A study on rheology mechanism of bimodal nano-particle dispersions by DNS

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直接数値計算による二峰性ナノ粒子分散液の流動メカニズムの検討

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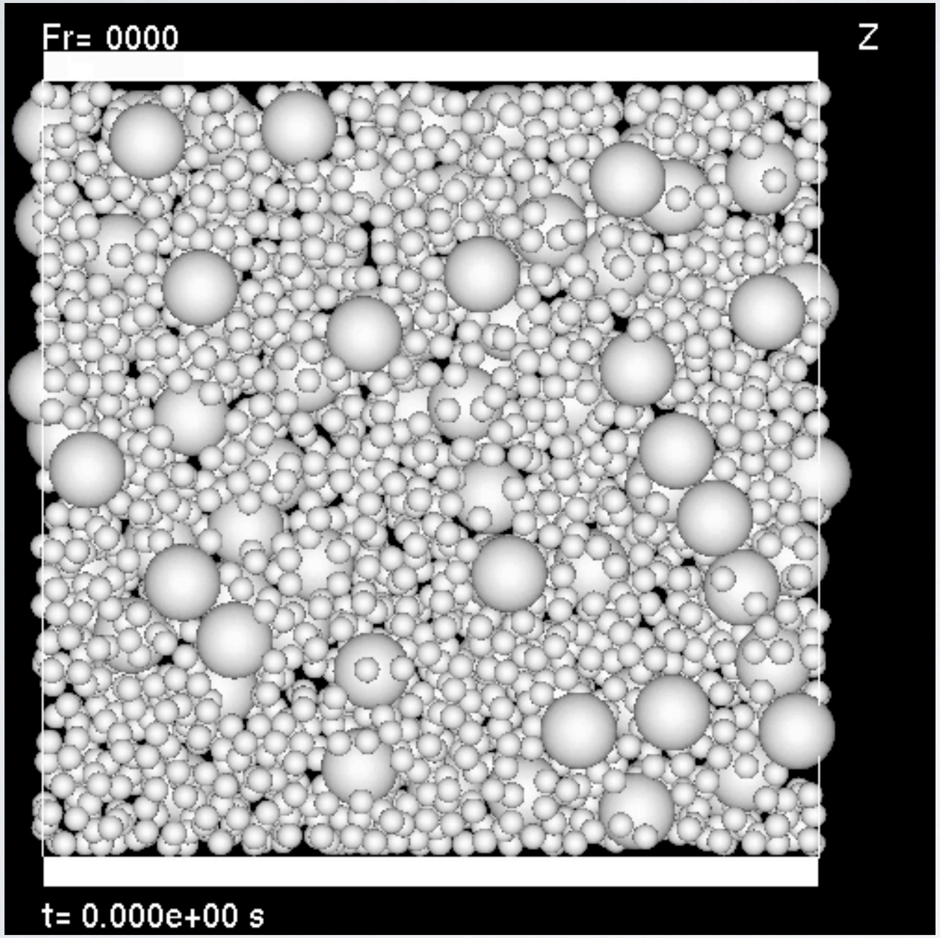
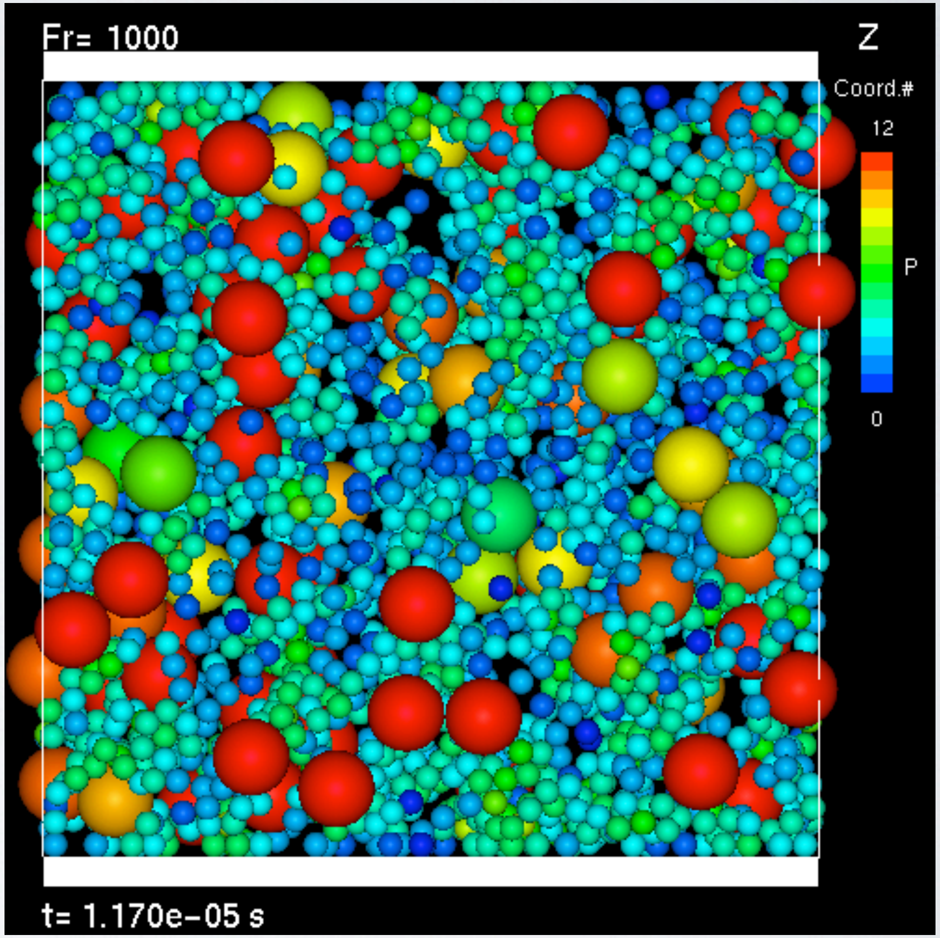
Flow of Bimodal Suspension

