Direct numerical simulation of pressure driven flow of rod-like fine particle dispersions

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棒状微粒子分散液の圧力駆動流れの直接数値シミュレーション

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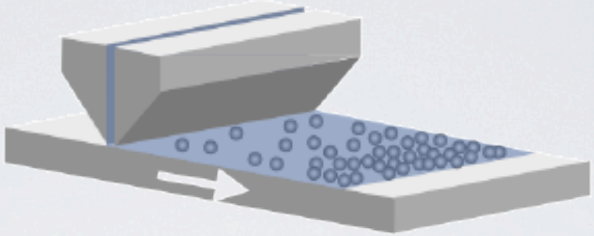
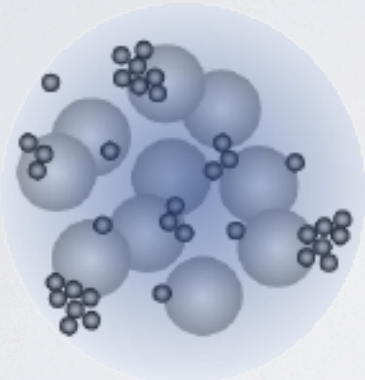
Colloidal Suspensions in Industrial Use

Kneading
Dispersing



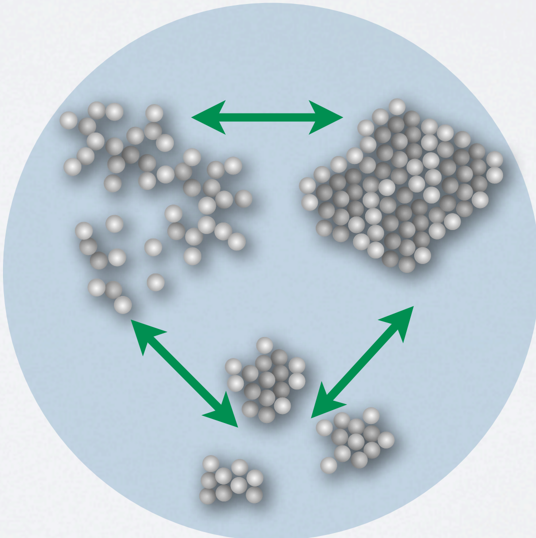
Coating

Chemical
Mechanical
Polishing



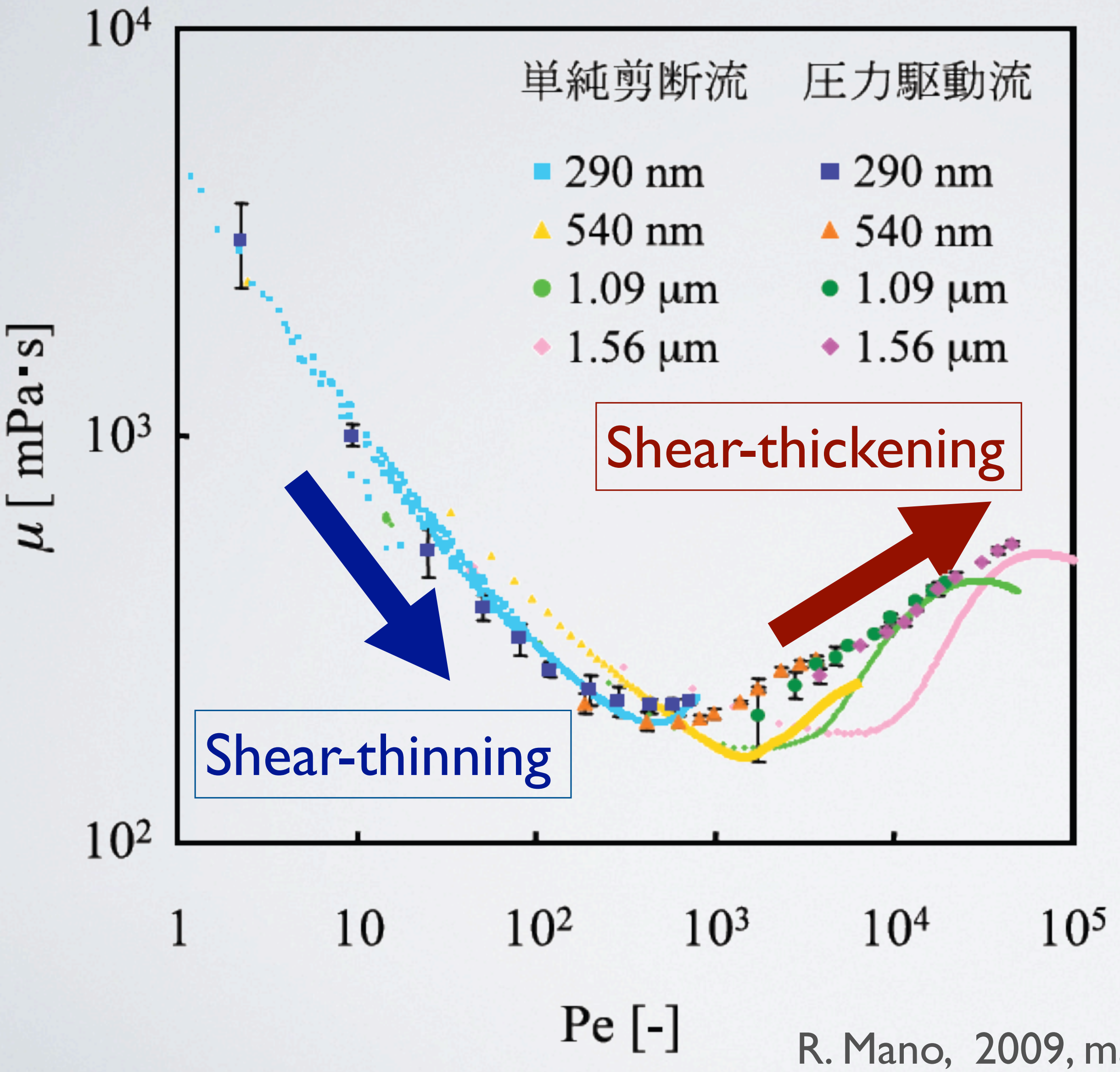
Flow field can induce athermal Particle structures

