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Estimation of the drying characteristics of colloidal suspensions by numerical simulation

数値シミュレーションによる微粒子分散液の乾燥特性の予測

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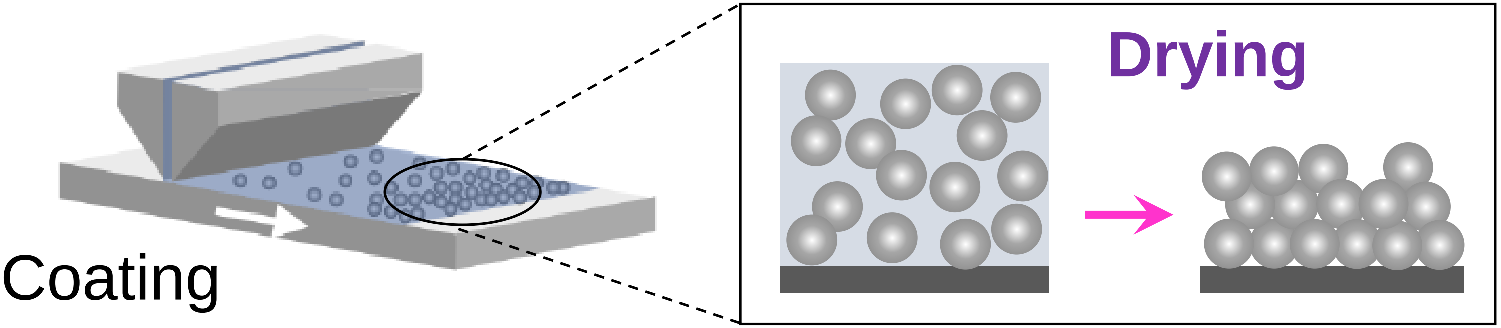
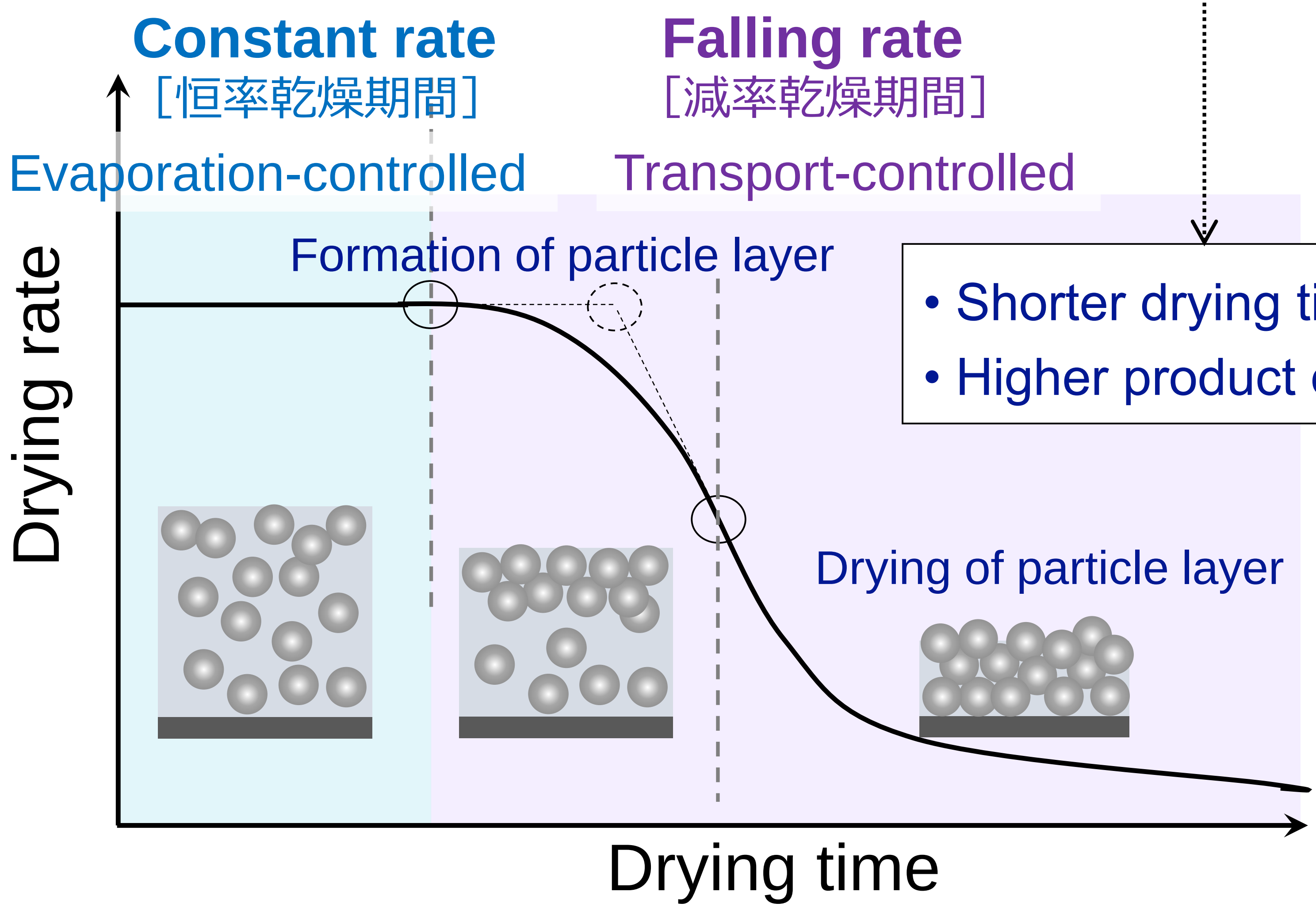