Demo (attractive system)



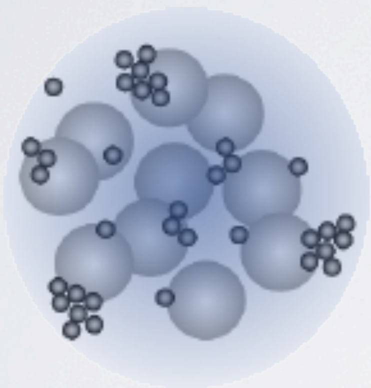


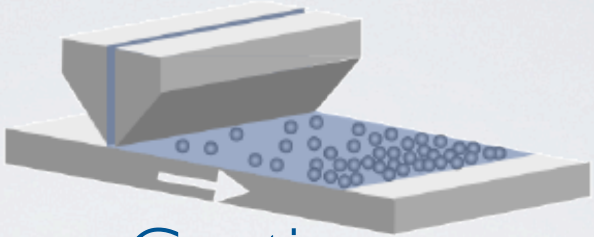
Size ratio, λ : 3

Coordination number

Colloidal Suspensions in Industrial Use

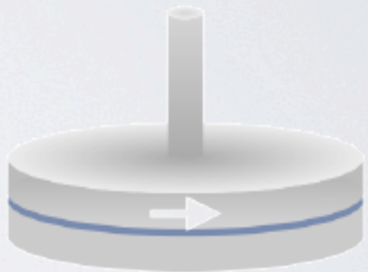
Kneading
Dispersing



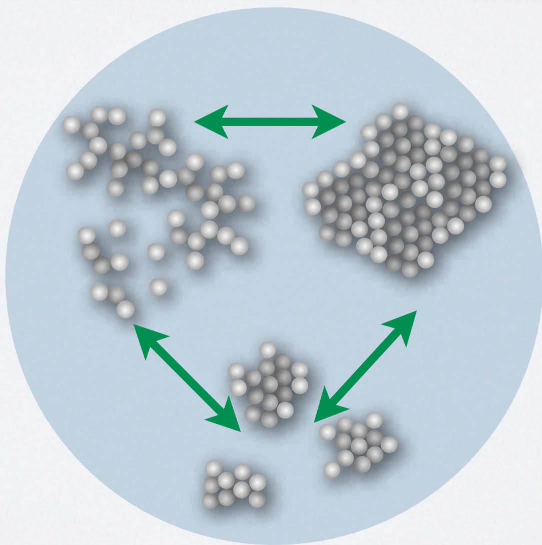


Coating