Contact network
Orietation



Viscosity
Thermal/electrical conductivity
Optical property
Mass diffusivity

Rheology of Suspension



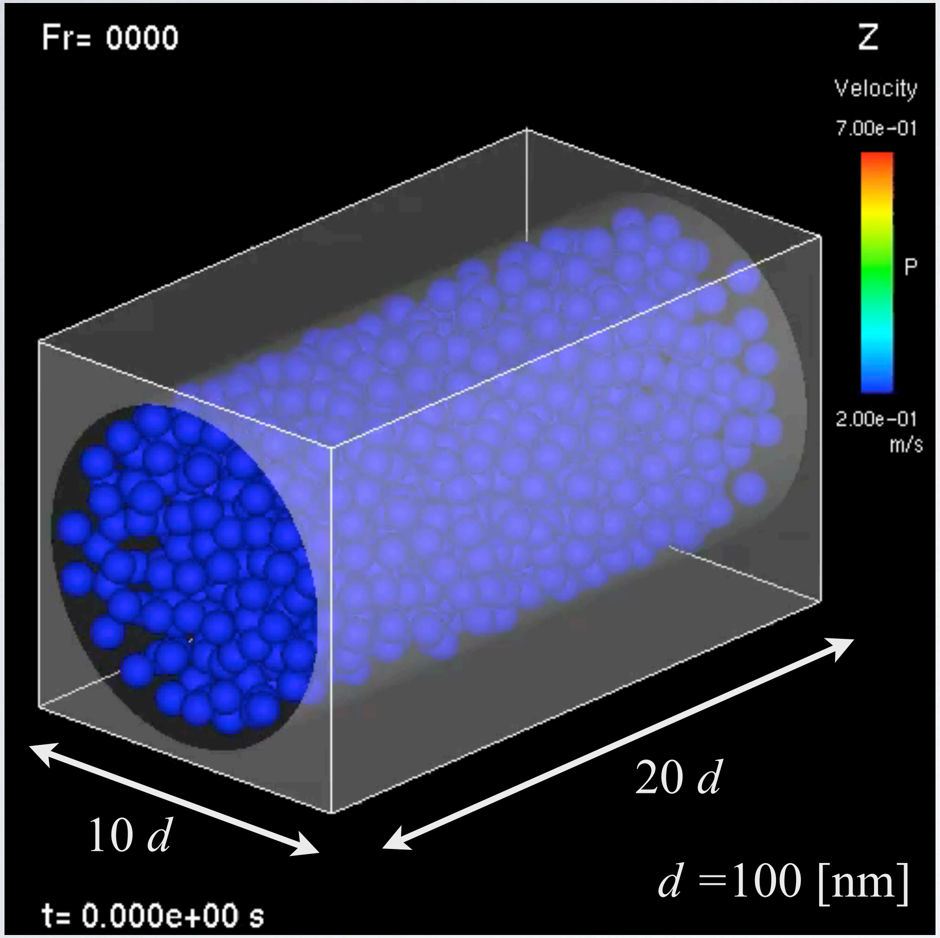
$$Pe = \frac{\dot{\gamma} d^2}{D} \longrightarrow \frac{3\pi\eta_s\dot{\gamma}d^2}{k_B T / d}$$

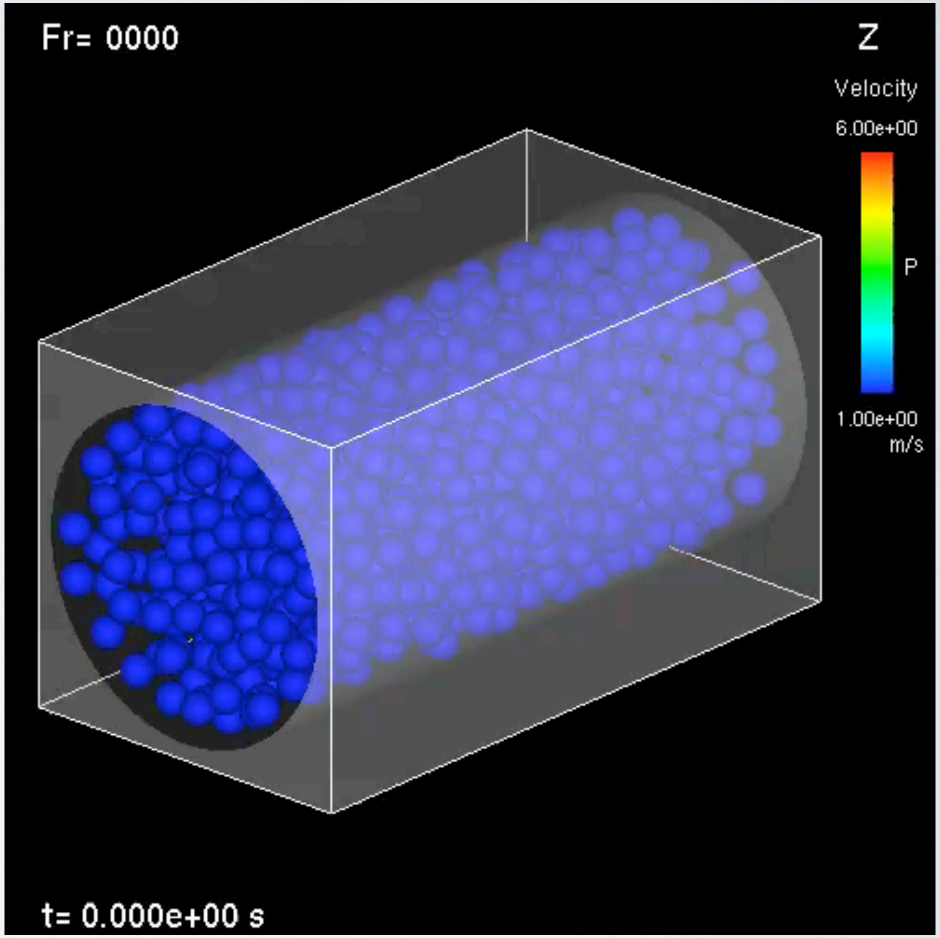
$$\frac{\text{Hydorodynamic force}}{\text{Thermal force}}$$

