Flow and Drying Simulation of Nanoparticle Suspension on Substrate

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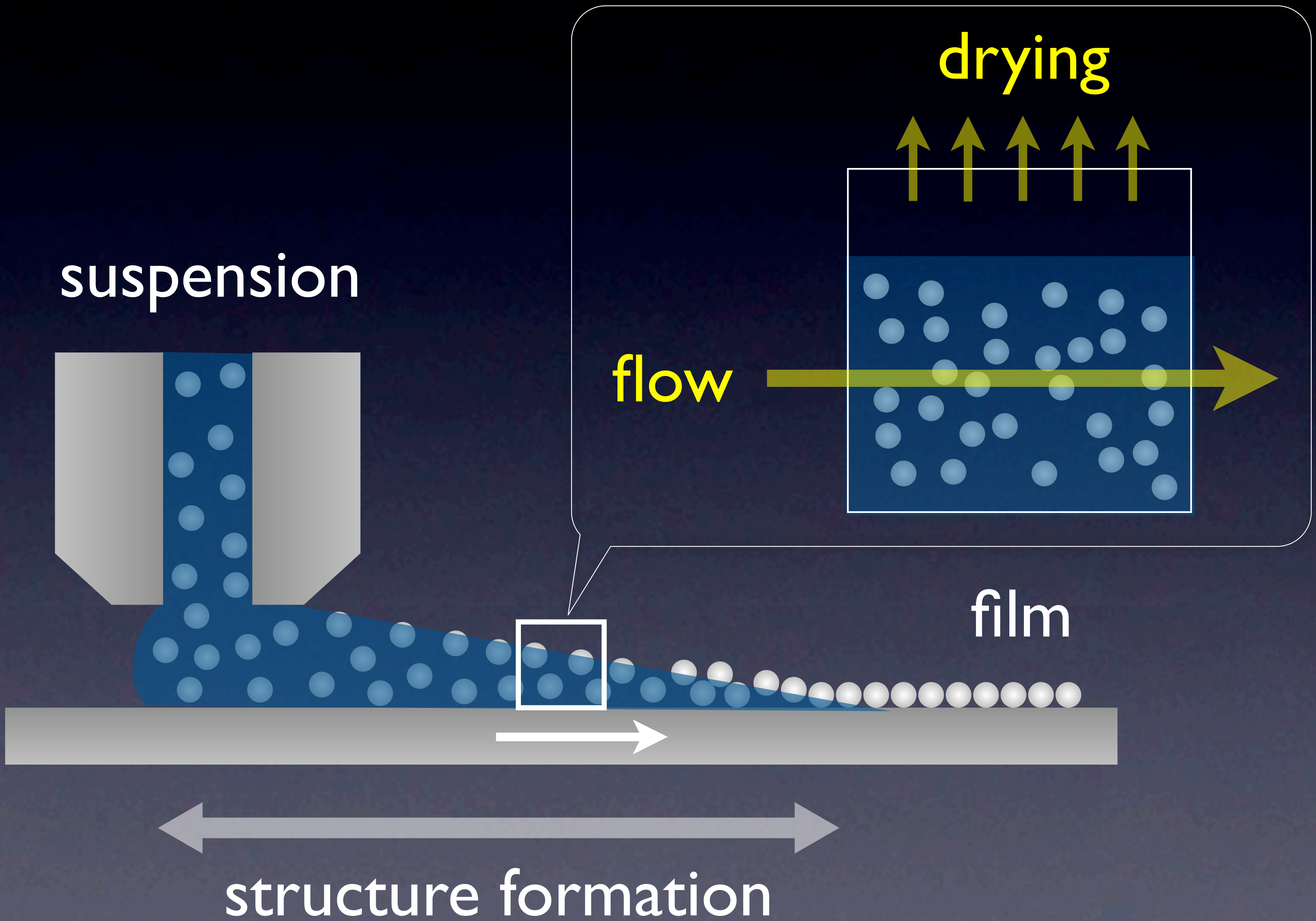
Outline