Chemical
Mechanical
Polishing

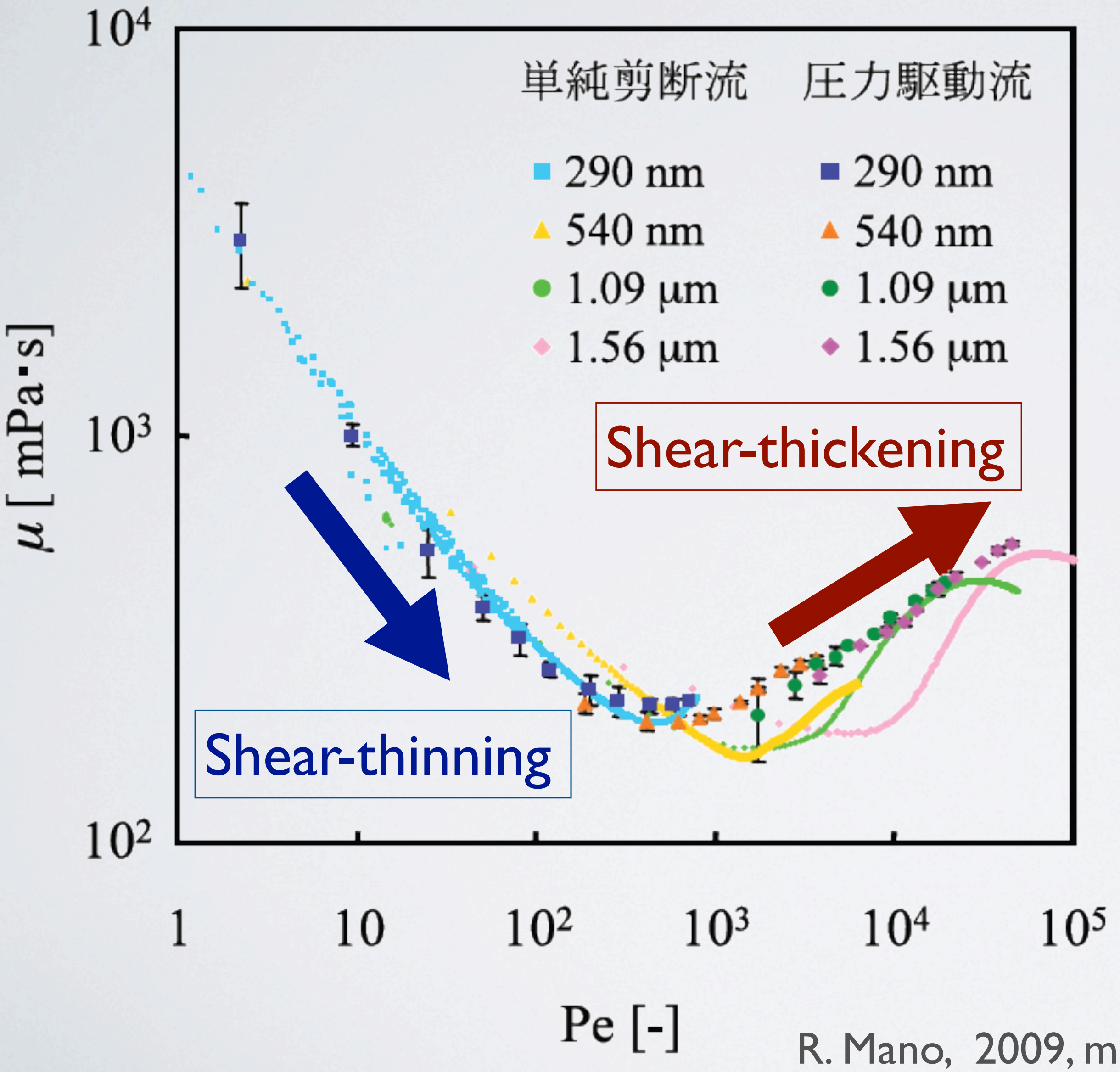


Flow field can induce athermal Particle structures



Rheology of Suspension

Mono-dispersed system



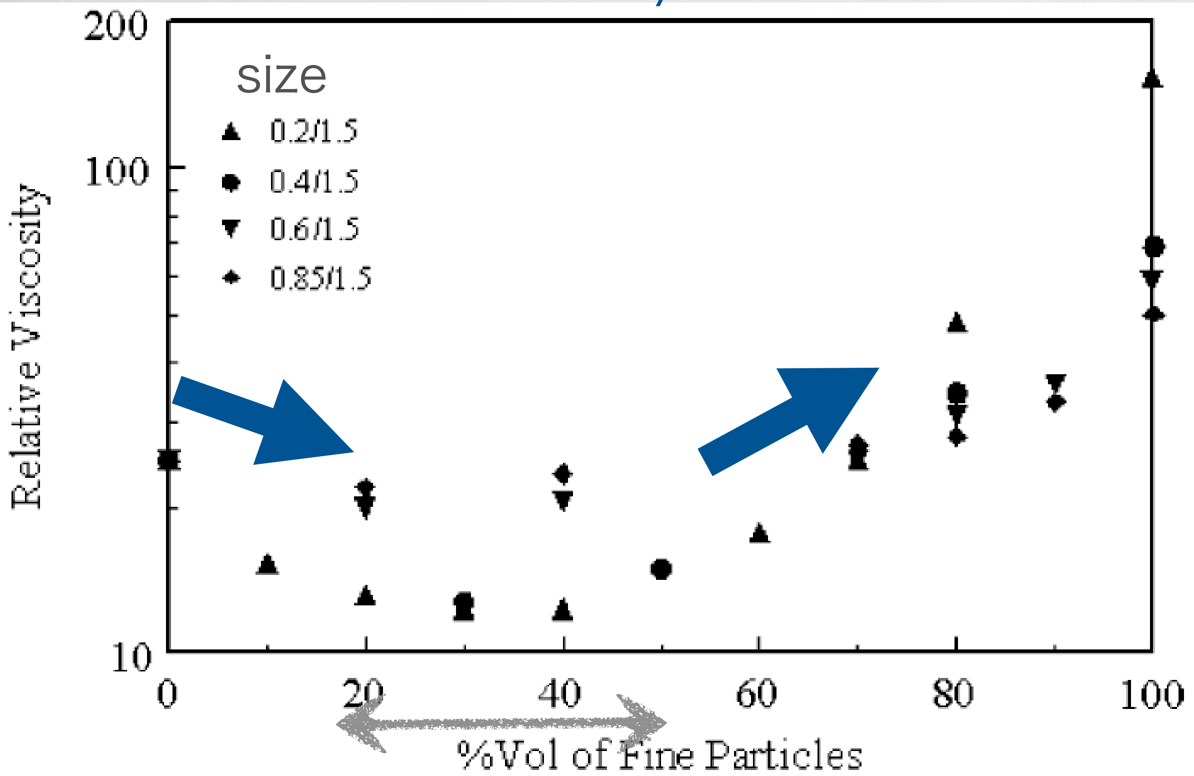
$$Pe = \frac{\dot{\gamma} d^2}{D} \rightarrow \frac{3\pi \eta_s \dot{\gamma} d^2}{k_B T / d}$$

