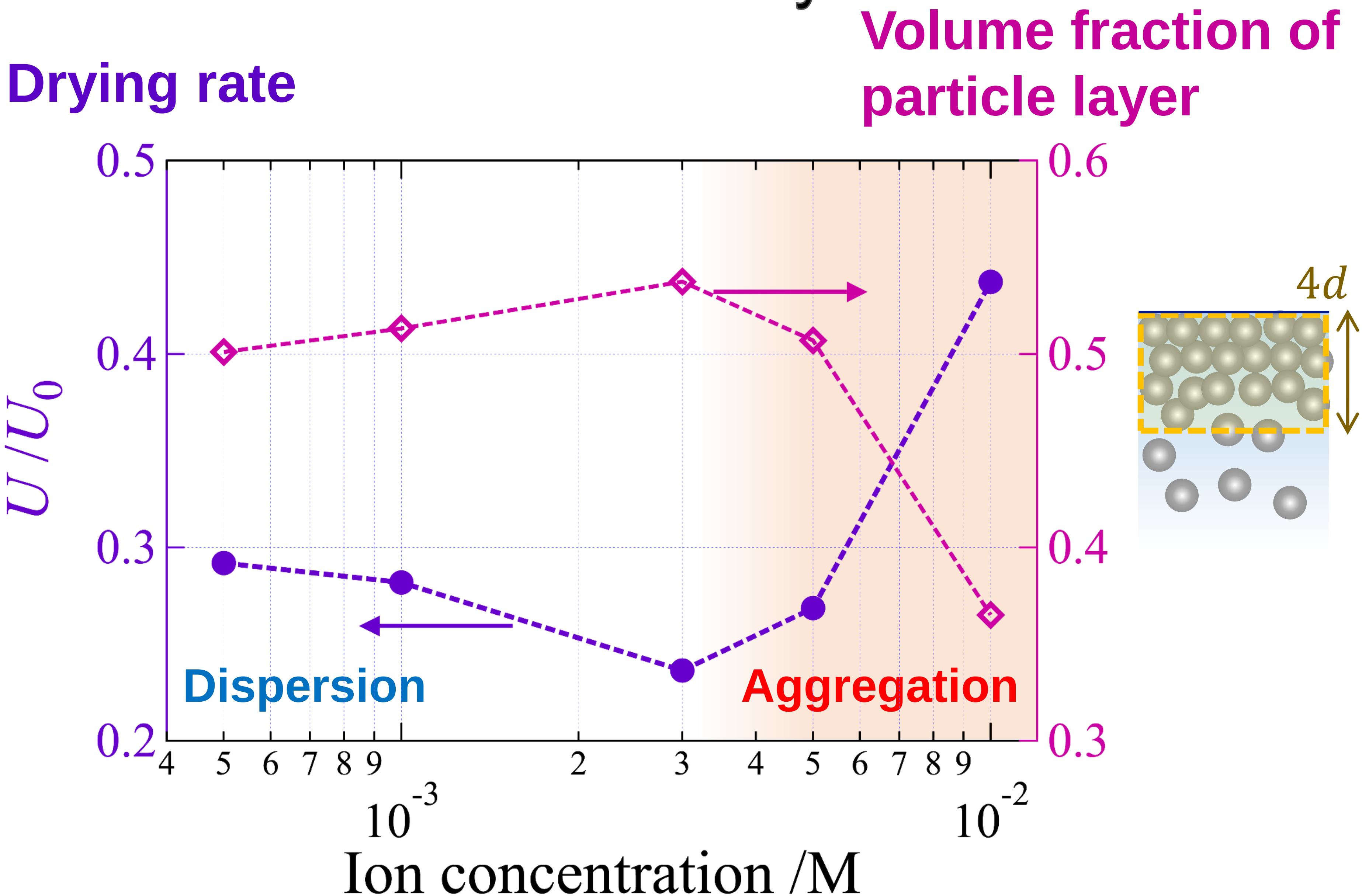


Particle Distribution



Time unit: $U_0 t/d$

Summary



Volume fraction of particle layer
Drying rate
0.5
0.4
0.3
0.2
0.6
0.5
0.4
0.3
U /U0
Dispersion
Aggregation
4
5
6
7
8
9
2
3
4
5
6
7
8
9
10-3
10-2
Ion concentration /M
4d

Summary

- Construction of a model to calculate the drying curves of colloidal suspensions

- Dispersion/aggregation control to reduce drying time
  - Aggregation: stronger attraction
    → higher porosity → higher drying rate
  - Dispersion : stronger repulsion
    → slower particle layer growth
    → higher drying rate