クロスフロー精密膜ろ過シミュレーションによる高せん断場での膜面堆積粒子の挙動

Behavior of particles deposited on the membrane surface at high shear field by a cross-flow microfiltration simulation

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Introduction

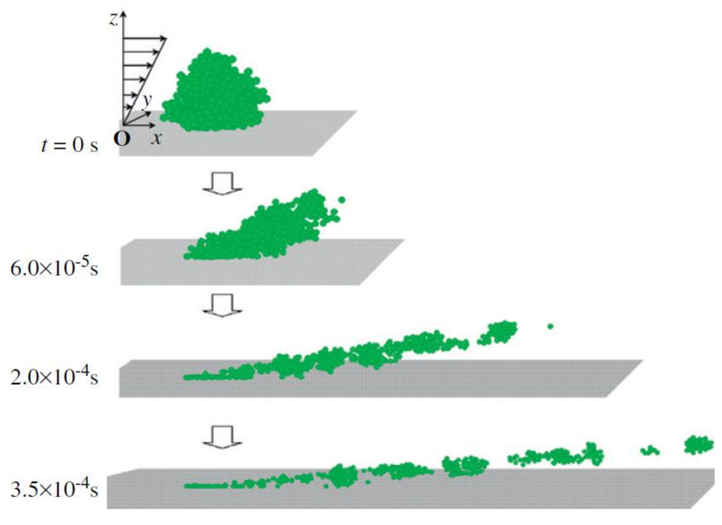


Fig. 8. Snapshots of entrainment process of Deposit-I from the plate surface $A_s/A = 1.0$ under the shear stress of $\mu\dot{\gamma}_s$ = 267 Pa.

Behavior of adherent aggregated particles on wall in shear flow field [1)]

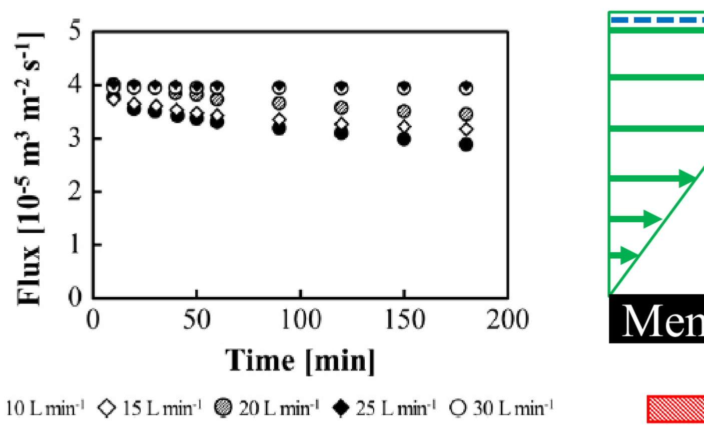
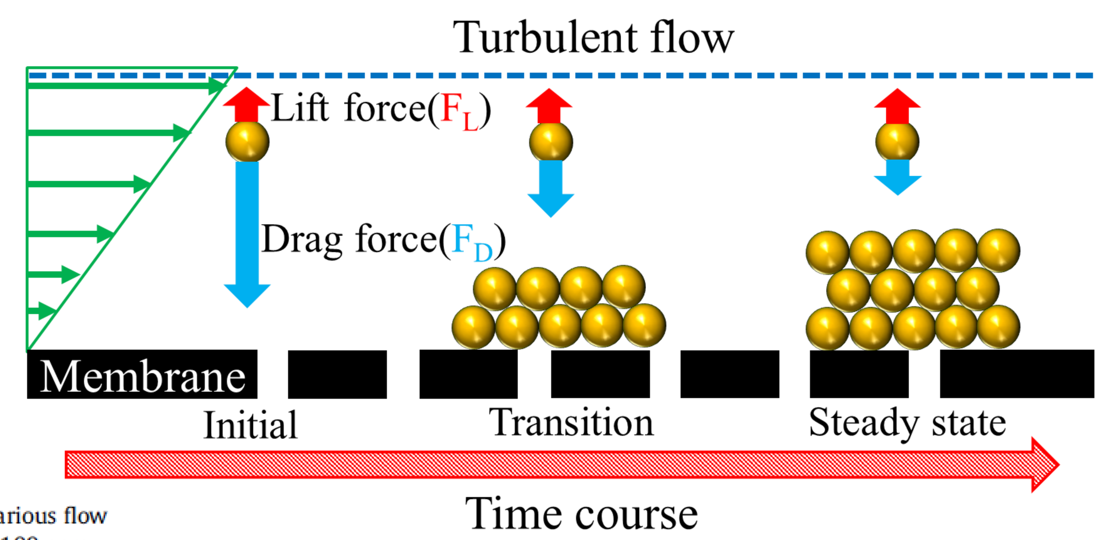