Drying Curve of Colloidal Suspensions

Drying characteristics ↔ Structure



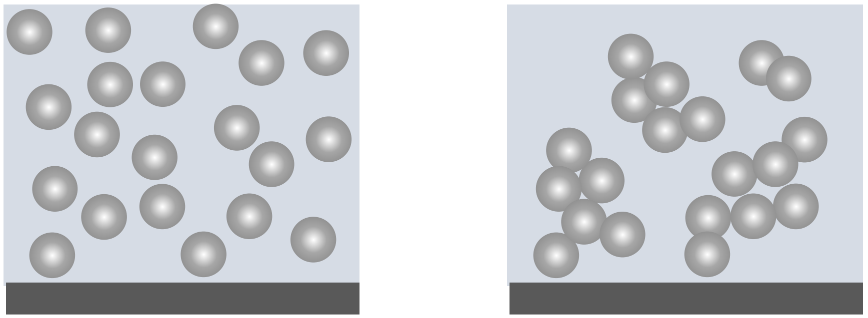
- Shorter drying time
- Higher product quality

山口由岐夫，「ものづくりの化学工学」(2015).

Objective

- Estimation of the drying curve of colloidal suspensions by numerical simulation (SNAP-L)

- Effects of particle dispersion/aggregation on the drying curve

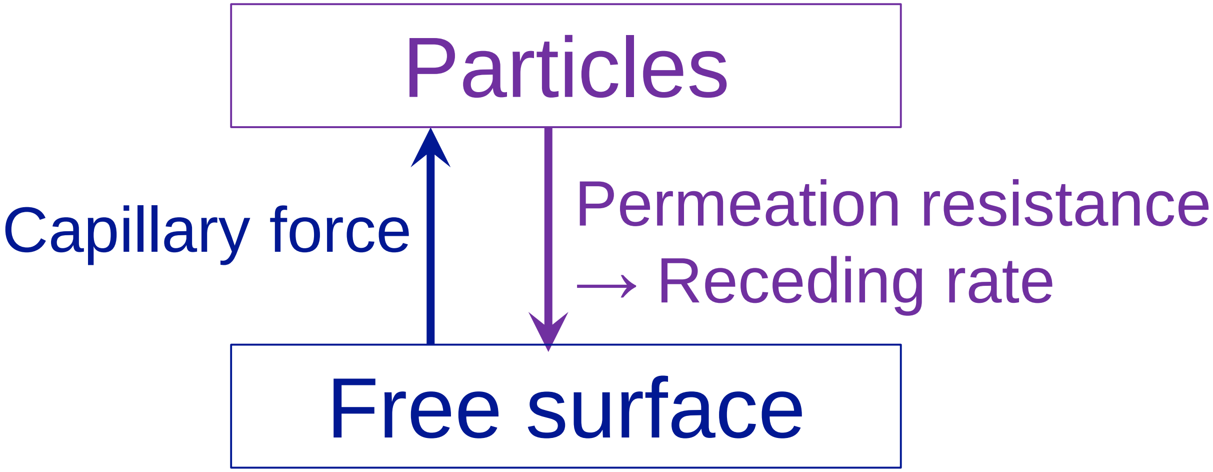


Dispersion Aggregation

Drying characteristics ↔ Structure

Model

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

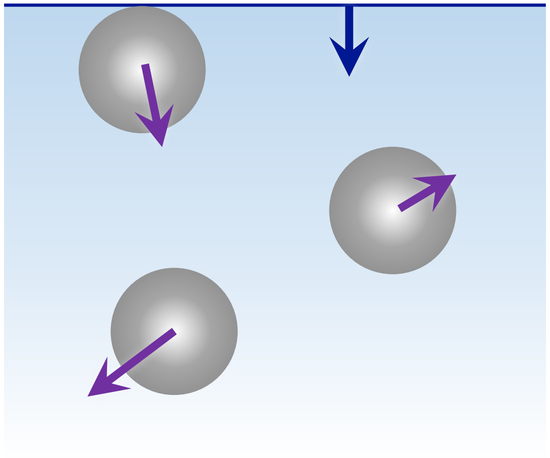


Particles

Capillary force

Permeation resistance
→ Receding rate

Free surface



Particles' Brownian Motion

Langevin equation

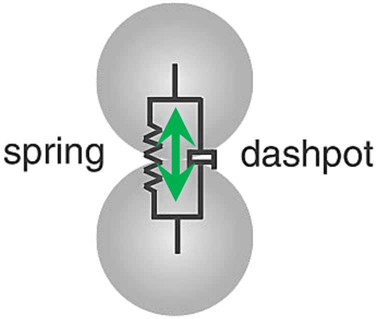
$$M_i \dot{\boldsymbol{V}}_i = -\xi \boldsymbol{V}_i + \boldsymbol{F}_i^{\mathrm{R}} + \boldsymbol{F}_i^{\mathrm{cnt}} + \boldsymbol{F}_i^{\mathrm{cpl}}$$

Fluid Interparticle Free surface

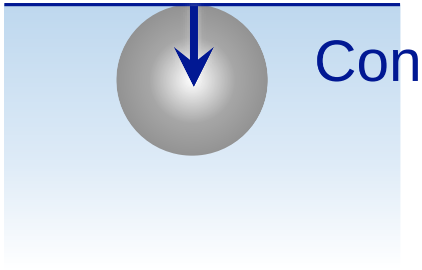
- **Drag force**: $-\xi \boldsymbol{V}_i$ Stokes' law: $\xi = 3\pi\eta d$
- **Random force**: $F_{i\alpha}^{\mathrm{R}}(t) \sim N(0, 2\xi k_{\mathrm{B}} T \Delta t)$ (Gaussian dist.)