R. Mano, 2009, master thesis

Pressure Driven Flow of Suspension

Spherical repulsive particle

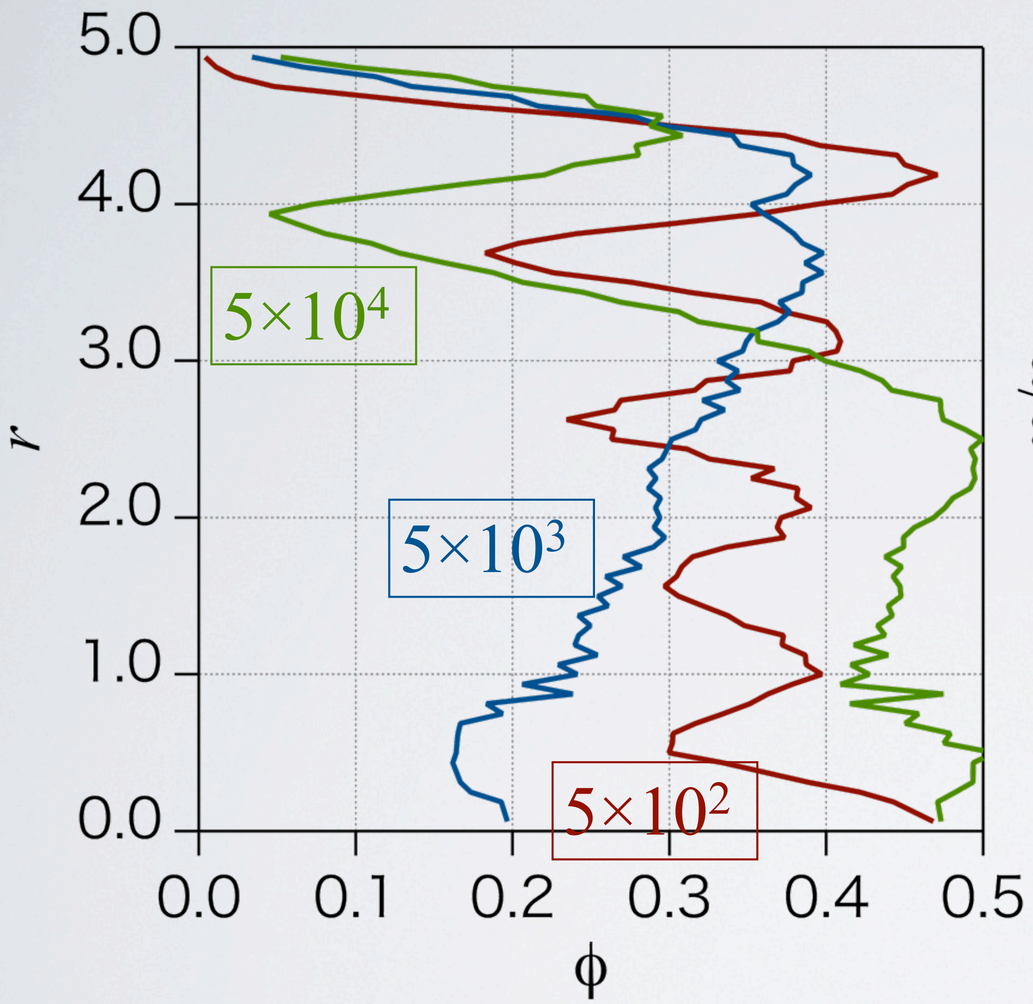




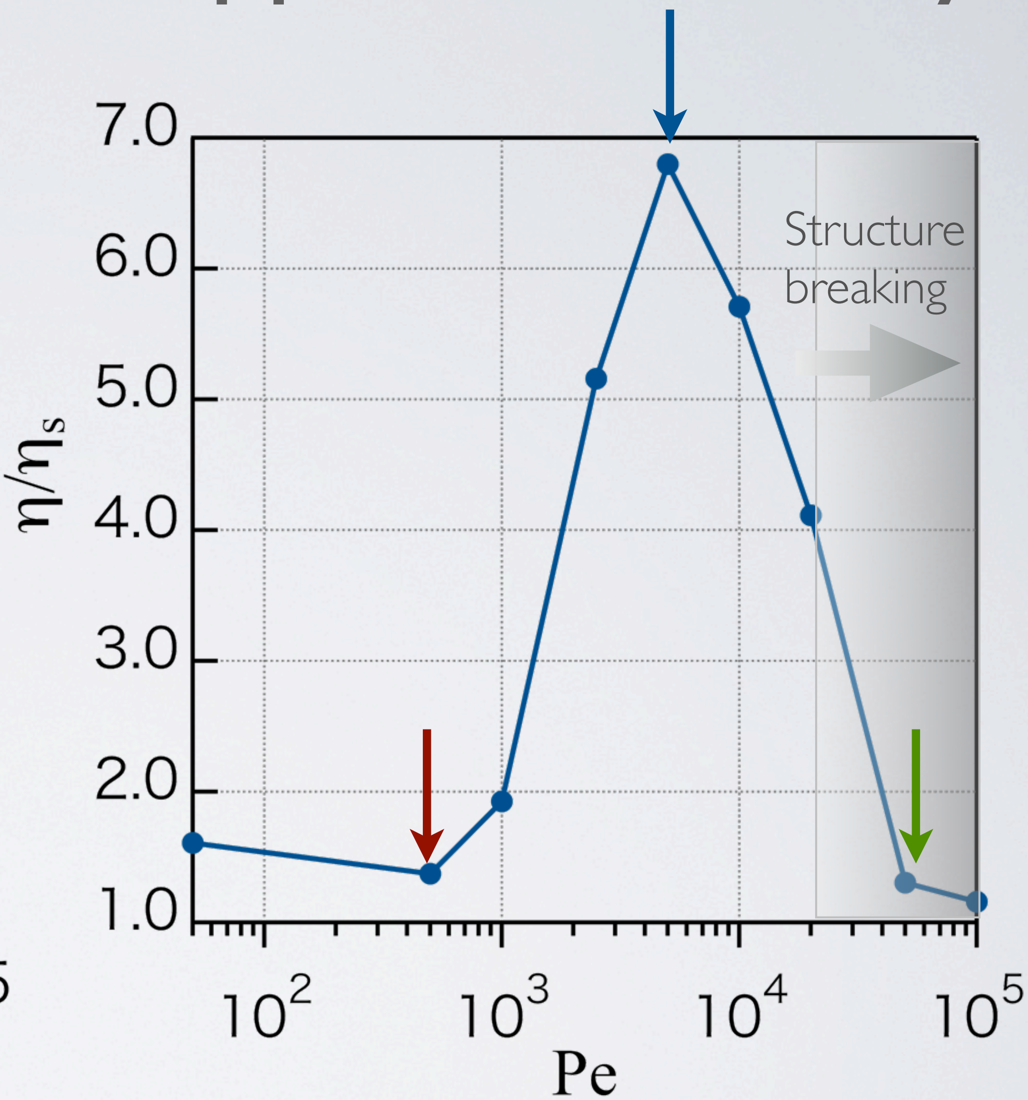
$\mathrm{Pe} = 2\times10^4$ $\varphi_\mathrm{p} = 0.3$ $\mathrm{Pe} = 5\times10^4$

