SIMULATION MODEL OF DRYING COLLOIDAL SUSPENSION ON SUBSTRATE

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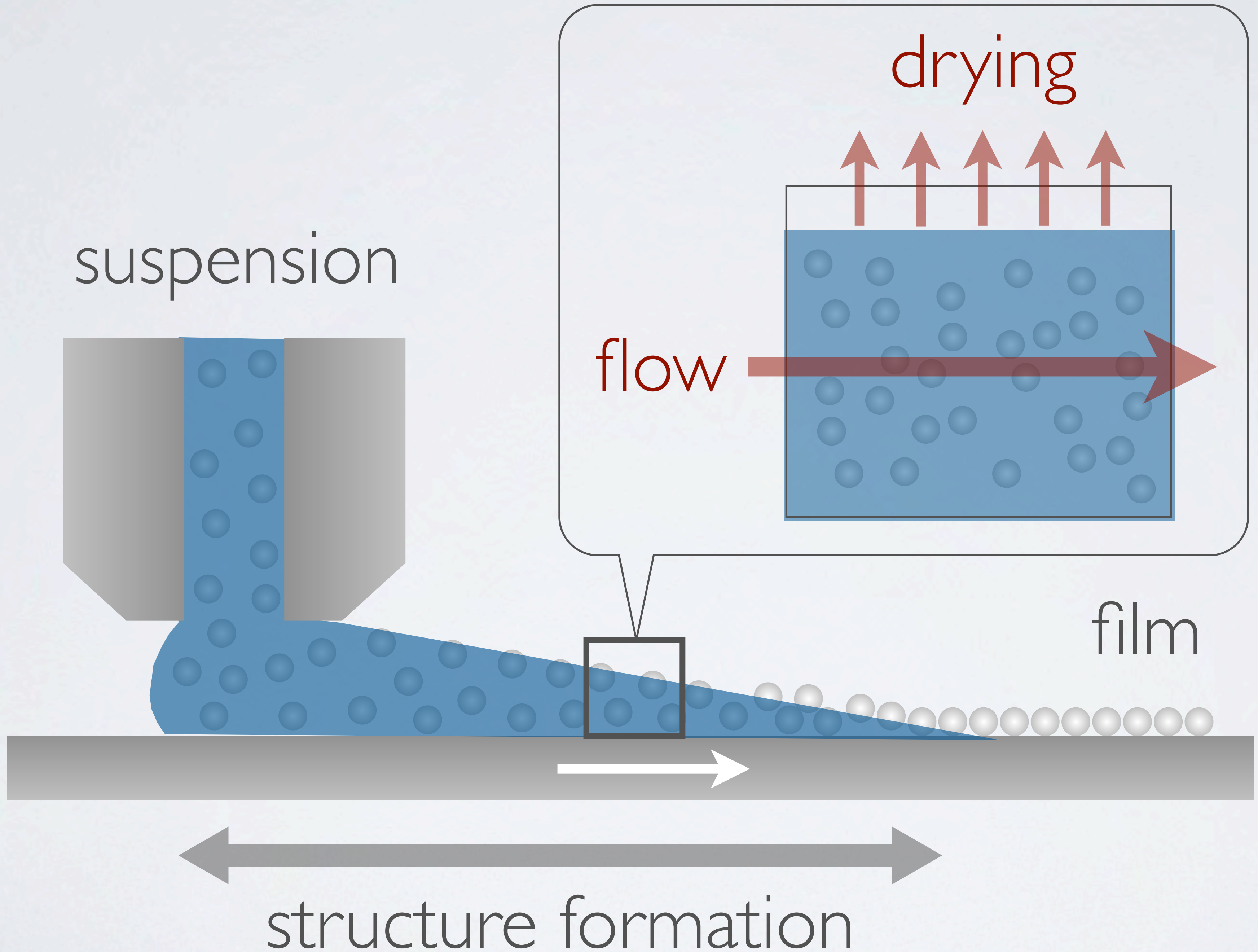
OUTLINE

- Continuous coating of colloidal suspension on substrate
- Direct simulation model for drying colloidal suspension
- Demonstration of present simulation model