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

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



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



Contact angle $\alpha = 0$

Drying Rate

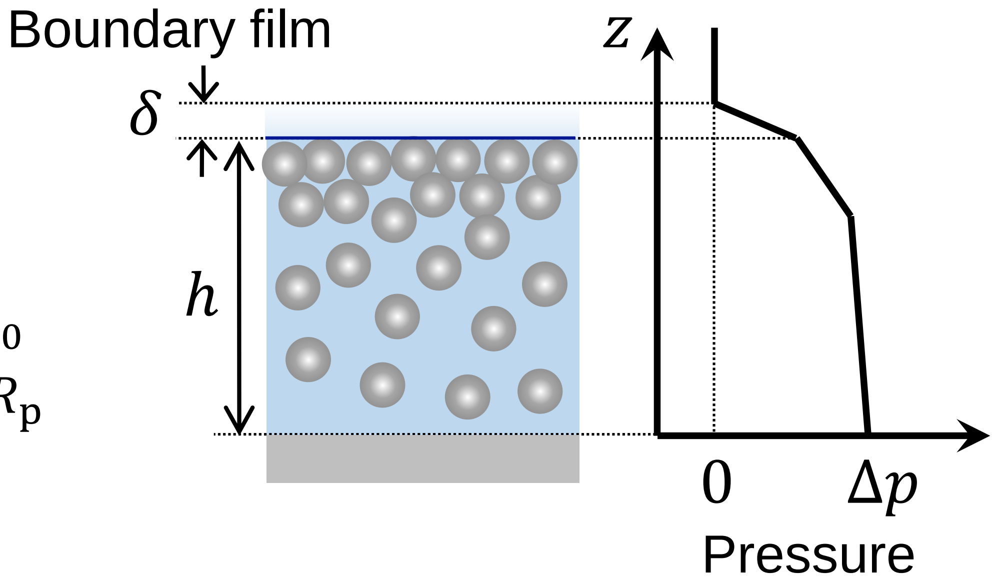
Darcy's law

Drying rate: $u = \dfrac{\Delta p}{\eta\left(R_0 + R_\mathrm{p}\right)}$

Resistance of evaporation: R_0

Resistance of suspensions: R_p

Viscosity of liquid: η



Resistance of evaporation

Drying rate of the liquid containing no particles:

$$u_0 = \frac{D_\mathrm{v}}{\delta}\frac{v_\mathrm{l}}{k_\mathrm{B}T}\Delta p = \frac{\Delta p}{\eta R_0}$$

Diffusion coefficient of vapor: D_v

Molecular volume of liquid: v_l

Drying Rate

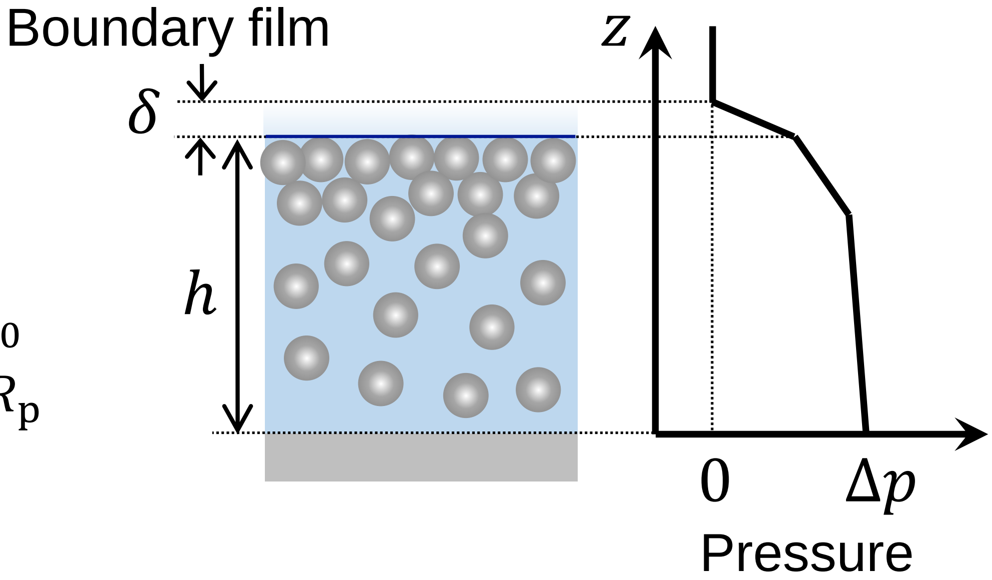
Darcy's law

Drying rate: $u = \dfrac{\Delta p}{\eta(R_0 + R_p)}$

Resistance of evaporation: R_0

Resistance of suspensions: R_p

Viscosity of liquid: η



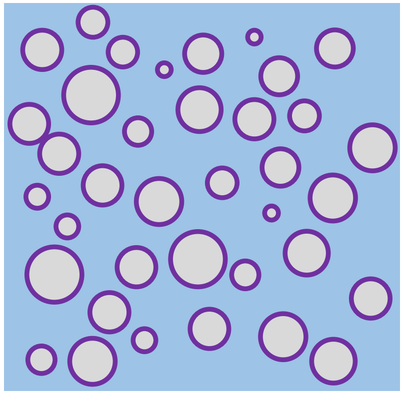
Resistance of suspensions

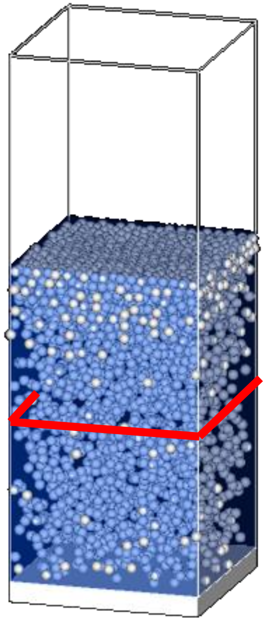
$$R_p = \int_0^h r(z)\mathrm{d}z \qquad r(z) = \frac{80}{[D_H(z)]^2}\frac{S_{tot}}{S_f(z)}$$