Fig. 3. Time courses of flux in the case of silica particles (1.5 μm) with various flow rates, an initial flux of 4.0 × 10⁻⁵ m³ m⁻² s⁻¹ and feed concentration of 100 ppm.

Time courses of flux with various flow rates[2)]



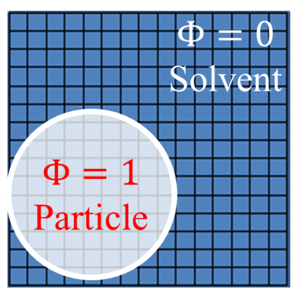
Schematic of particle deposition mechanism on membrane surface in cross-flow microfiltration

In recent years, studies on dispersion and aggregation of particles in the liquid phase and separation operation have been conducted[1)]. With cross flow microfiltration, particles accumulating on the membrane surface do not increase as filtration proceeds[2)]. As the filtration progresses, it is considered that the lift and the drag force acting on the particles are balanced. In this study, we investigated what happens on the membrane surface by high shear field.

1) K. Iimura *et al.*, Chemical Engineering Science 64 1455 - 1461 (2009).
2) R. Makabe *et al.*, Sep. Purif. Technol., 160, 98-105 (2016).

Simulation model

In this research, simulation was carried out using a simulator (SNAP-F) [3),4)] which simultaneously simulates particle and fluid motion.

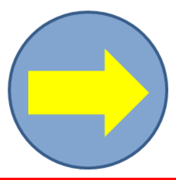


Navier-Stokes equation in fluid

$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\Delta \boldsymbol{v} + \frac{1}{\rho}\nabla\cdot\boldsymbol{s} - \frac{1}{\rho}\boldsymbol{D} + \Phi\boldsymbol{\alpha} \quad (1)$$

t : Time, $\boldsymbol{v}$: Velocity, ρ : Density, p : Pressure, μ : viscosity,
$\boldsymbol{S}$: Thermal fluctuating stress tensor, $\boldsymbol{D}$: Pressure gradient vector, Φ : Volume fraction of solid phase,
$\boldsymbol{\alpha}$: Acceleration vector associated with the Velocity of particle on the grid

Translational motion of particle



$$m\frac{dV}{dt} = \boldsymbol{F}^c + \boldsymbol{F}^e + \boldsymbol{F}^v + \boldsymbol{F}^h \quad (2) \qquad \boldsymbol{F}^h = -\int \varphi^p(\rho\boldsymbol{\alpha} + \boldsymbol{D})dr$$

m : mass [kg], $\boldsymbol{V}$: Velocity [m/s],
$\boldsymbol{F}^c$: contact force [N], $\boldsymbol{F}^e$: electrostatic force [N], $\boldsymbol{F}^v$: van der Waals force [N], $\boldsymbol{F}^h$: hydrodynamic force [N],
φ^p : volume fraction of the particle, whose sum is Φ

Rotational motion of particle

$$I\frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{T}^c + \boldsymbol{T}^h \quad (3) \qquad \boldsymbol{T}^h = -\int \varphi^p(\boldsymbol{r}\times\rho\boldsymbol{\alpha})dr$$

I : moment of inertia [kgm²], $\boldsymbol{\omega}$: angular velocity [rad/s],
$\boldsymbol{T}^c$: contact torque [Nm], $\boldsymbol{T}^h$: hydrodynamic torque [Nm]