- Continuous coating of nanoparticles suspension on substrate
- Direct simulation model for nanoparticles suspension in flow and drying
- Demonstration of present simulation model

Continuous coating on substrate



Peclét numbers for flow and drying

flow Peclét number

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

drying Peclét number

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

ratio of Peclét numbers

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

$$\frac{\mathrm{Pe_f}}{\mathrm{Pe_d}} \sim 1$$

→ Both flow and drying influence structure formation

Objectives of this study

- Develop direct simulation model for nanoparticles suspension in flow and drying
- Perform flow and drying simulations of nanoparticles suspension on substrate
- Quantify structure formation of nanoparticles and evaluate effect of ratio of Peclét numbers

Direct simulation model

- Solves gas-liquid two phase flow on lattice using VOF method
- Solves translational motion and rotational motion of each particle
- Couples motion of particle with flow of solvent using fictitious domain method

→ Interparticle hydrodynamic interaction is included without analytical model

Equations of fluid motion

fluctuating stress

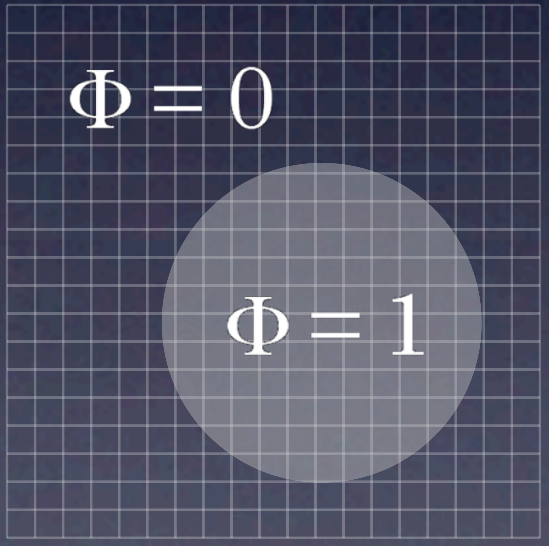
$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla p + \nabla \cdot \mu \{ \nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T \} + \nabla \cdot \boldsymbol{S} + \rho \boldsymbol{g} + \Phi \alpha$$

acceleration

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

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

VOF function



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

evaporation rate

Equations of particle motion

$$m\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}^{\mathrm{co}} + \boldsymbol{F}^{\mathrm{D}} + \boldsymbol{F}^{\mathrm{ca}} + \boldsymbol{F}^{\mathrm{h}} + \left(\rho_{\mathrm{p}} - \rho\right)V_{\mathrm{p}}\boldsymbol{g}$$