Hydraulic diameter: $D_H = \dfrac{4S_f}{L_f}$

Cross-sectional area of the flow: S_f

Wetted perimeter: L_f



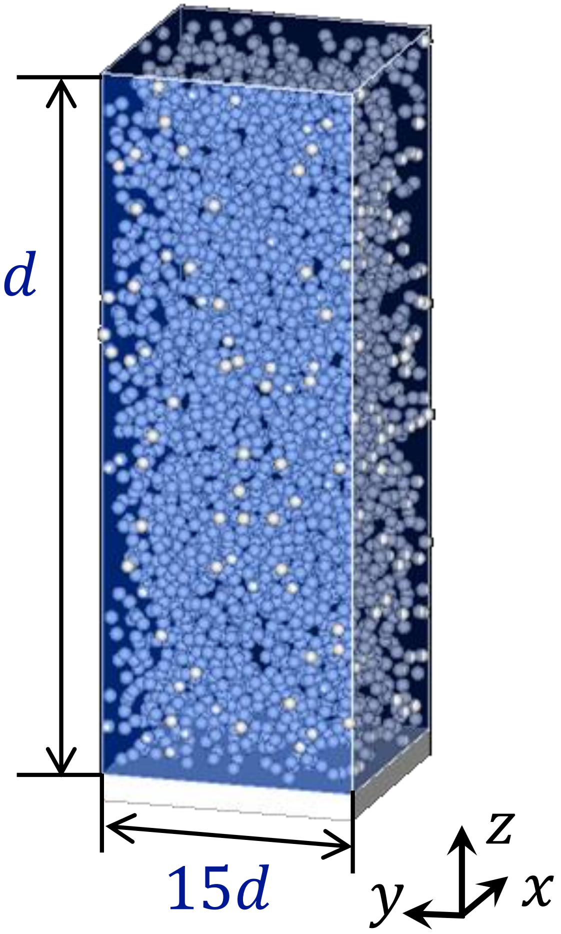


Simulation Conditions

- Particle diameter d
- Initial volume particle fraction 0.1
- Resistance of evaporation $R_0 d = 200$
- Initial particle drying Péclet number

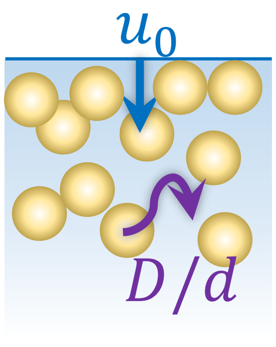
$$\mathrm{Pe}_0 = \frac{(\text{Drying rate})}{(\text{Diffusion rate})} = \frac{u_0}{D/d} = \frac{u_0 d}{D} = 100$$

- Interparticle force: Dispersion/Aggregation



Corresponding system

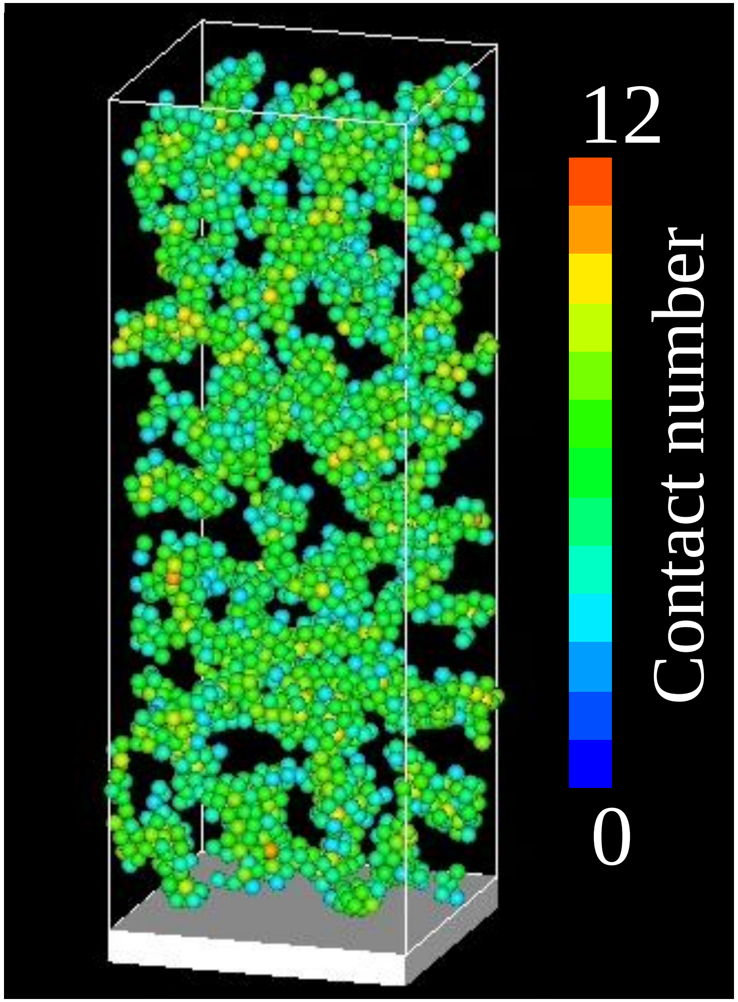
- Particles: $d = 100\ \mathrm{nm}$
- Medium: Water
- Condition: $T \approx 330\ \mathrm{K}$,
  $u_0 \approx 5 \times 10^{-3}\ \mathrm{m/s}$