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

R. Mano, 2009, master thesis

Rheology of Suspension

Bimodal system



ig. 10. Relative viscosity as a function of the amount of fine particle
ı bidisperse suspensions of silica particles at 55 vol% containing 1.5 μr
oarse particles (25°C, pH = 9.5, 0.01*M* NaCl).

Trimodal system

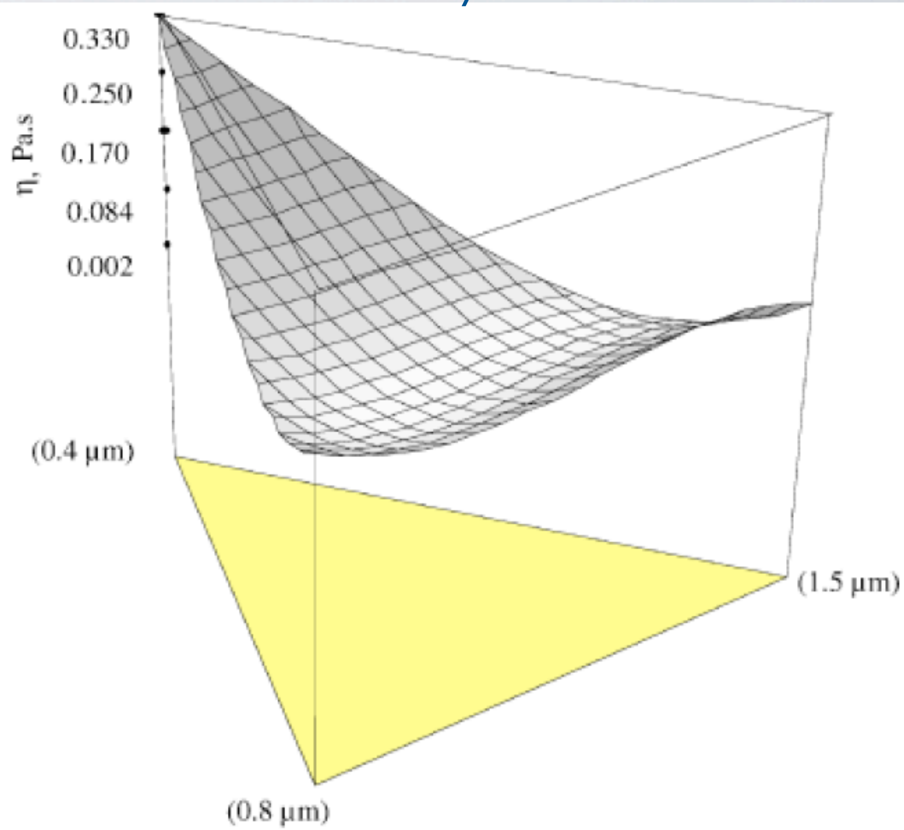


Fig. 15. Three-dimensional surface response plot for the viscosity of trimodal silica suspensions at 55 vol% at a shear rate of 1000 s^{-1} (25°C, pH = 9.5, 0.01*M* NaCl).

*Shear rate 10^3 [s^{-1}]

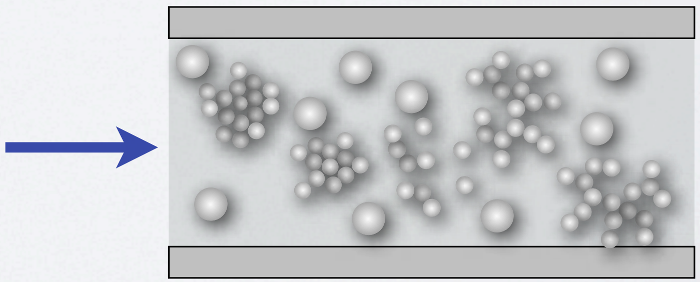
A. A. Zaman & C. S. Dutcher,
J. Am. Ceram. Soc., 89 (2006) 422

Objective

- To Obtain key factors in constructing rheology of bimodal nano-particle dispersions