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

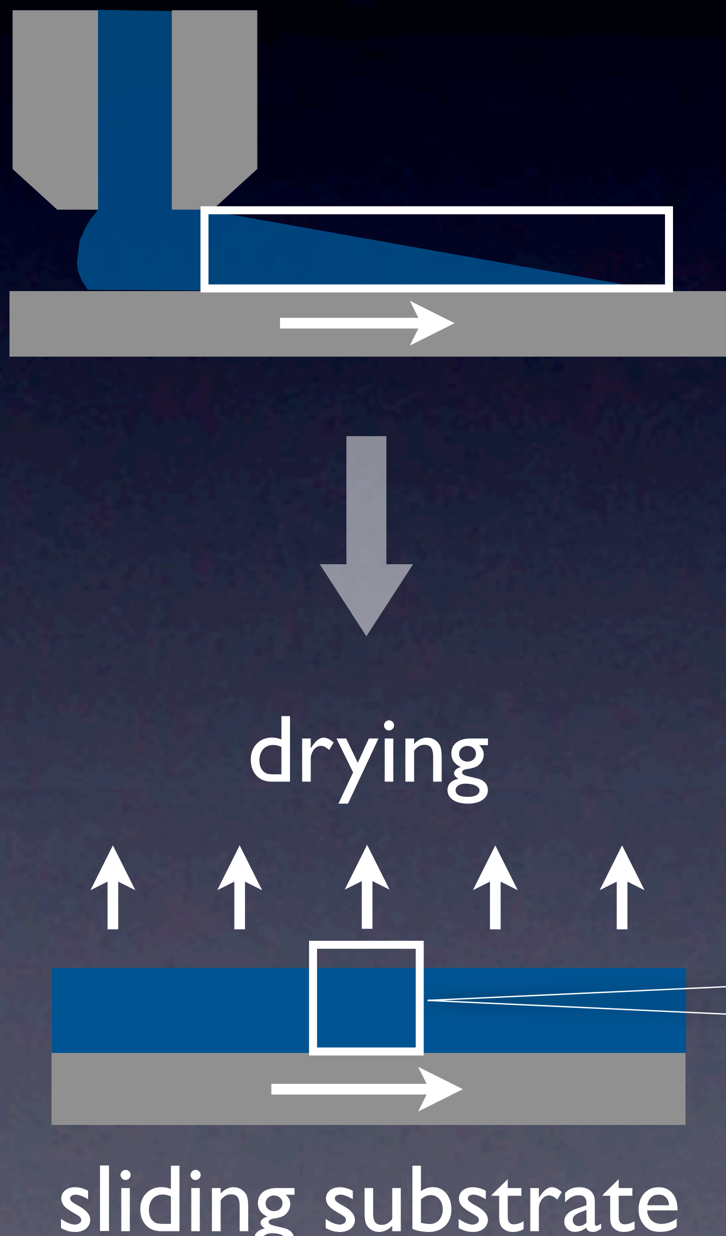
$$\boldsymbol{F}^{\mathrm{h}} = -\int_{V_{\mathrm{p}}} \rho\Phi\underline{\boldsymbol{\alpha}}\,d\boldsymbol{r}$$