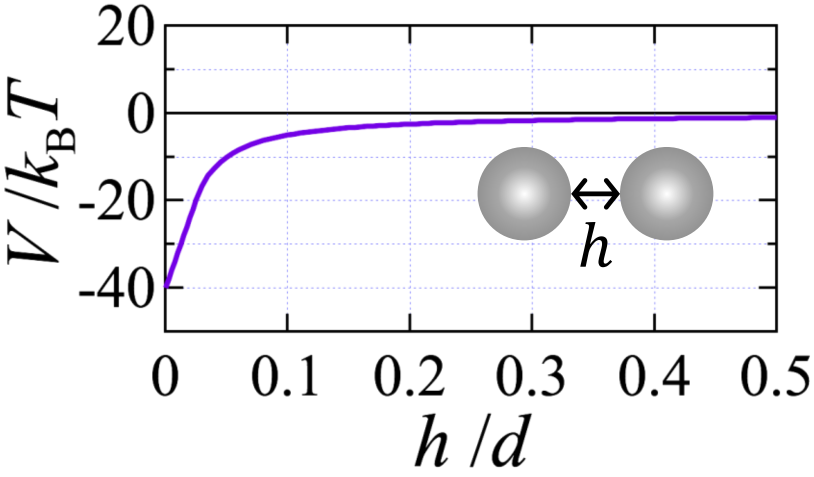


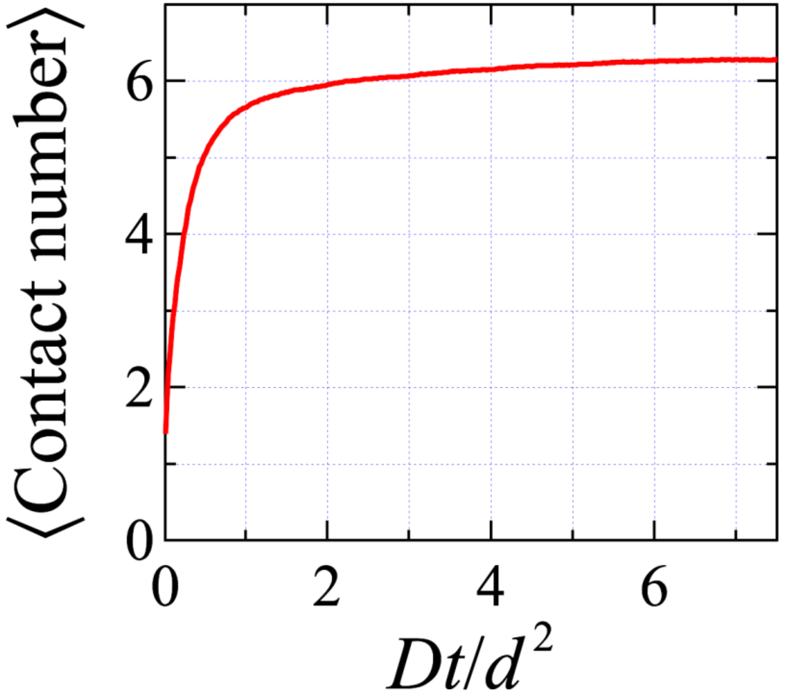
Periodic boundaries: x, y

Aggregation

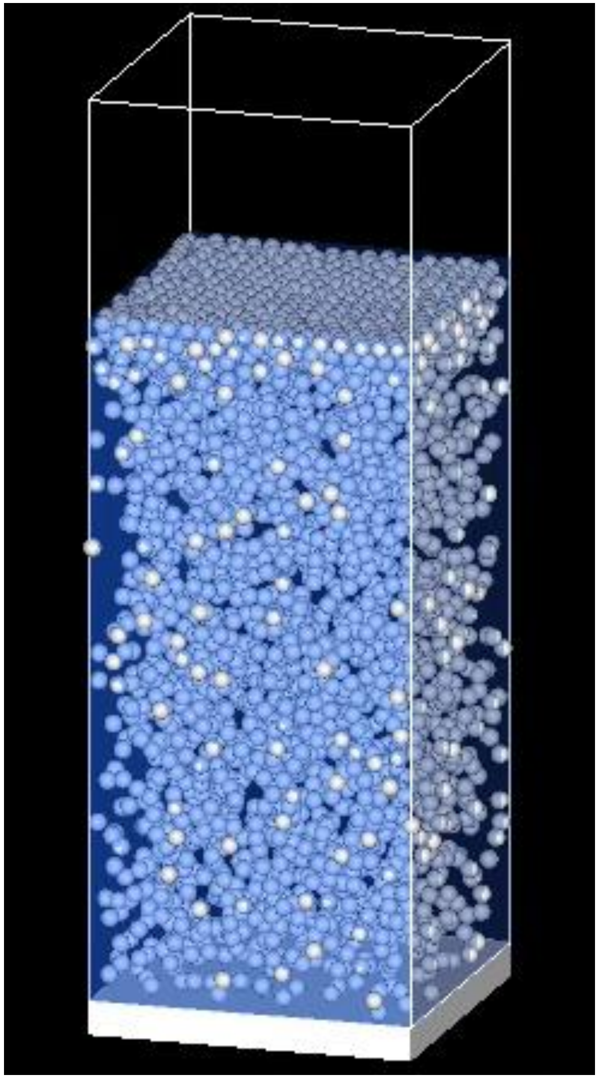
Van der Waals potential
between particles