CONTINUOUS COATING ON SUBSTRATE



PECLÉT NUMBERS

coating Peclét number

$$\mathrm{Pe_c} = \frac{cd^2}{Dh}$$

drying Peclét number

$$\mathrm{Pe_d} = \frac{eh}{D}$$

Peclét numbers ratio

$$\frac{\mathrm{Pe_c}}{\mathrm{Pe_d}} = \frac{c}{e}\left(\frac{d}{h}\right)^2$$

$$\frac{\mathrm{Pe_c}}{\mathrm{Pe_d}} \sim 1$$ → Both flow and drying influence structure formation

OBJECTIVES OF THIS STUDY

- Develop direct simulation model for drying colloidal suspension
- Perform flow simulations of colloidal suspension on sliding substrate with drying of solvent
- Quantify coating-drying dynamics
  - structure of particles
  - variable drying rate

DIRECT SIMULATION MODEL

- Solves gas-liquid two phase flow on lattice using VOF (volume of fluid) method
- Solves translational/rotational motion of particles subject to contact, DLVO, capillary interactions
- Couples motion of particles with flow of solvent using immersed boundary method

→ Interparticle hydrodynamic interaction is included without analytical model

EQUATIONS OF FLUID MOTION

fluctuating stress

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla p - \frac{2}{3} \nabla \cdot \left\{ \mu (\nabla \cdot \boldsymbol{v}) \boldsymbol{I} \right\} + \nabla \cdot \mu \{ \nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T \} + \nabla \cdot \boldsymbol{S} + \Phi \boldsymbol{\alpha}$$

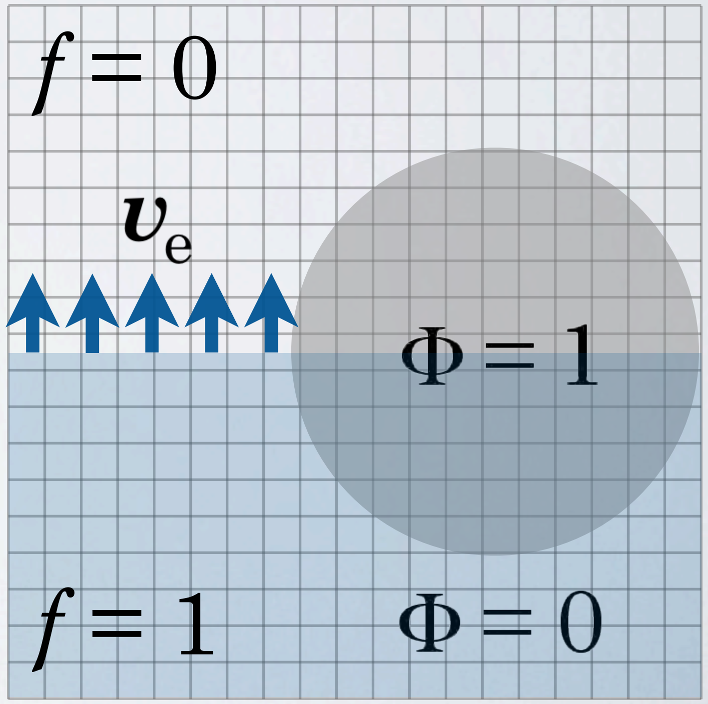
acceleration

$$\boldsymbol{\alpha} = \rho \frac{\boldsymbol{v}^{\mathrm{p}} - \boldsymbol{v}}{\Delta t} + \rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \nabla p + \frac{2}{3} \nabla \cdot \left\{ \mu (\nabla \cdot \boldsymbol{v}) \boldsymbol{I} \right\} - \nabla \cdot \mu \{ \nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T \} - \nabla \cdot \boldsymbol{S}$$

$$\rho = f \rho_{\mathrm{l}} + (1 - f) \rho_{\mathrm{g}}, \quad \mu = f \mu_{\mathrm{l}} + (1 - f) \mu_{\mathrm{g}}$$

$$\frac{\partial f}{\partial t} + (\boldsymbol{v} + \boldsymbol{v}_{\mathrm{e}}) \cdot \nabla f = 0 \qquad \nabla \cdot \boldsymbol{v} = \frac{\rho_{\mathrm{l}} - \rho_{\mathrm{g}}}{\rho} \boldsymbol{v}_{\mathrm{e}} \cdot \nabla f$$

local drying velocity



EQUATIONS OF PARTICLE MOTION

$$m\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}^{\mathrm{co}} + \boldsymbol{F}^{\mathrm{D}} + \boldsymbol{F}^{\mathrm{ca}} + \boldsymbol{F}^{\mathrm{h}}$$

$$I\frac{d\omega}{dt} = \boldsymbol{T}^{\mathrm{co}} + \boldsymbol{T}^{\mathrm{h}}$$