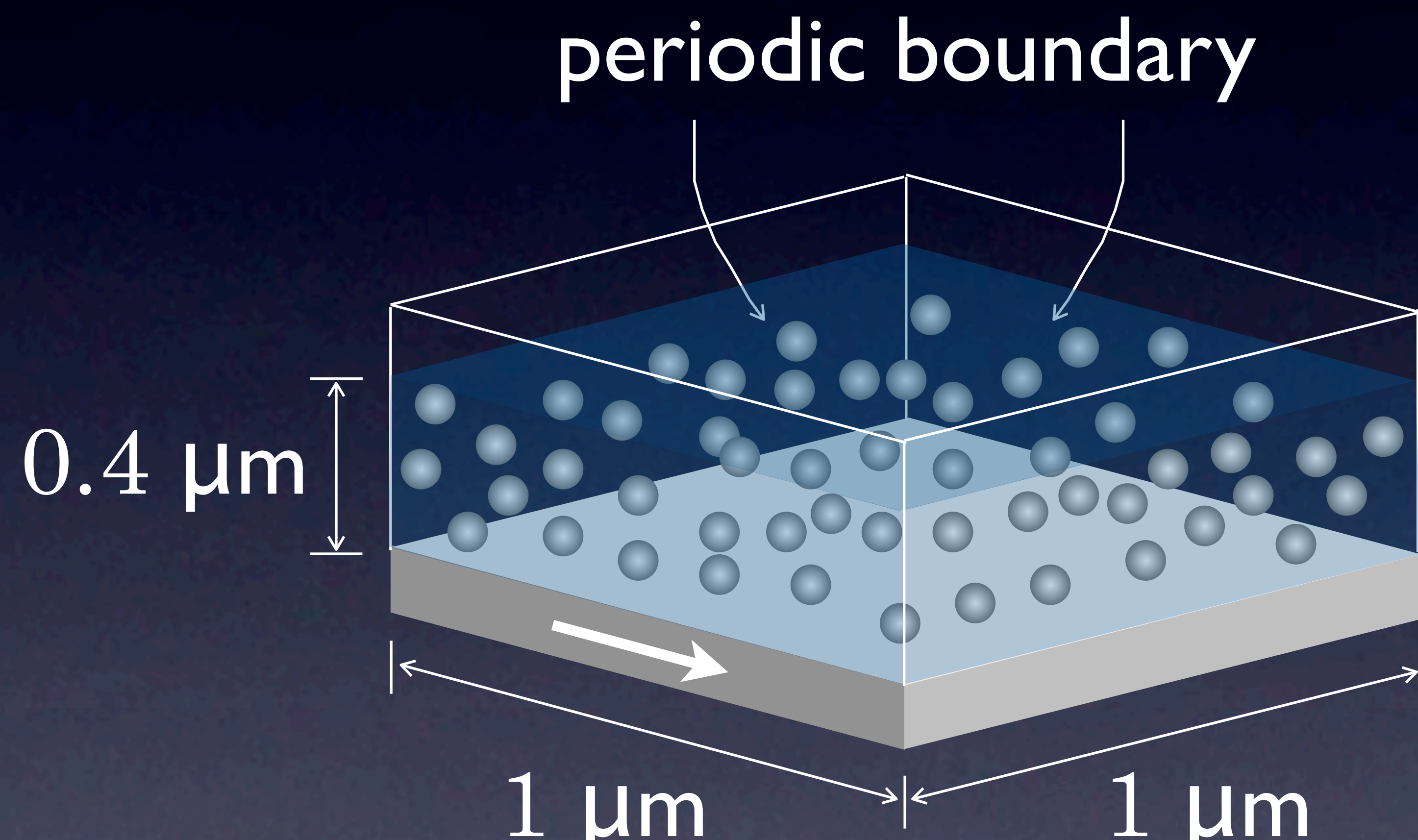
acceleration

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

acceleration

Simulation domain





lattice points = 80 x 80 x 40

Simulation conditions

concentrated repulsive system

- nanoparticles

  $d = 0.1$ μm, $\phi_0 = 15$ vol%, ζ-potential = -50 mV

- solvent