小池・藤田・山口，化工学会第44回秋季大会（2012）

Particle Distribution & Apparent Viscosity



Distribution varies
with flow strength



$$\mathrm{Pe} = \frac{A/d}{k_B T/d}\left(\frac{3\pi\eta_s\dot{\gamma}d^2}{A/d}\right) \approx 10^{(0-1)}\left(\frac{3\pi\eta_s\dot{\gamma}d^2}{A/d}\right)$$

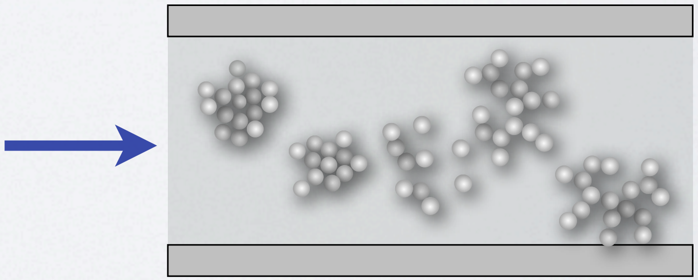
小池・藤田・山口，化工学会第44回秋季大会（2012）

Objective

- To obtain structure formation process of rodlike fine particle dispersions under pressure driven flow
- Is there any difference from the case of spherical ones?

Method

- Direct Numerical Simulation by IBM + DEM (SNAP-F)
- Pressure driven flow inside a plane-parallel channel



Equation of Fluid Motion

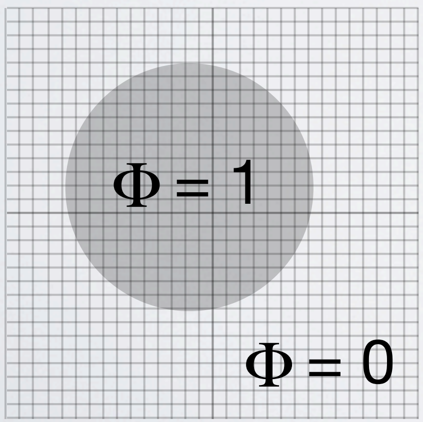
Immersed Boundary Method

Mass : $\nabla \cdot \boldsymbol{v} = 0$

Random force

Momentum: $\dfrac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla p + \nu \nabla^2 \boldsymbol{v} + \dfrac{1}{\rho_{\mathrm{f}}} \nabla \cdot \boldsymbol{S} + \Phi \boldsymbol{\alpha}$

Coupling term of fluid with solid : $\alpha = \dfrac{\boldsymbol{v}_{\mathrm{p}} - \boldsymbol{v}}{\Delta t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} - \nu \nabla^2 \boldsymbol{v} - \dfrac{1}{\rho_{\mathrm{f}}} \nabla \cdot \boldsymbol{S}$



$$\boldsymbol{F}^{\mathrm{h}} = -\int_V \rho_{\mathrm{f}} \phi_{\mathrm{p}}(\boldsymbol{x}) \alpha(\boldsymbol{x}) dV$$

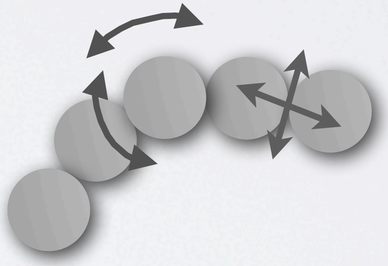
$$\boldsymbol{T}^{\mathrm{h}} = -\int_V \left\{ \boldsymbol{r}_{\mathrm{p}}(\boldsymbol{x}) \times \rho_{\mathrm{f}} \phi_{\mathrm{p}}(\boldsymbol{x}) \alpha(\boldsymbol{x}) \right\} dV$$

Equation of Bead Motion

DLVO

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

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



DEM ＋ Coulomb's friction

$$\left|\boldsymbol{F}_\mathrm{t}^\mathrm{co}\right| = \min\left(\left|\boldsymbol{F}_\mathrm{t}^\mathrm{co}\right|, \mu\left|\boldsymbol{F}_n^\mathrm{co}\right|\right)$$

Nonslip condition inside rod

$$\boldsymbol{v}_i + a\boldsymbol{\omega}_i \times \boldsymbol{n}_{ij} = \boldsymbol{v}_j + a\boldsymbol{\omega}_j \times \boldsymbol{n}_{ji}$$