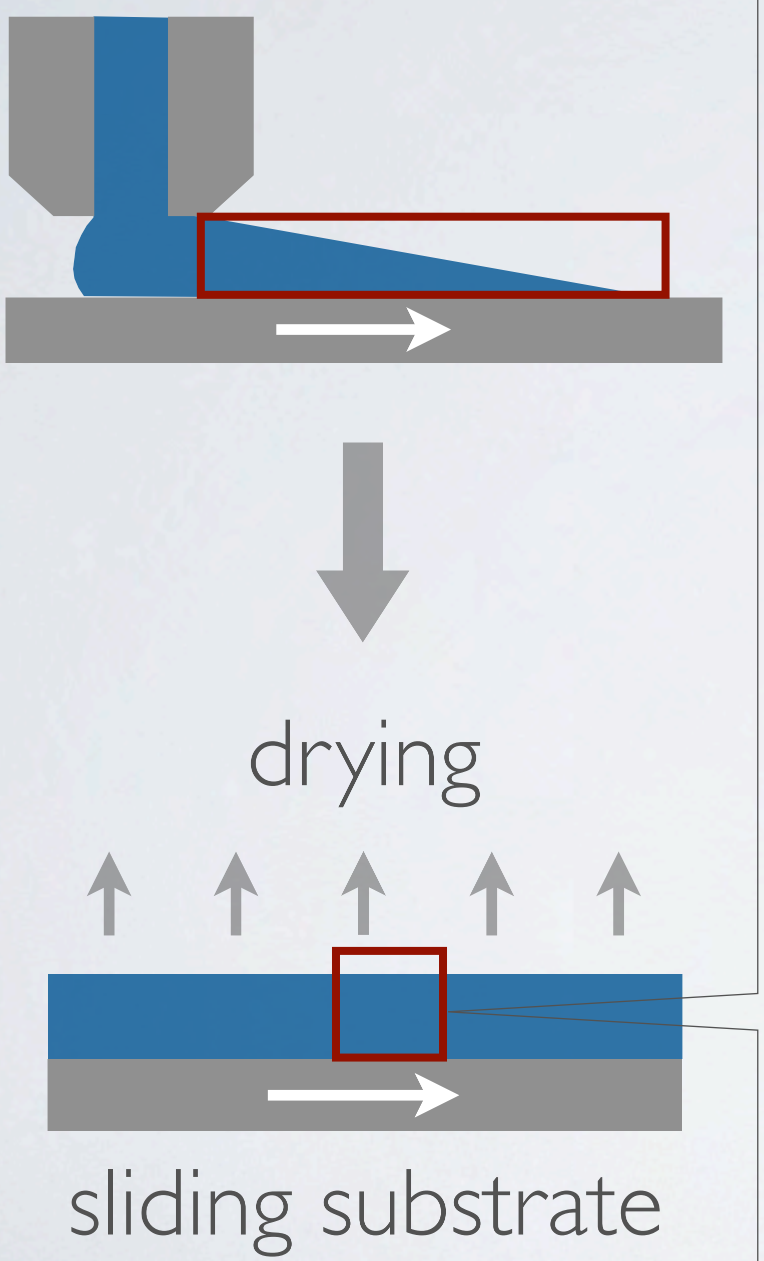
$$\boldsymbol{F}^{\mathrm{h}} = -\int_{V_{\mathrm{p}}} \rho\Phi\underline{\boldsymbol{\alpha}}\,d\boldsymbol{r}$$