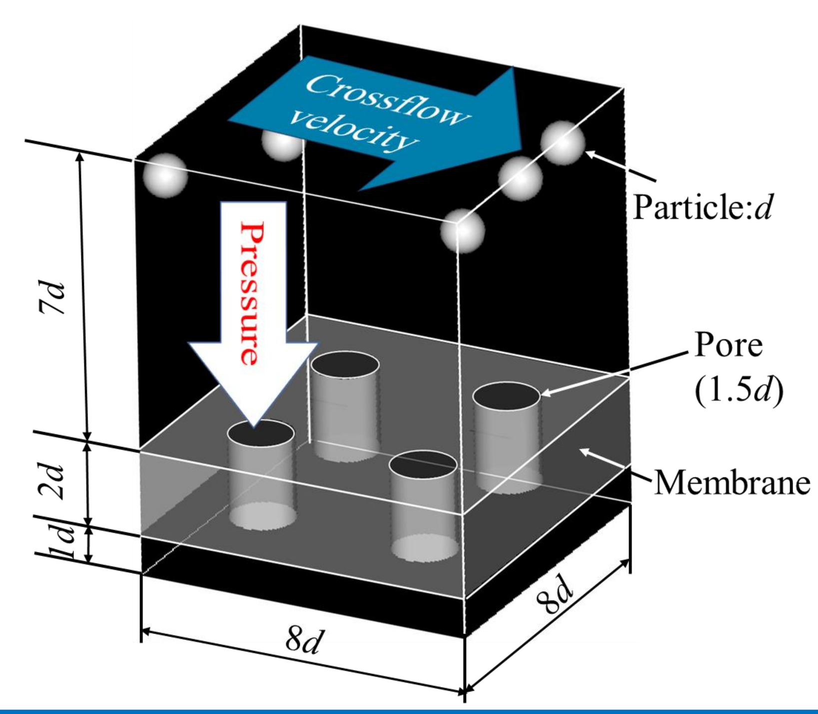
3) M. Fujita, Y. Yamaguchi, Phys. Rev. E, 77, 026706 (2008).
4) T. Ando *et al.*, J. Membr. Sci., 48, 392-393 (2012).

Simulation conditions

Initial condition	
Particle diameter, d [μm]	0.1
Pressure gradient, D [GPa/m]	200
Shear rate, $\dot{\gamma}$ [× 10⁶s⁻¹]	4.86
Particle volume concentration, Φ[vol%]	5

High shear conditions	
Particle diameter, d [μm]	0.1
Pressure gradient, D [GPa/m]	0
Shear rate, $\dot{\gamma}_1$[× 10⁶s⁻¹]	25.0
Shear rate, $\dot{\gamma}_2$[× 10⁶s⁻¹]	34.0
Particle volume concentration, Φ[vol%]	0

Simulation area

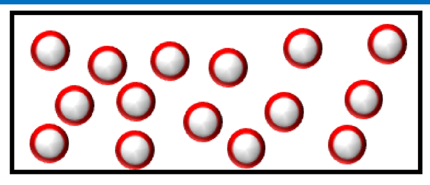


Evaluation method of structure (Nondimensional Boundary Area)

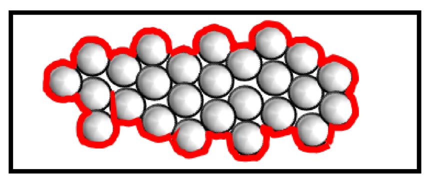
$$\mathrm{NBA} = \frac{1}{N}\left[\frac{1}{c_{max}}\sum_{c=0}^{c_{max}}(c_{max} - c)n(c)\right]$$

c : Coordination number ($c_{max} = 12$)
$n(c)$: Number of particles with coordination number c
N : Total particle number

$$\mathrm{NBA} = \frac{\text{Surface area of aggregate}}{\text{Sum of the surface area of the particle}}$$