Simulation Condition

Particle

d [nm] : 100

φ_{p} : 0.1

ζ [mV] : -50

Fluid

c [M] : 10^{-1}

Pe $/10^4$: 2, 5

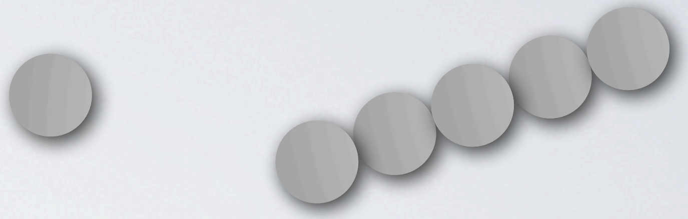
T [K] : 293.15

*Shear rate 4.3×10^{6} [s^{-1}]

for Pe $/10^4 = 1$

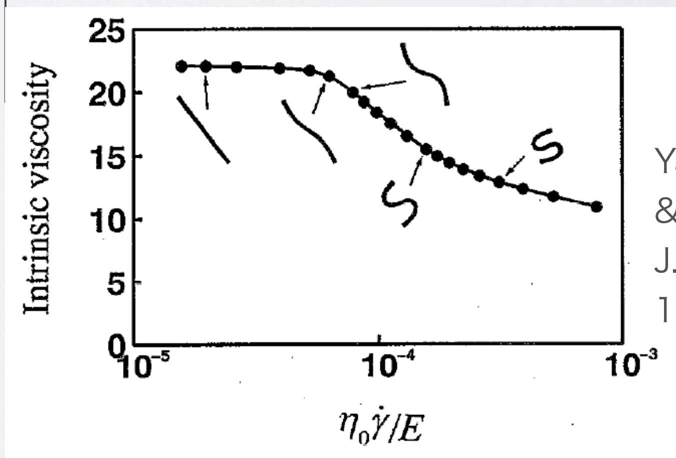
Aspect ratio

r_{p} : 1, 5



Field strength / rod strength

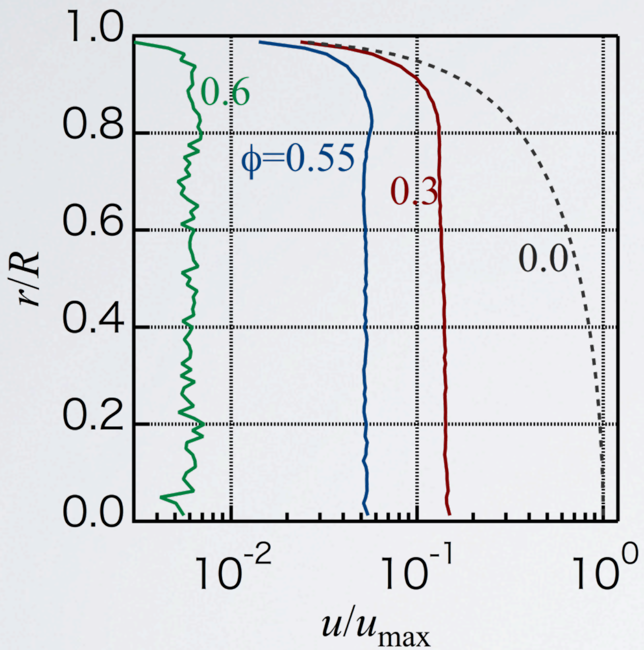
$$\frac{\eta_s\dot{\gamma}}{E} \sim 10^{-5} : \text{rigid}$$



Yamamoto & Matsuoka J. Chem. Phys. , 100 (1994) 3317

Apparent Viscosity

Apparent viscosity : $\eta = \dfrac{Q_{\phi=0}}{Q}\eta_s$



: Indirect but simple method

$$Q_{\phi=0} = \frac{SH^2}{g\eta_s}\left|\nabla P\right|$$

: flow rate without solids

Estimate η
by volume flow rate Q

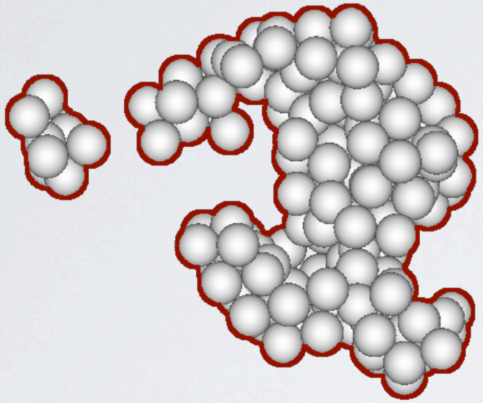
S : corss section of flow path,

H : height of flow path

$g = 12\ (32)$: channel (pipe)