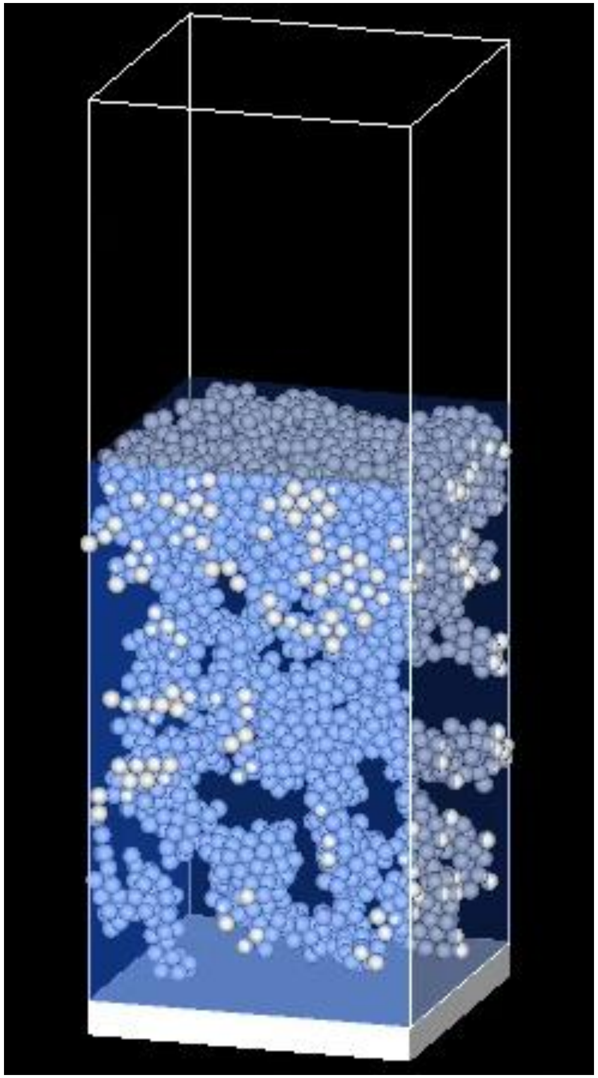




Particle Distribution



Dispersion

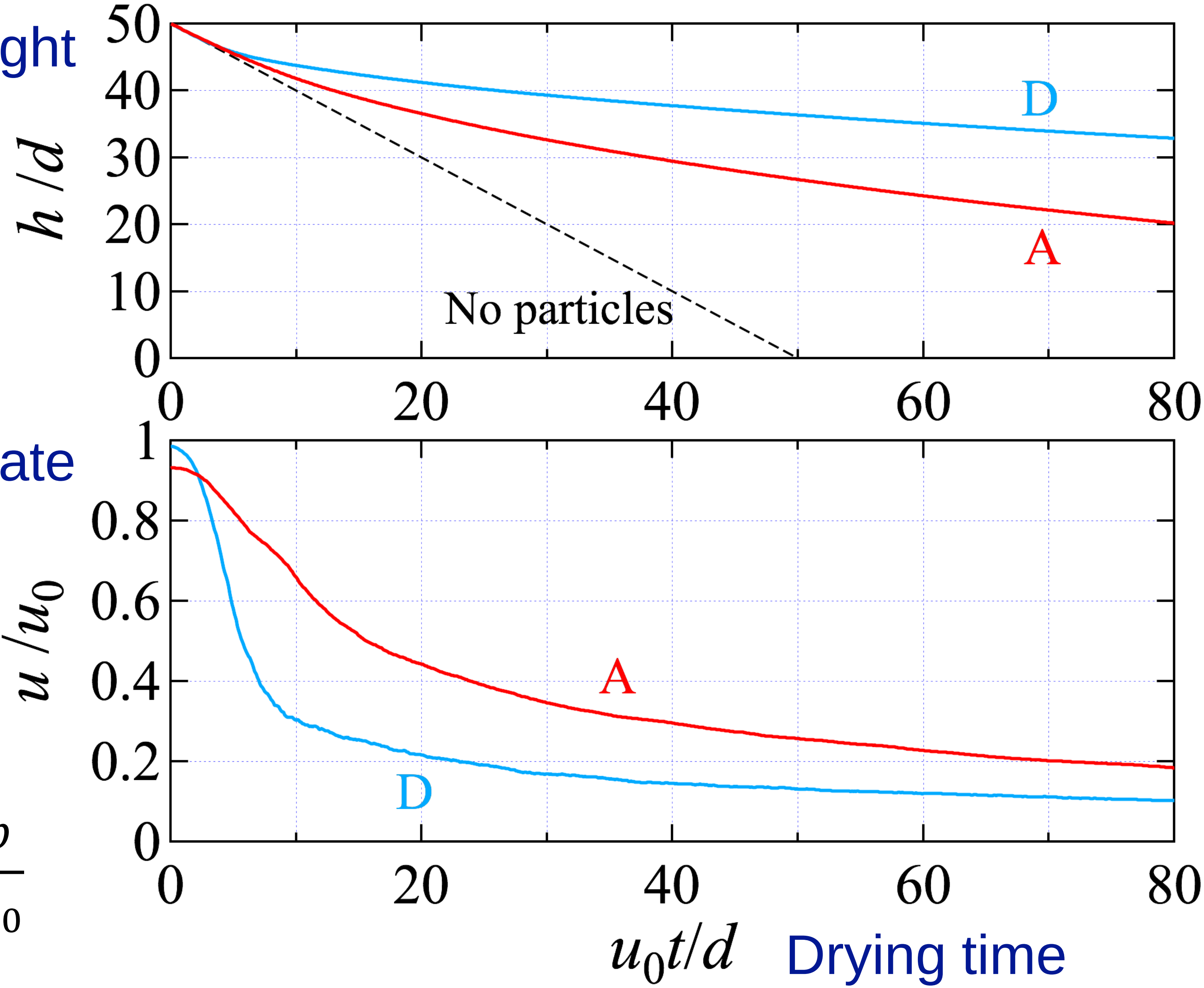


Aggregation

Drying Characteristics

Film height

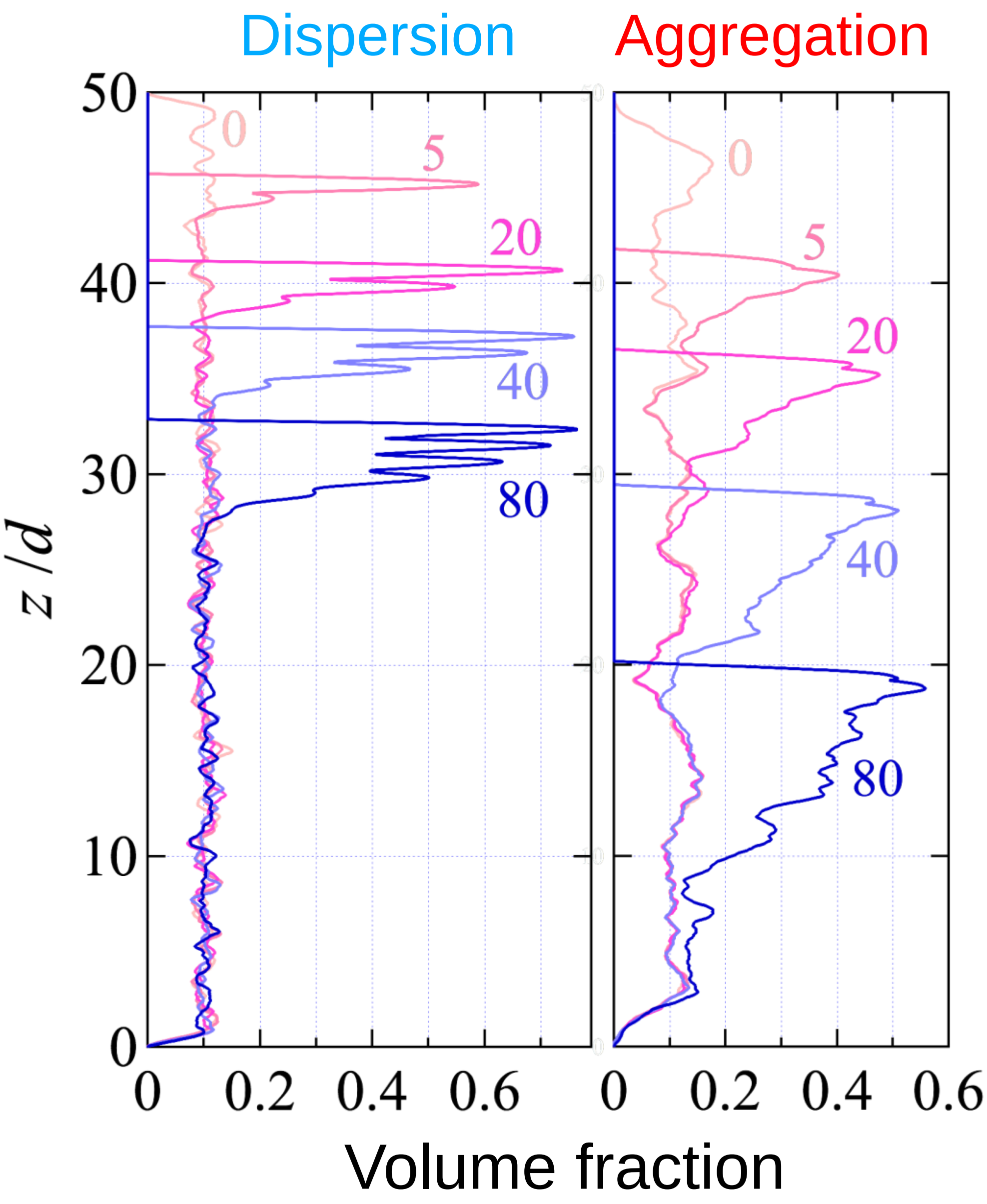
Drying rate