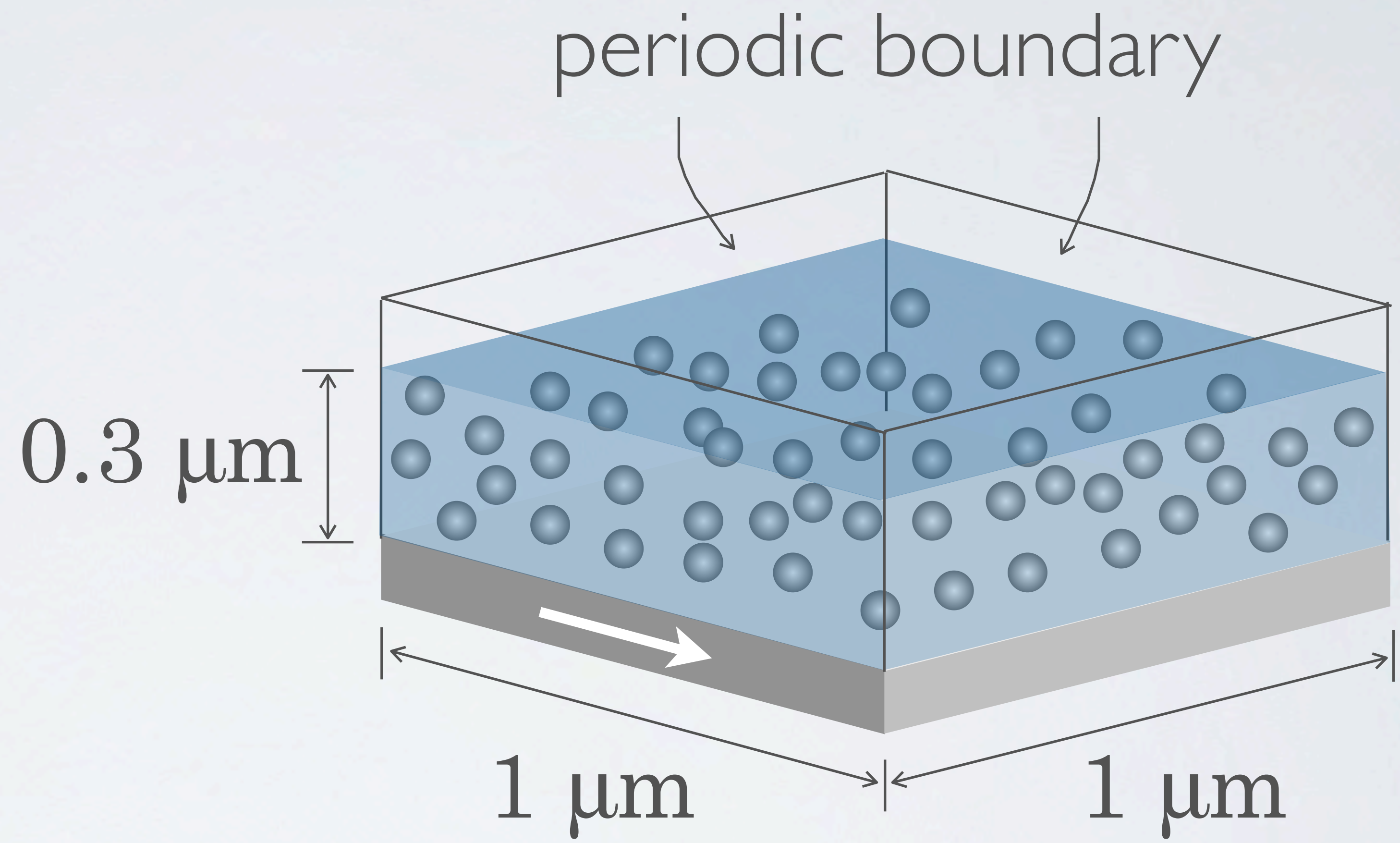
acceleration

$$\boldsymbol{T}^{\mathrm{h}} = -\int_{V_{\mathrm{p}}} (\boldsymbol{r}\times\rho\Phi\underline{\boldsymbol{\alpha}})\,d\boldsymbol{r}$$

acceleration

SIMULATION CONDITION





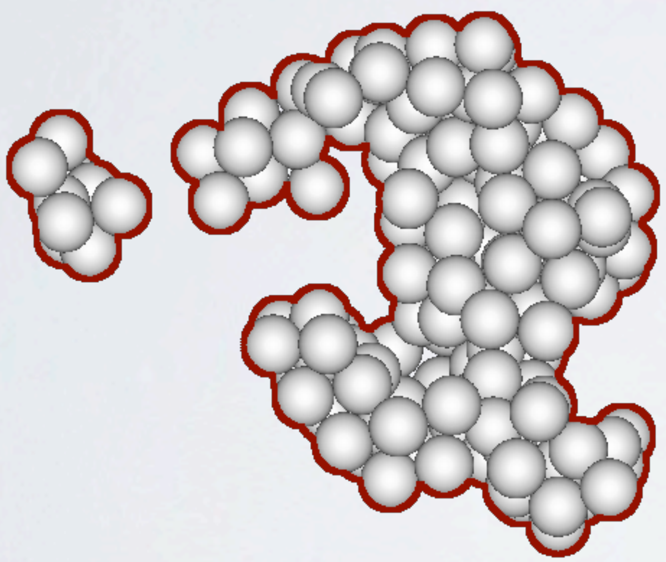
$d = 0.1\ \mu\text{m}$, $\phi_0 = 20$ vol%, $\zeta = -50/0$ mV