Nondimensional Boundary Area

NBA



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

Definition of NBA

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

$n(c)$ ：number of particles with coordination number of c

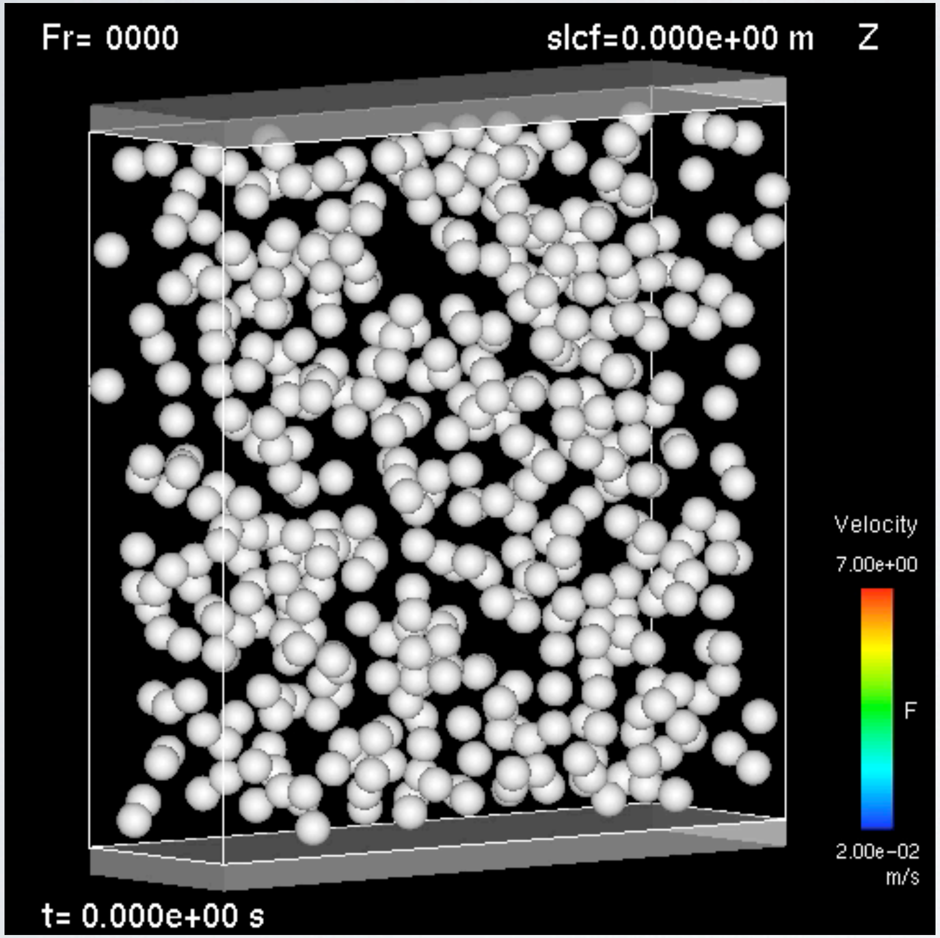
N ：total number of particles

NBA = 1 : completely dispersed

NBA = 0 : close-packed

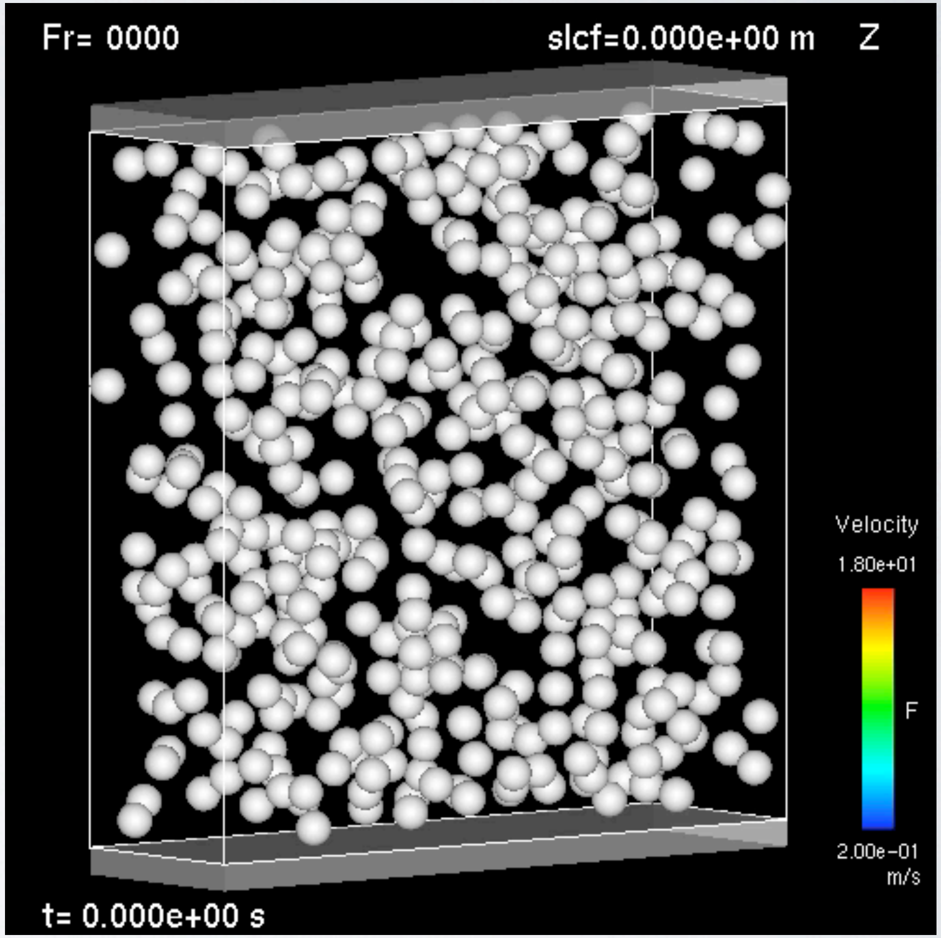
Result　Case: 