Method

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



Equation of Fluid Motion

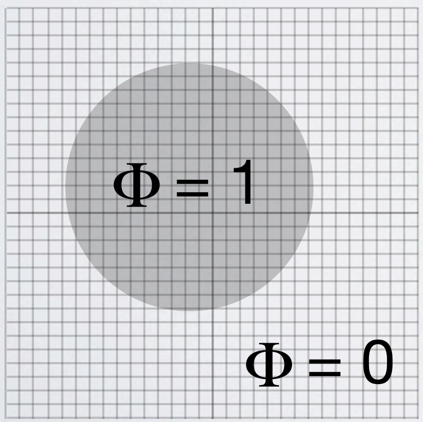
Immersed Boundary Method

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

Random force

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

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



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

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

Equation of Particle Motion

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

DLVO

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

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

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

DEM ＋ Coulomb's friction

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

Simulation Condition

Case A

Particle

d [nm] : 200, 100

φ_p : 0.4

ζ [mV] : -50

Fluid

c [M] : 10^{-3}, 10^{-1}

Pe : 8×10^4

T [K] : 293.15

*Shear rate 4×10^6 [s^{-1}]

Case B

Particle

d [nm] : 1000, 500

φ_p : 0.5

ζ [mV] : -50

Fluid

c [M] : 10^{-2}

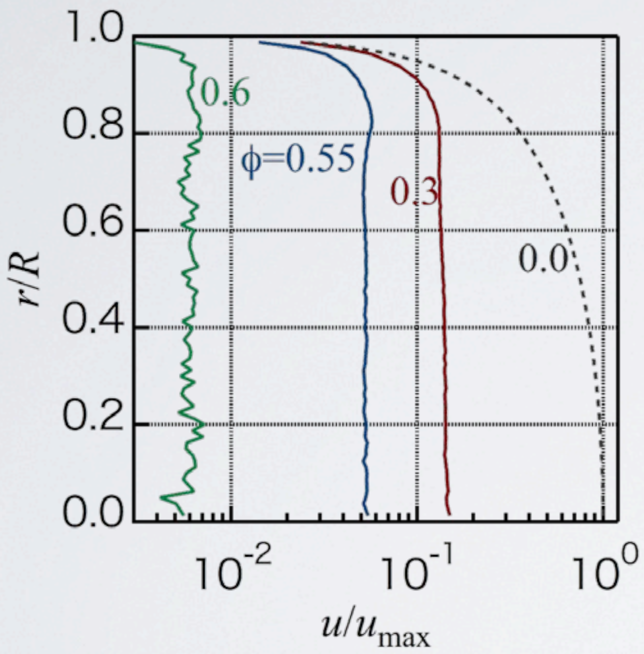
Pe : $(2, 10)\times10^4$

T [K] : 293.15

*Shear rate $(8, 40)\times10^3$ [s^{-1}]