  water in normal temperature, $\mathrm{Pe_d} = 930$

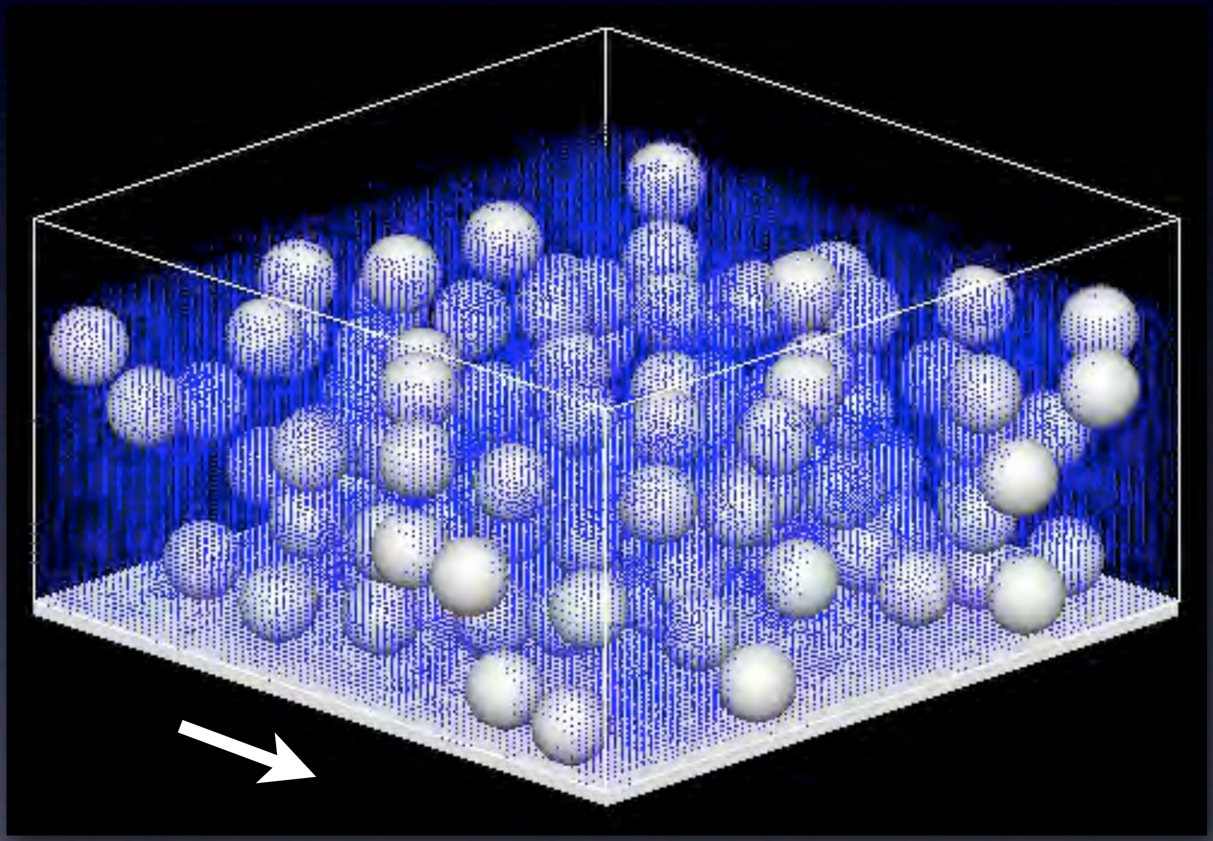
- sliding substrate

  ζ-potential = -50 mV, $\mathrm{Pe_f} = 93, 930$

→ $\mathrm{Pe_f}/\mathrm{Pe_d} = 0.1, 1$

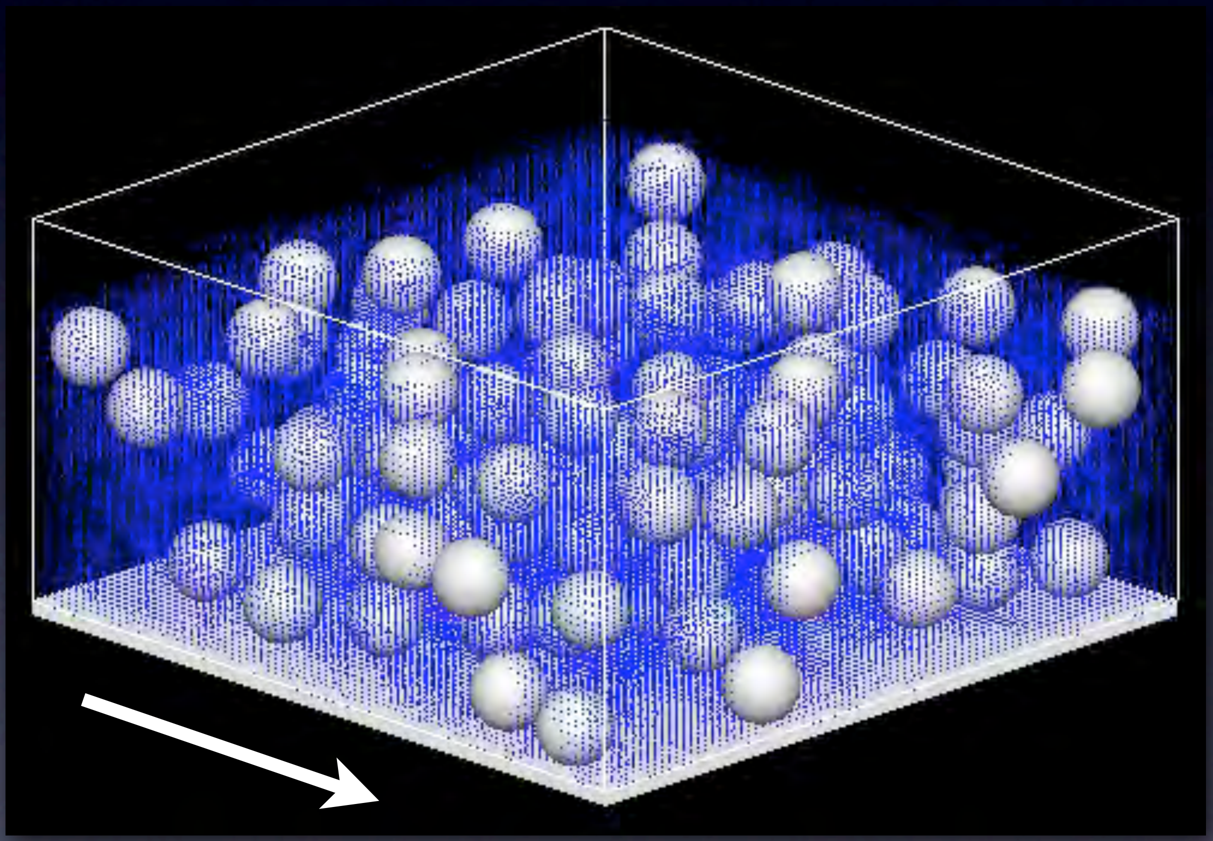
Simulation results

$Pe_f / Pe_d = 0.1$



low speed coating

$Pe_f / Pe_d = 1$