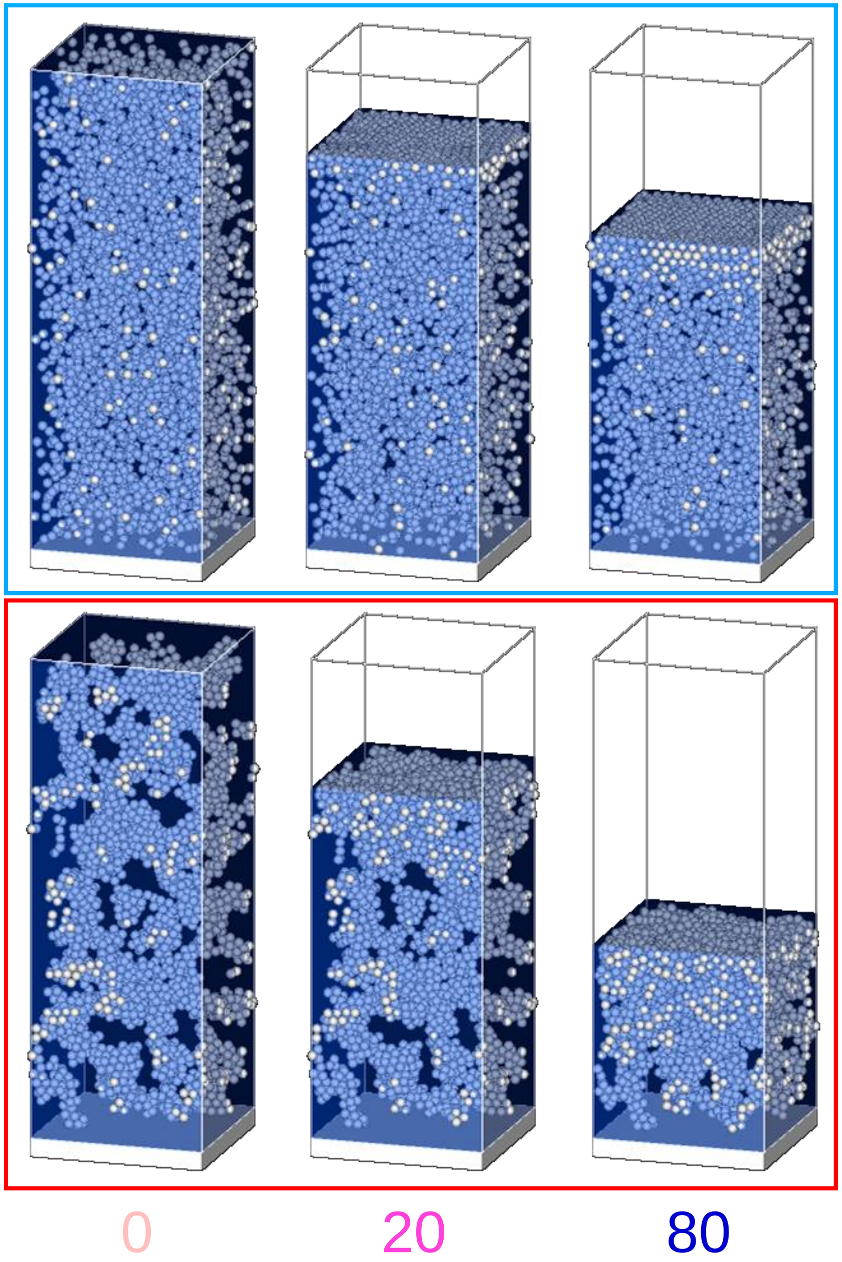


Drying time

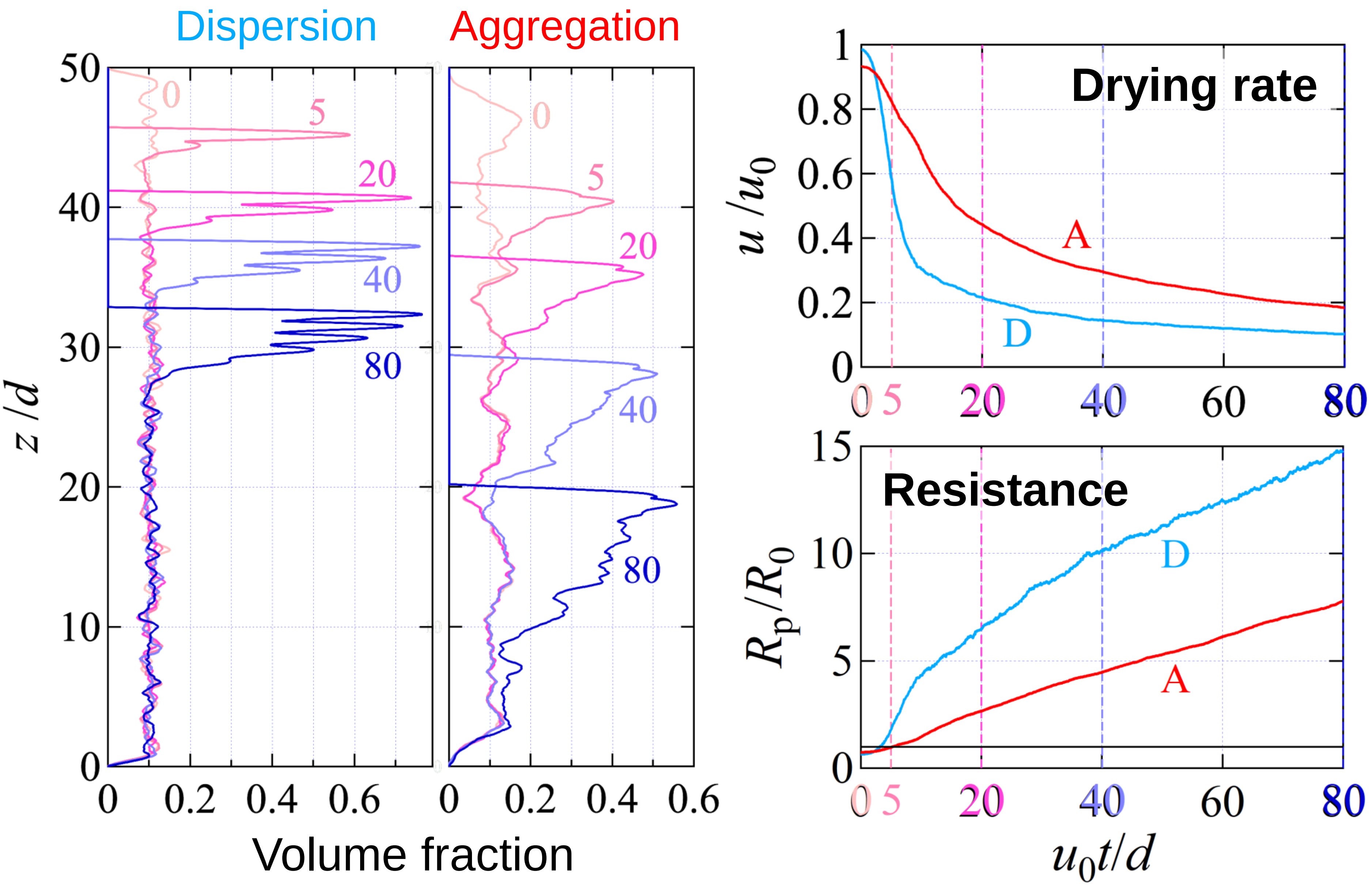
$$u_0 = \frac{\Delta p}{\eta R_0}$$

Particle Distribution





Particle Distribution



Summary

- ◆ Model to estimate the drying characteristics:

$$u = \frac{\Delta p}{\eta\left(R_0 + R_\mathrm{p}\right)}$$

- ◆ Effects of particle dispersion/aggregation on the drying characteristics
  - Aggregation: higher porosity → higher drying rate
  - Dispersion/aggregation control to reduce drying time