Apparent Viscosity

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



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

：flow rate without solids

Estimate η
by volume flow rate Q

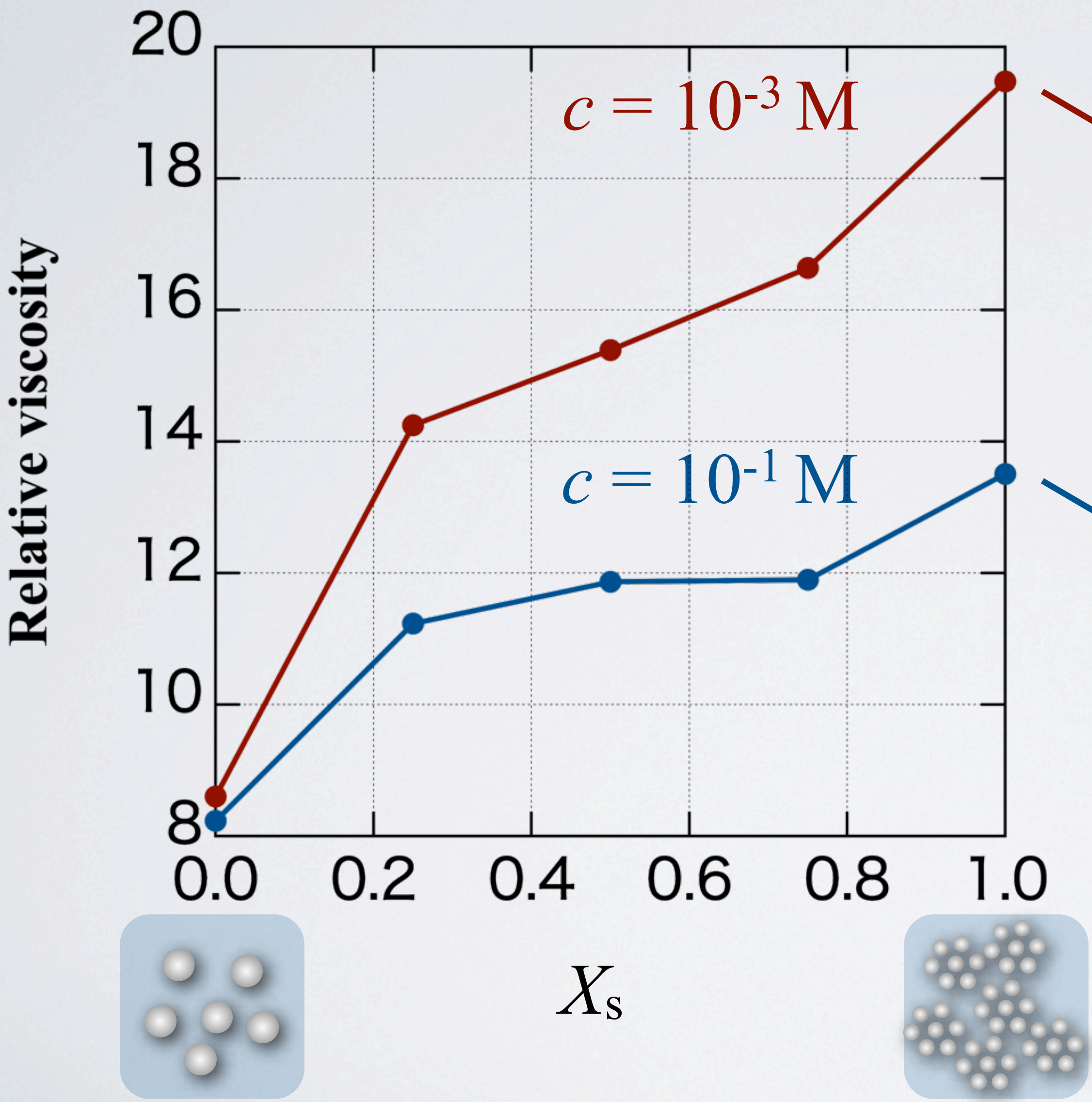
S ： corss section of flow path,

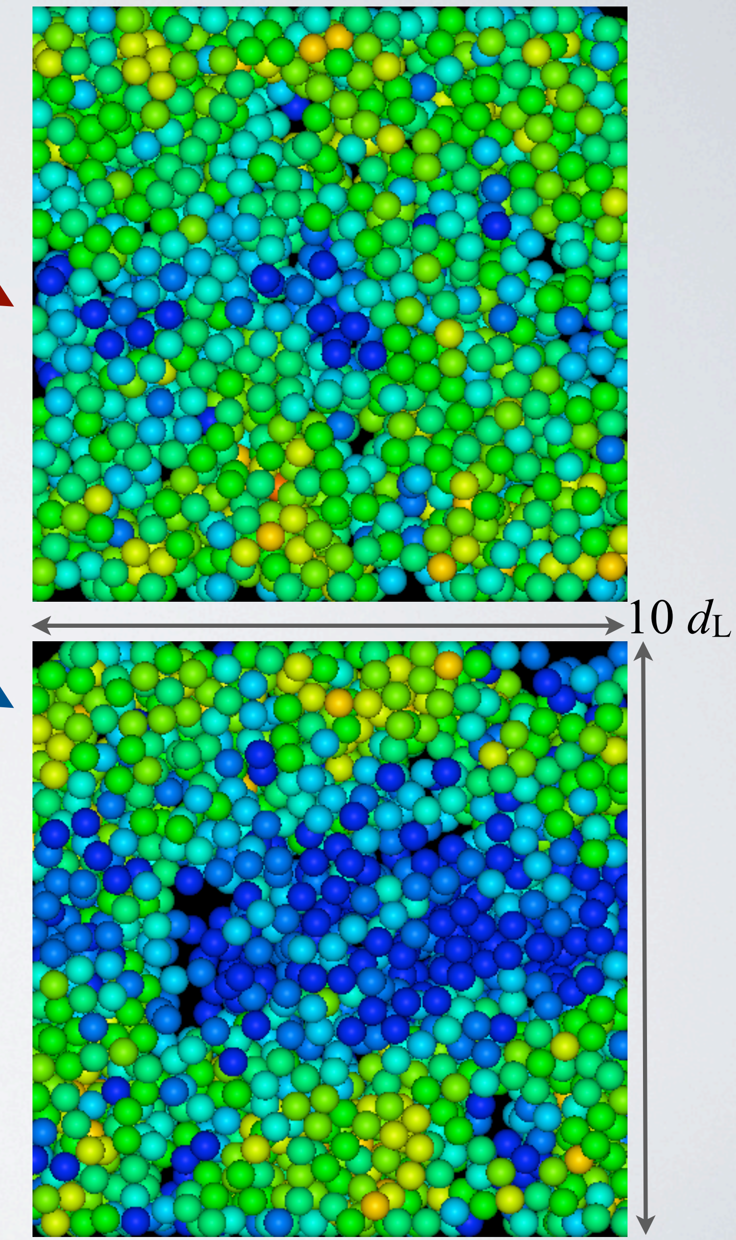
H ： height of flow path

$g = 12\ (32)$ ：channel (pipe)