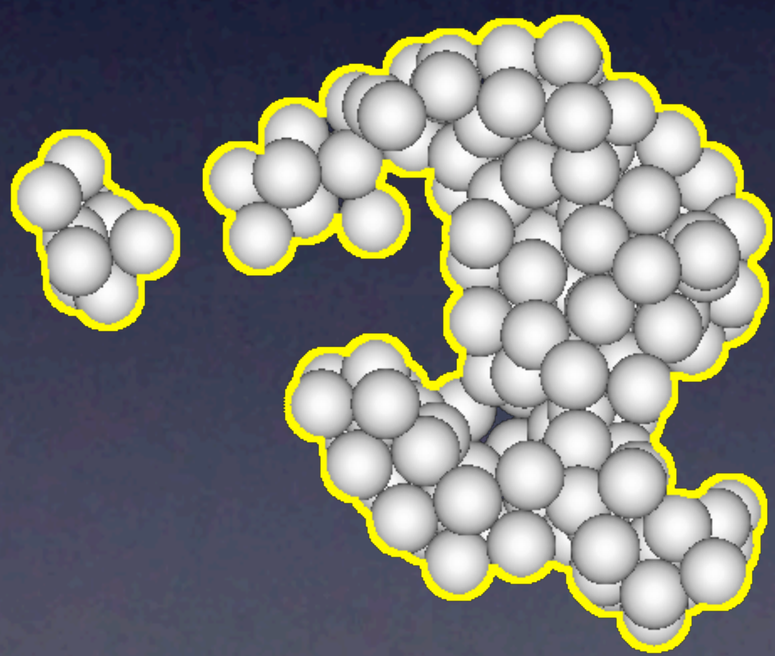


high speed coating

Quantification of structure formation

Non-dimensional Boundary Area (NBA)

$$\mathrm{NBA} = \frac{\text{area of aggregates}}{\text{total area of particles}}$$



$$\mathrm{NBA} = \frac{1}{12N}\sum_{k=0}^{12}\left\{\left(12-k\right)n(k)\right\}$$