Agglomerates



$Pe = 2\times10^4$

Disperses

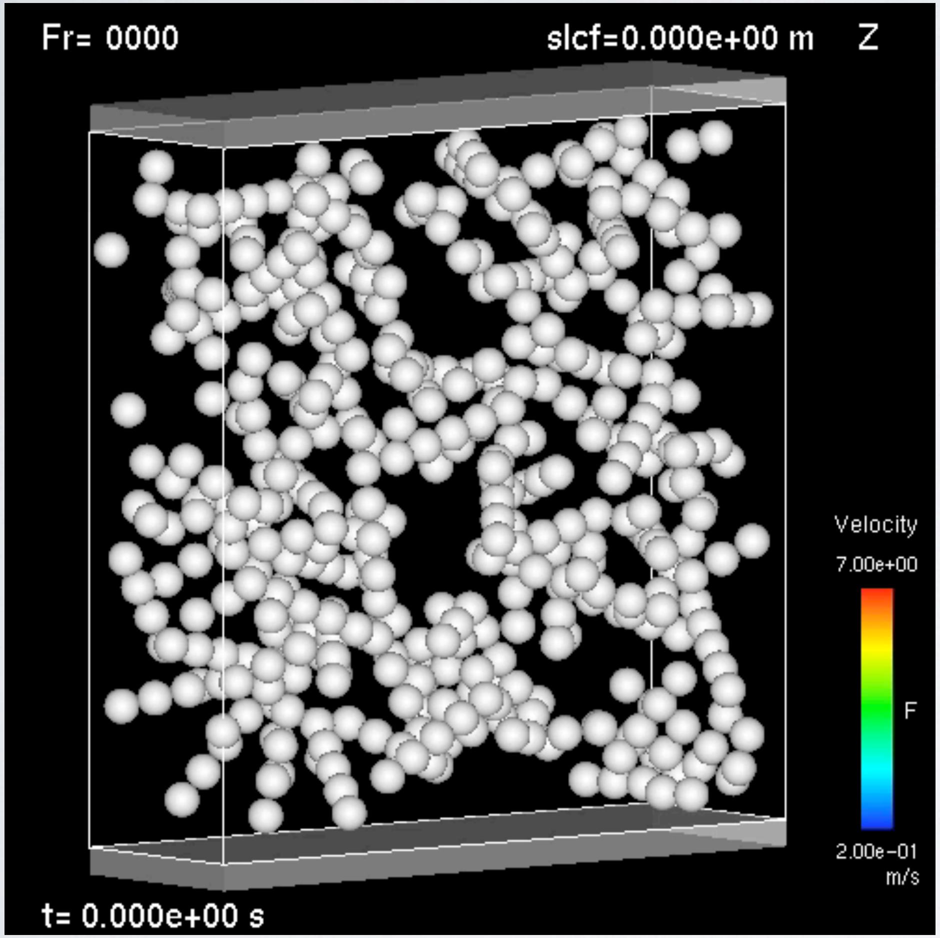


$Pe = 5\times10^4$

$\varphi_p = 0.1$

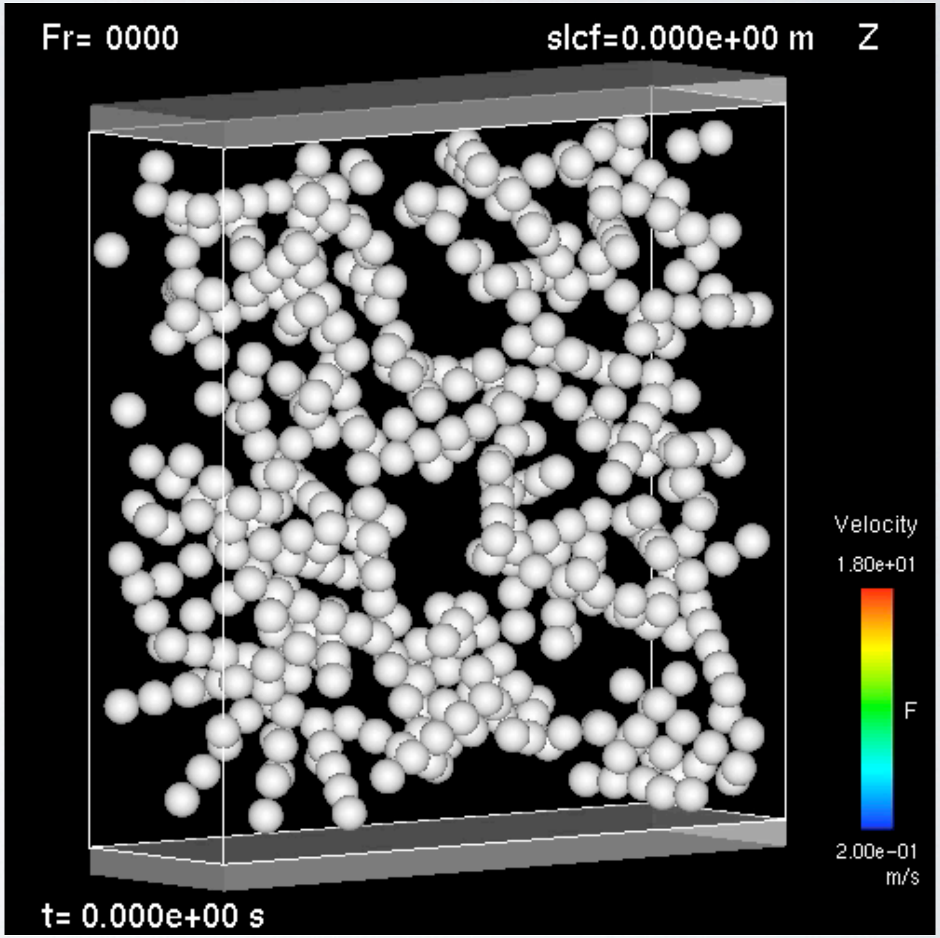
Result Case:

Agglomerates



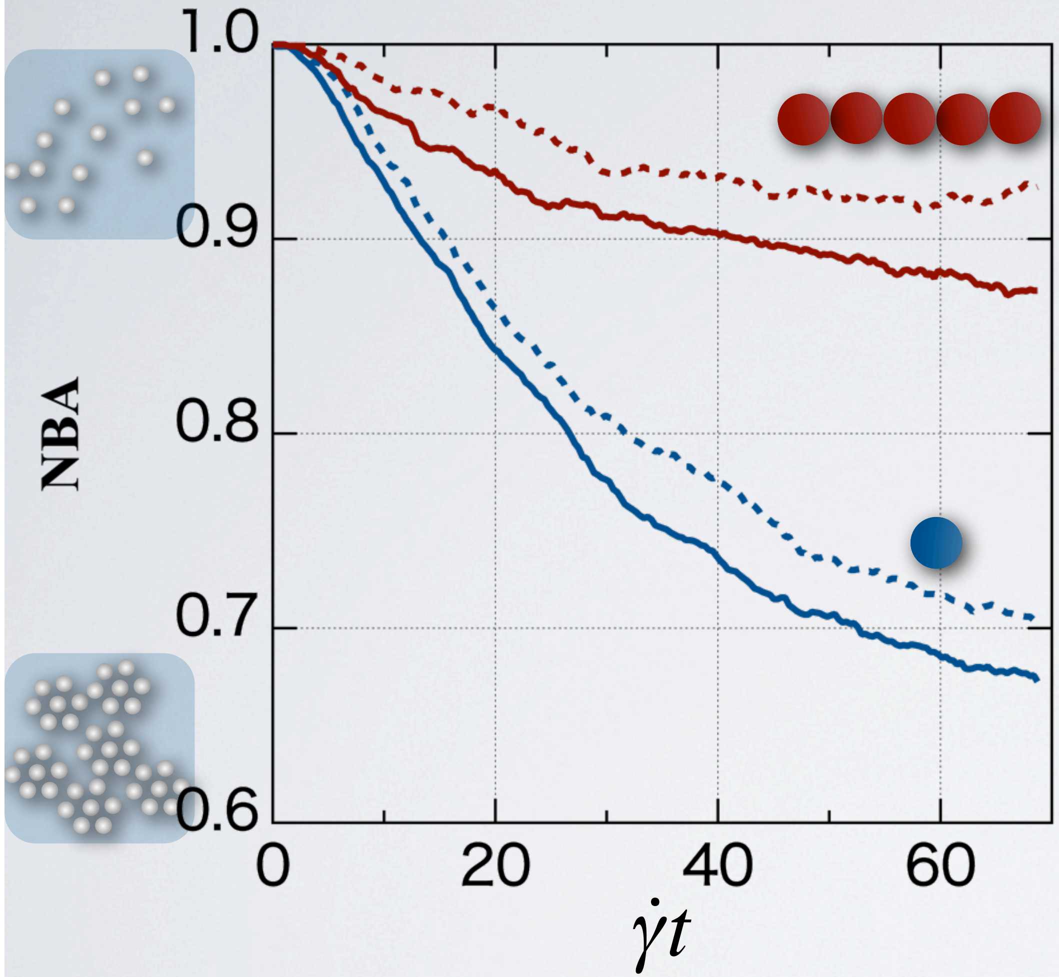
$Pe = 2 \times 10^4$

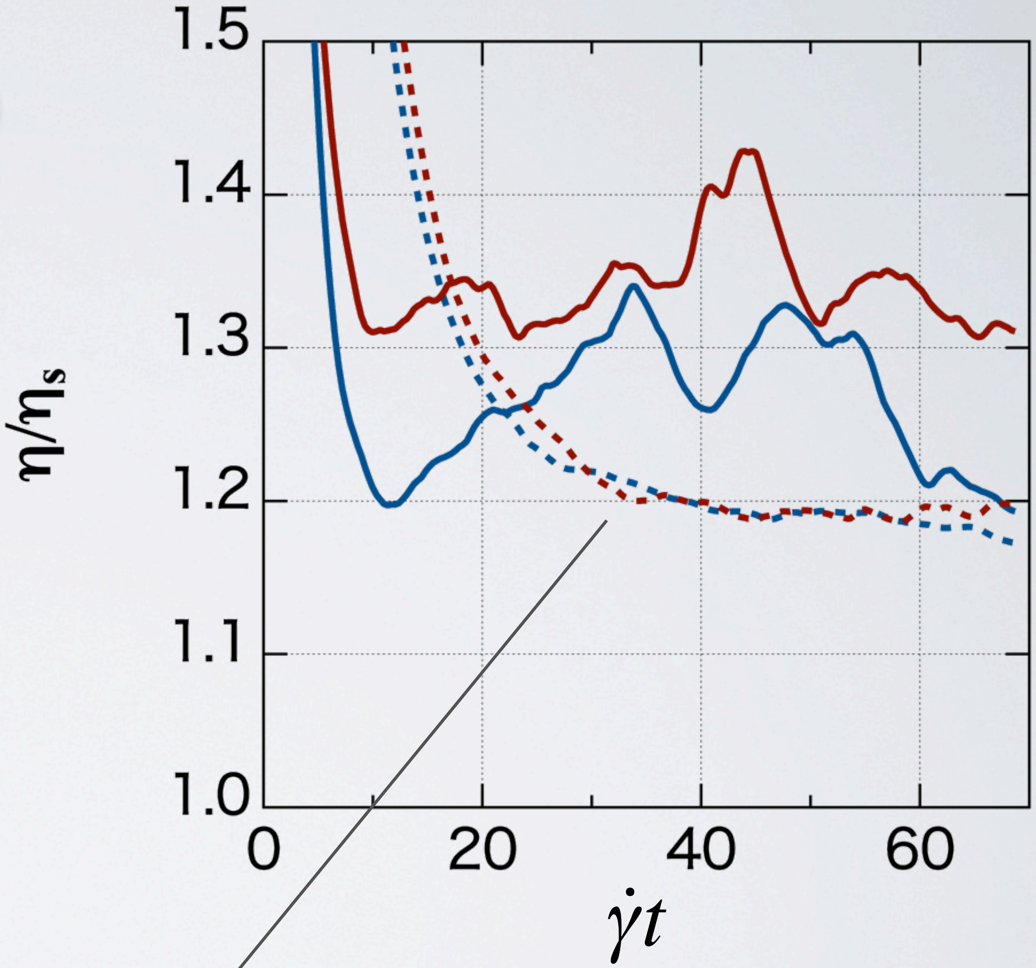
Disperses



$Pe = 5 \times 10^4$

NBA & Apparent Viscosity





$\mathrm{Pe} = 5\times10^4$ - - - - - - - - - - - -

$\mathrm{Pe} = 2\times10^4$ ————————

Higher shear increases the fluidity of dispersion

Concluding Remarks

- DNS gives the micro-scale structures
  of fine particle dispersions under flow
- DNS can give us criterion of orientation/deformation
  specific to rodlike particles
- Is there any difference from the case of spherical ones?
  >> Basically same :
  Criterion for agglomerating or dispersing