$c = 13$ cm/s, $e = 1.4$ cm/s ➡ $\mathrm{Pe_c} / \mathrm{Pe_d} = 1$

QUANTIFICATION OF STRUCTURE

Non-dimensional Boundary Area (NBA)

$$\mathrm{NBA} = \frac{\text{surface area of aggregates}}{\text{total surface area of particles}} = \frac{1}{12N}\sum_{k=0}^{12}\left\{\left(12-k\right)n(k)\right\}$$



k : coordinate number

$n(k)$: number of particles with coordinate number of k

N : total number of particles

NBA=0 : 3D hexagonal close-packed

NBA=0.5 : 2D hexagonal close-packed

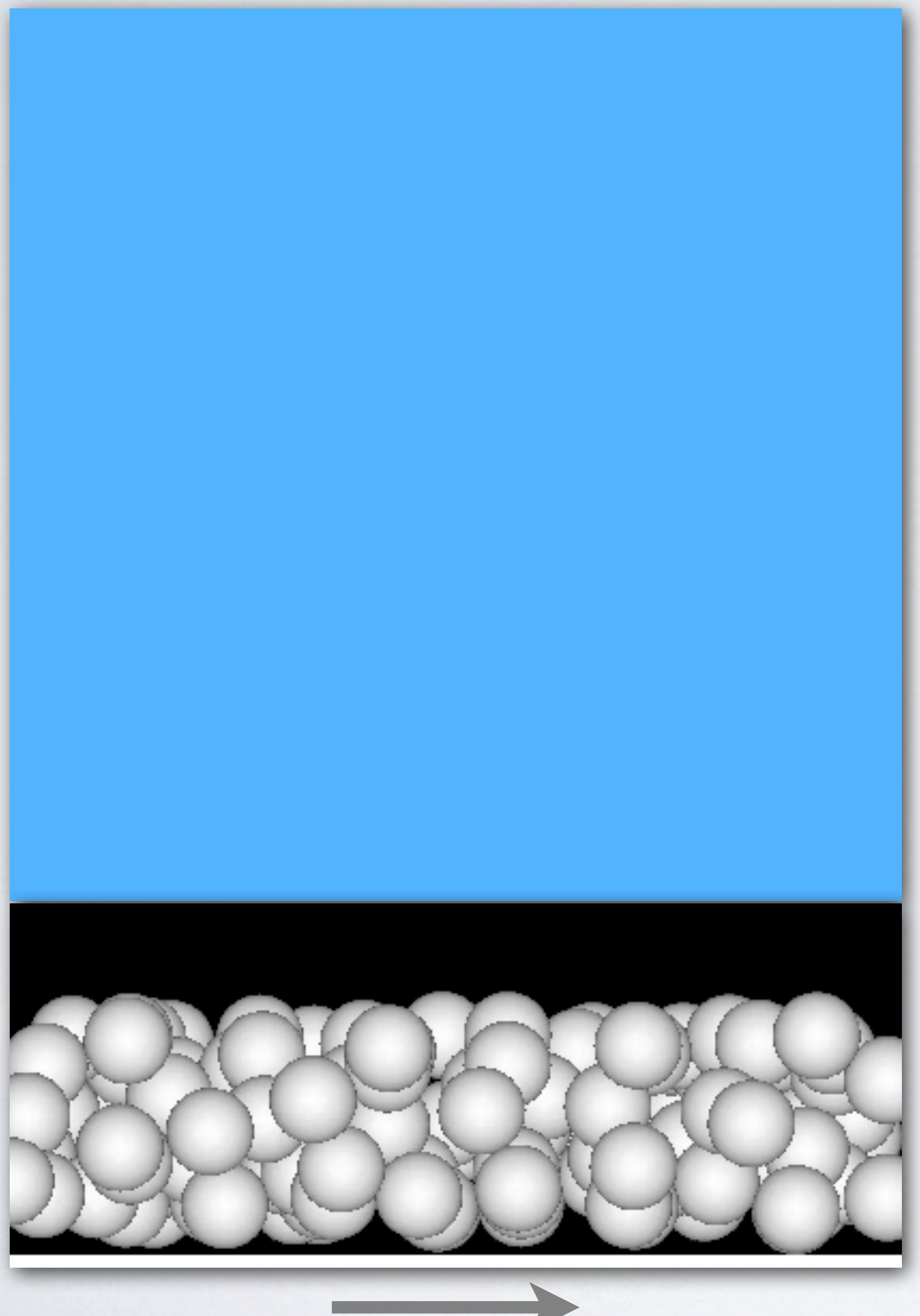
NBA=1 : complete-dispersed

STRUCTURE OF PARTICLES

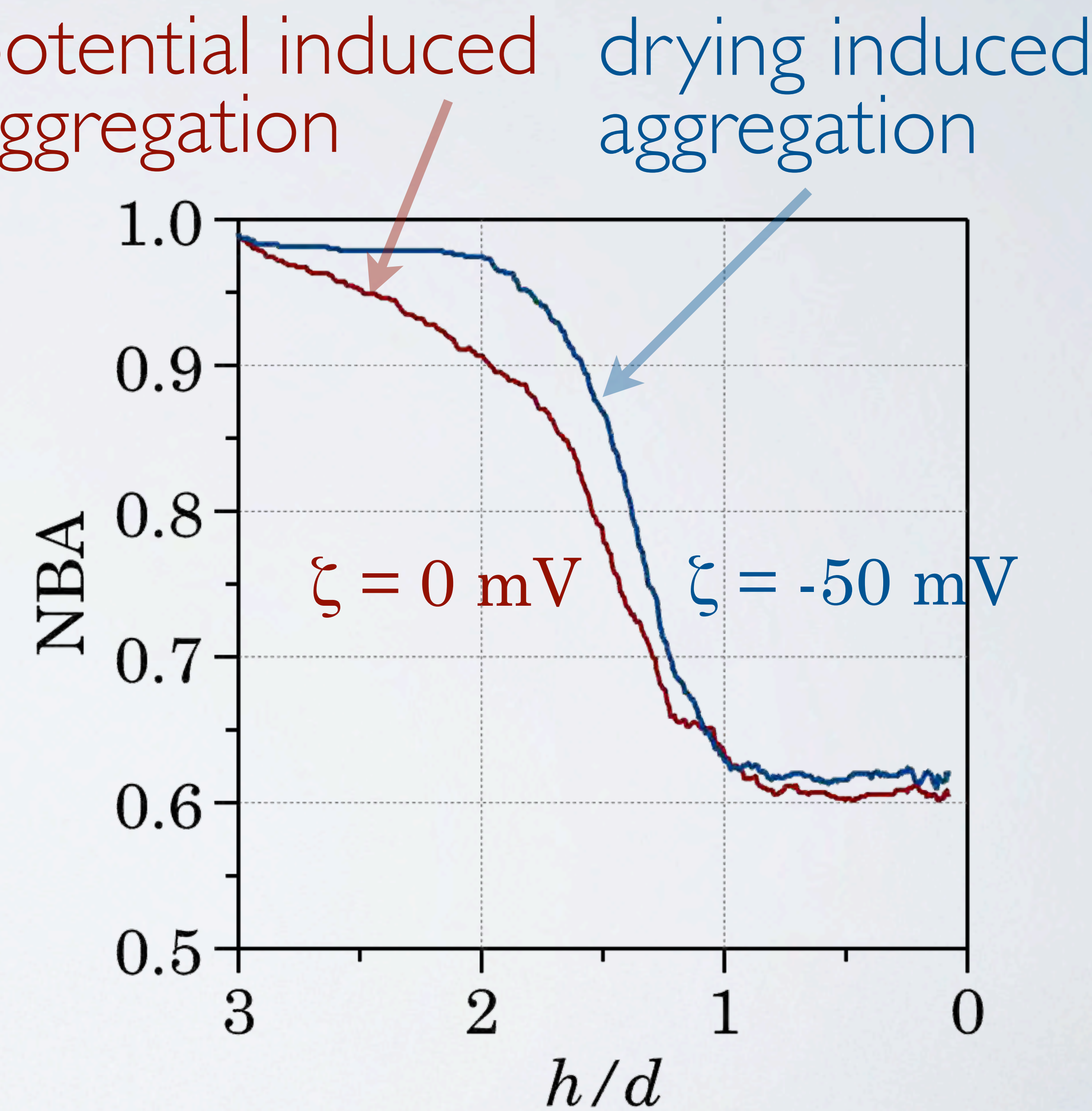
ζ = -50 mV

plan

side

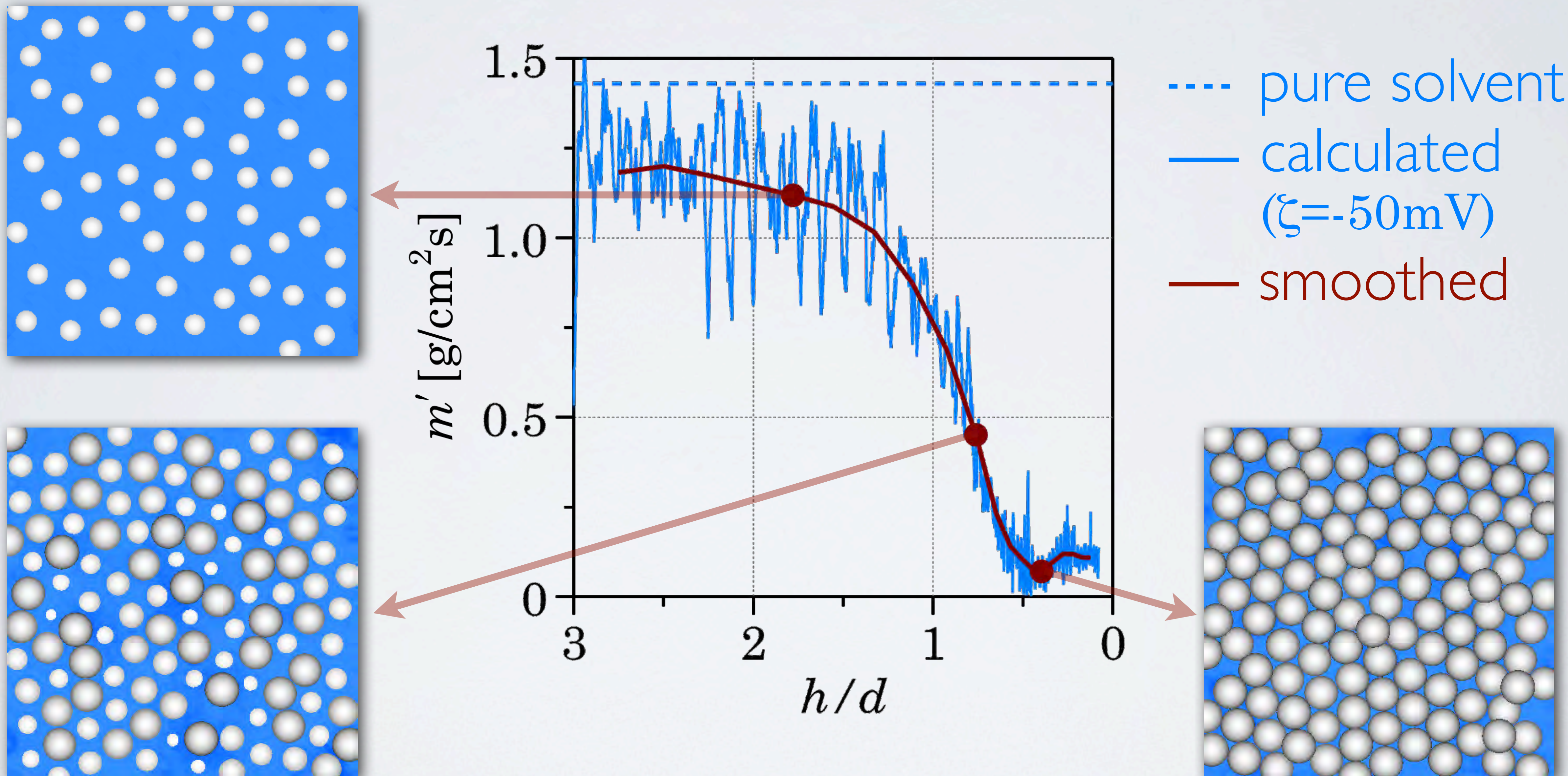


NBA vs interface height



VARIABLE DRYING RATE

drying rate vs interface height



CONCLUSION

- Developed direct simulation model for drying colloidal suspension
- Quantify structure formation of particles using NBA
- Quantify variable drying rate in which constant rate of drying changes to decreasing rate of drying.