Result - Case A -

Pe = 8×10^4



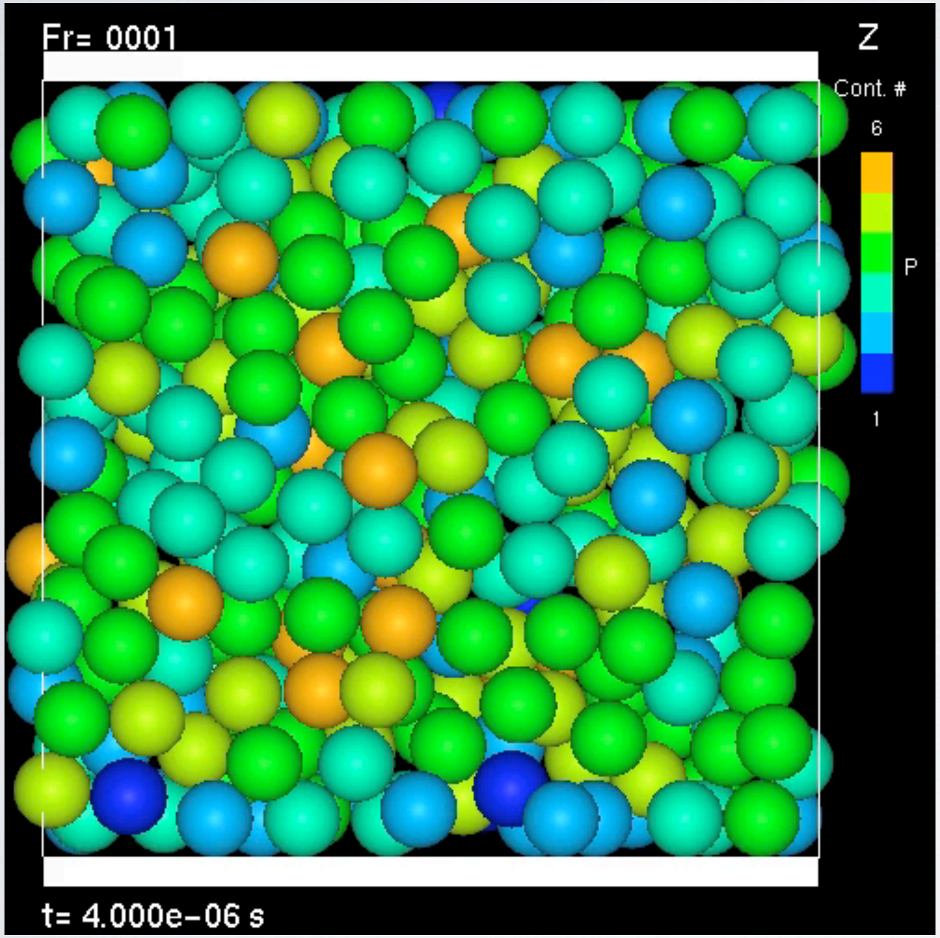


d = 200, 100 [nm], $\varphi_p = 0.4$

Result - Case B -

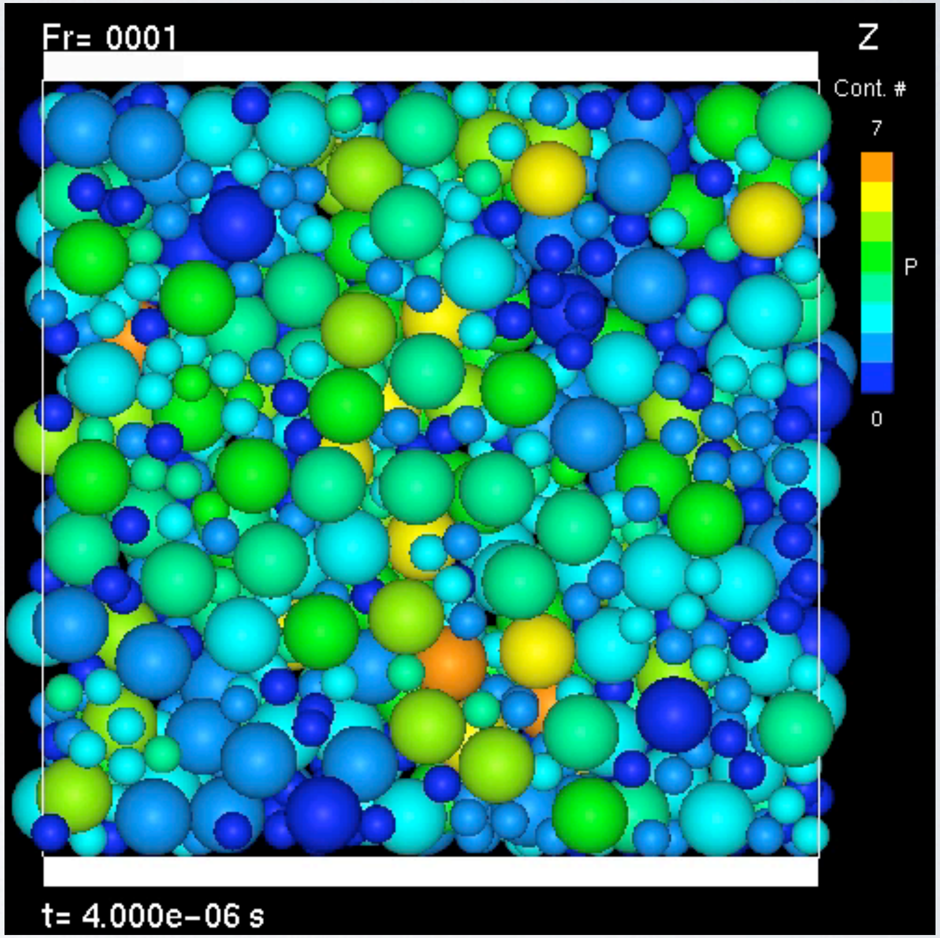
$Pe = 2\times10^4$

$X_S = 0.0$



Stagnates

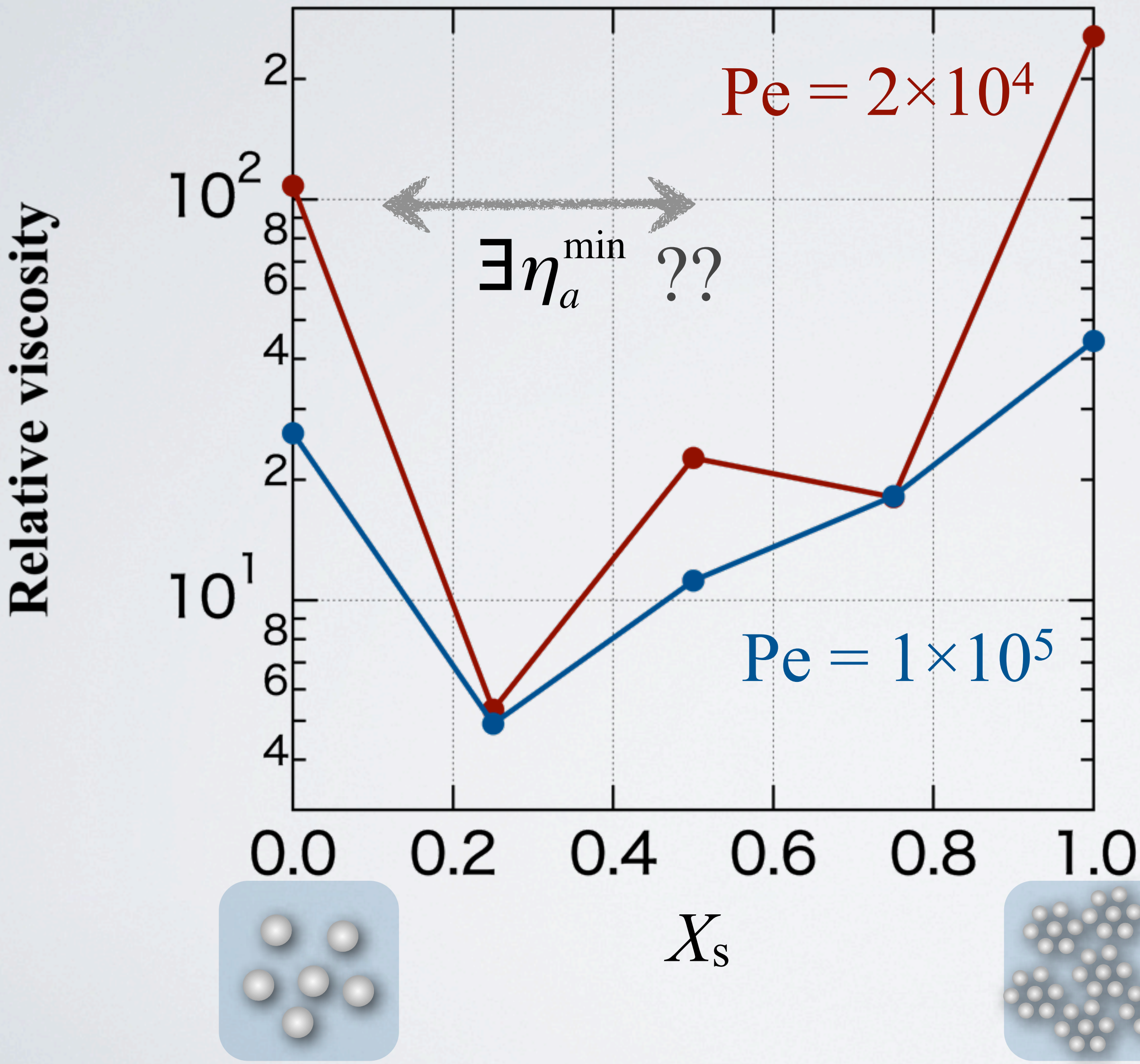
$X_S = 0.25$



Flows

$d = 1000, 500$ [nm], $\varphi_p = 0.5$

Result - Case B -



Higher shear reduces the viscosity gap $\Delta\eta$

Concluding Remarks

- Present simulation could lead us to a general function of the suspension viscosity:

$$\eta_a = F(\varphi_{\mathrm{p}},\ \lambda_{\mathrm{p}},\ X_s;\ \ \mathrm{Pe}, \Delta W(d_i))$$

Realistic variables ... Case A

Ideal variables ... Case B

- What's the origin of bimodal particle structure induced by shear flow field ? .... future work