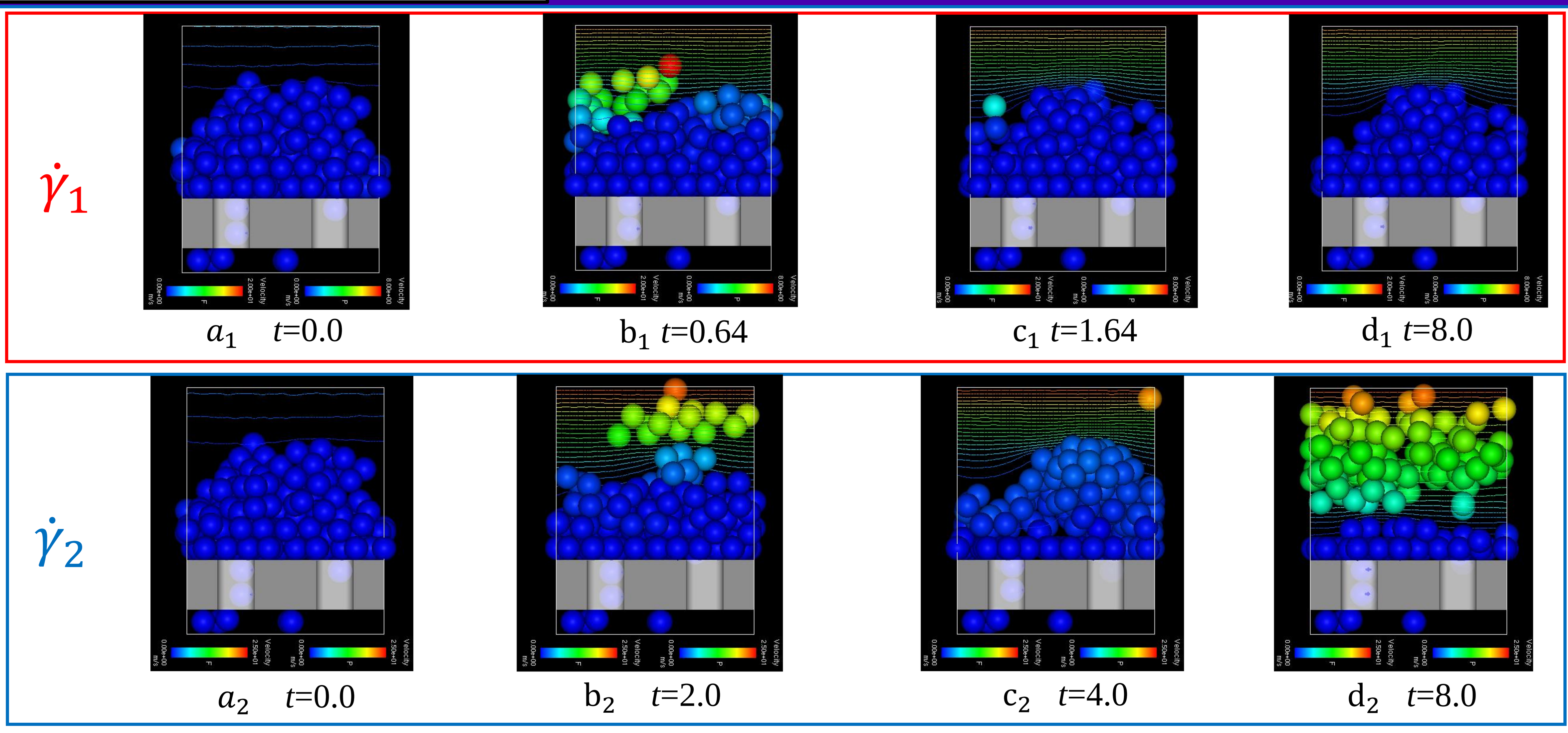


NBA=1
Complete dispersion

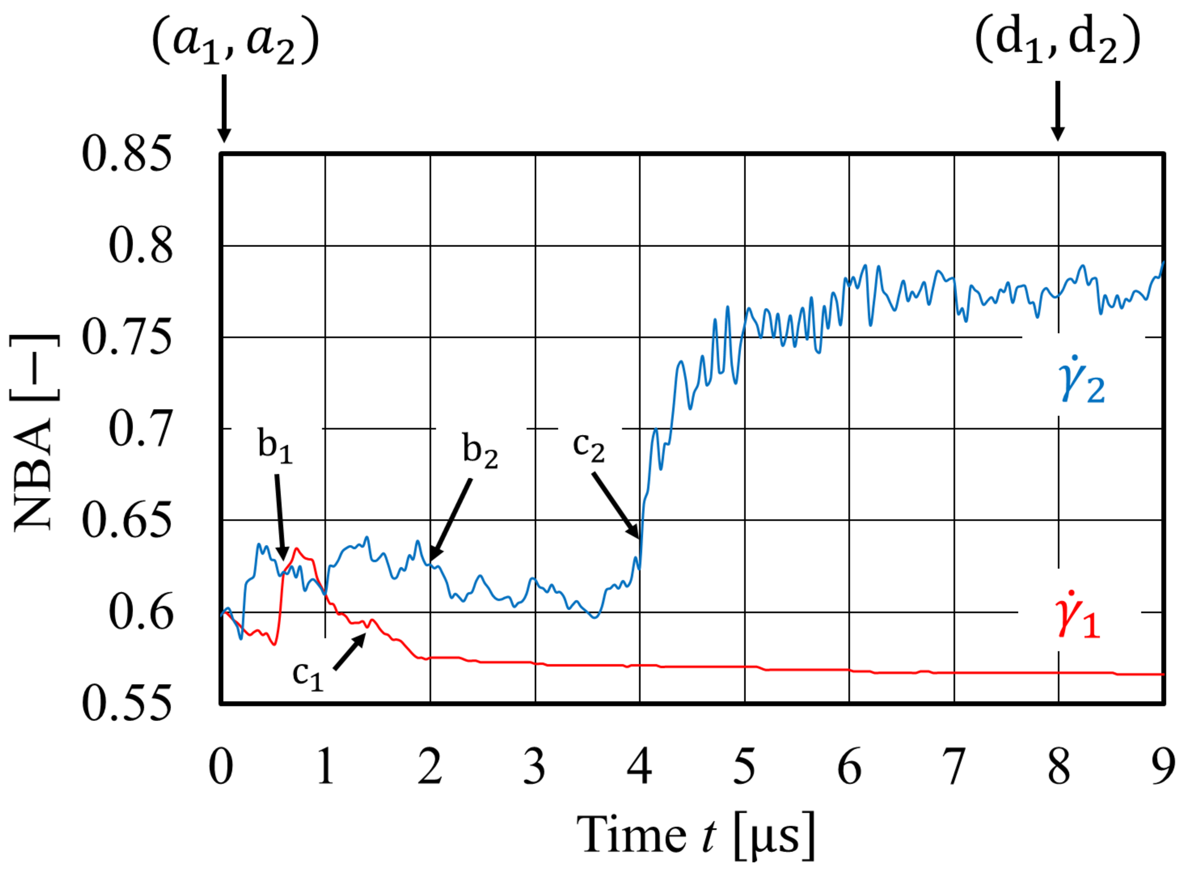


The NBA approaches 0 as it cohesion.

Simulation results



Particle separating situation



Relationship between NBA and time by high shear field

Consideration/Summary

Rumpf equation

$$\sigma = \frac{\varphi_p n_c F^v}{\pi d^2}$$

Newton's viscosity equation

$$\sigma = \mu \times \dot{\gamma}$$

$$\frac{\varphi_p n_c F^v}{\pi d^2} = \mu \times \dot{\gamma}$$

$$F^h = \frac{\mu \times \dot{\gamma} \times \pi d^2}{\varphi_p n_c}$$

$$F^v = \frac{A \times 0.5d}{12 H_{lm}^{\ 2}} = 1.96 \times 10^{-10}[\mathrm{N}]$$

$$F^h = \frac{\mu \times \dot{\gamma}_2 \times \pi d^2}{\varphi_p n_c} = 5.41 \times 10^{-10}[\mathrm{N}]$$

Calculation condition	
Paticle volume fraction: φ_p	≅0.41
Average coordination number: n_c	≅ 4.82
Inter-surface distance: H_{lm}	0.01d
Hamaker constant: A [J]	4.7×10^{-20}

$F^v \geq F^h$

Particle fouling

$F^v \ll F^h$

Particle Separating

- It was found that accumulated particle on membrane surface were separated by high shear rate.
- It can be thought that particle separation depends on the correlation between hydrodynamic force and van der Walls force.
- Shear rate and particle size are important for particle separation.