k : coordinate number

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

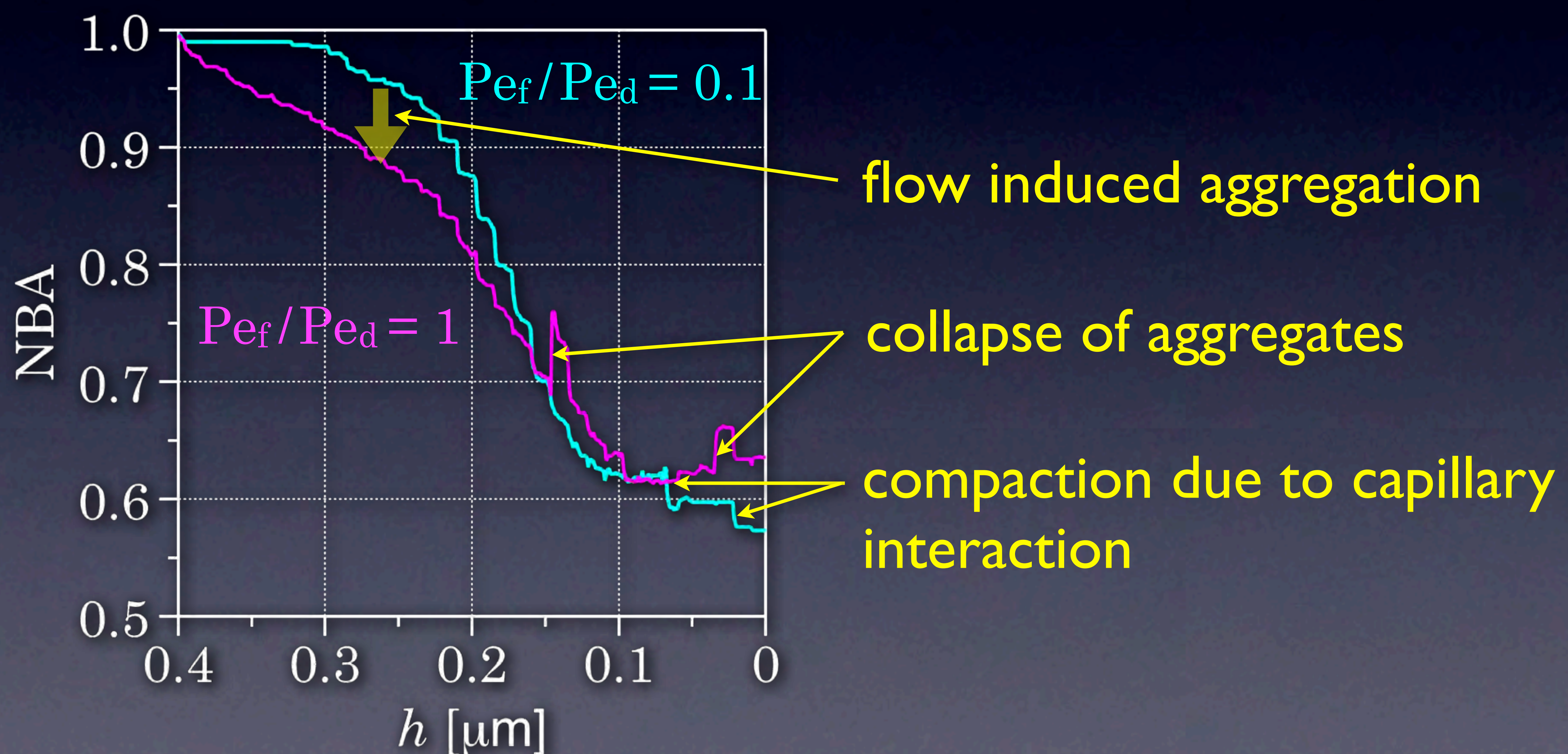
N : total number of particles

$\mathrm{NBA} = 0$: close-packed

$\mathrm{NBA} = 1$: dispersed

Effect of ratio of Peclét numbers

variation of NBA with thickness of wet film



Conclusion

- Developed direct simulation model for nanoparticles suspension in flow and drying
- Quantified structure formation of nanoparticles in flow and drying by use of NBA
- As ratio of Peclét numbers increases, compactness of final structure of nanoparticles decreases.