Numerical Simulation of Particle Settling and Cohesion in Liquid

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Abstract. In this study, the motions of particles and particle clusters in liquid were numerically simulated. The particles of two sizes (Dp=40µm and 20µm) settle while repeating cohesion and dispersion, and finally the sediment of particles are formed at the bottom of a hexahedron container which is filled up with pure water. The flow field was solved with the Navier-Stokes equations and the particle motions were solved with the Lagrangian-type motion equations, where the interaction between fluid and particles due to drag forces were taken into account. The collision among particles was calculated using Distinct Element Method (DEM), and the effects of cohesive forces by van der Waals force acting on particle contact points were taken into account. Numerical simulations were performed under conditions in still flow and in shear flow. It was found that the simulation results enable us to know the state of the particle settling and the particle condensation.

1. INTRODUCTION

Particulate operation has played the important role in chemical industry, electricity and electronic industry, medicine manufacture, and the product manufacture process of the information industry. In the design of fluid and particle process, solid liquid separation process and the manufacture process of solid dispersion system, it is required to grasp the state of particle motion and particle formation in fluid correctly.

For example, in the manufacturing process of a ceramic product, it is important to predict the state of the sediment after materials particles sediment in liquid. Although the materials particles of the ceramics of a sediment serve as the end products according to processes, such as compression, drying, dryness, fabrication, and sintering, the character of the end products is greatly influenced by the state of the sediment made first. The unevenness of void made when settling materials particles in liquid causes problems, such as an internal defect in the end products, and material strength unevenness. Therefore, in order to predict the quality of the end products, it is important to grasp the state of particle settling, particle condensation, and sediment of particles.

In this study, the numerical simulation of process in which the particles of two sizes sediment in the case of still flow and in the case of simple shear flow was performed. The particles of two sizes form a particle cluster, and they are distributed depending on the case. While the particles which sediment in liquid repeated condensation and distribution, process until it fabricates a sediment was pursued using the three-dimensional numerical simulation. In order to calculate the contact force of particles, Distinct Element Method (DEM) was used. The DEM is one of the trajectory models, is a simple numerical model by which interactions due to multi-body collisions can be calculated. The DEM has
been applied to many kinds of multi-body complex problems (Kawaguchi et al., 1992; Yuu et al., 1995). The effects of cohesive forces by van der Waals force acting on particle contact points were taken into account. Condensation of particles, the state of distribution, and the state of a sediment were considered from the simulation result.

2. CALCULATION METHOD
In this calculation, the three-dimensional Navier-Stokes equation which is a governing equation of fluid was used for the calculation for fluid phase, and the Lagrangian-type equation of motion was used for the calculation of the particle motion. The motion of fluid and particles was calculated by being allied and solving the equation of motion of fluid and particles. The drag force produced with both relative velocity as a dynamic interaction of fluid and particles was taken into account. In order to calculate the contact force of particles, DEM was used, and in order to calculate the adhesion between particles, van der Waals force was used. Moreover, in order to calculate the settling velocity of a particle cluster, the sphere equivalent diameter of a particle cluster was used.

2.1 Calculation of fluid phase
The governing equations for the fluid phase are the three-dimensional Navier-Stokes equations for the incompressible fluid with particle source terms, and the equation of continuity. These equations are expressed with a non-dimension as follows in consideration of existence of particles (Anderson et al., 1967).

\[
\frac{\partial \varepsilon u}{\partial t} + \nabla \cdot \varepsilon u = -\varepsilon \nabla p - \frac{\varepsilon}{Re} \nabla \cdot \tau - S_p
\]  

\[
\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \varepsilon = 0
\]

\( \tau \) in Eq. (1) is the viscous stress tensor expressed by Newton's law of viscosity. \( S_p \) in Eq. (1) is the particle source term, which indicate the mutual interaction between particles and fluid. \( S_p \) is resistance of Stokes produced with the relative velocity of particles and fluid, and motions of particles and fluid are linked through the interaction term \( S_p \). The equation of \( S_p \) term is expressed with a non-dimension as follows.

\[
S_p = \frac{3\pi \mu D_p D_n}{U_o \rho} (u - u_p)
\]

In actual numerical computation, by taking divergence of both sides of Eq. (1), the Poisson’s equation about pressure \( P \) was obtained and the Poisson’s equation was solved by the Relaxation method (Harlow et al., 1965; Rai et al., 1991). The fourth-order central difference scheme is used for the convection terms, and the second-order central difference scheme is used for other spatial derivative terms. The forward difference scheme is used for the time derivative terms. In addition, since it was difficult to calculate the flow between particles strictly, physical quantity, such as velocity, calculated the amount of partial averages, and calculated it in consideration of void fraction.

2.2 Calculation of particle motion
2.2.1 The equation for particle motion
The motion of the particles in the fluid is pursued with the Lagrangian type equation of motion. The Lagrangian type equation for particle motion is described as the following equation (Umekage et al., 2001).
In Eq. (4), the left side is the acceleration term of particles, the 1st term of the right-hand side is interaction force between particles, the 2nd term of the right-hand side is a drag force based on Stokes's law of resistance, the 3rd term is the force by the pressure slope of the circumference of the particles produced in order that fluid may accelerate by particles, the 4th term is the force required to accelerate added mass and the 5th term is gravity and lift. The Eq. (4) is an equation of motion about the translation motion of particles, and is not taking rotational motion of particle into consideration in this calculation.

2.2.2 Calculation of contact force using Distinct Element Method

In the process of particle settling, particles collide with many other particles repeatedly. Therefore, it is important to calculate particles collision. In this study, the particle-particle interactions due to multi-body contacts were simulated using Distinct Element Method (DEM) (Cundall et al., 1979). The DEM, which is one of the trajectory models, is a simple numerical model to calculate the multi-body contacts (Yuu et al., 2000). In DEM, the contact force of particles is calculated in all contact points. In order to estimate the contact force of particles, an elastic spring and viscous dashpot are introduced. The contact model of DEM is shown in Fig. 1. The increments of the normal and shear forces, \( \Delta F_n \) and \( \Delta F_s \), modeled with the elastic spring are calculated as follows using the normal and shear relative displacement increments, \( \Delta n \) and \( \Delta s \).

\[
\Delta F_n = k_n \Delta n , \quad \Delta F_s = k_s \Delta s
\]  

(5)

The normal stiffness \( k_n \) is estimated from the Hertz contact theory. The shear stiffness \( k_s \) is \( k_s = (1/3)k_n \) in this calculation. The increments of the normal and shear damping forces, \( \Delta D_n \) and \( \Delta D_s \), modeled with the dashpots are calculated as follows using the normal and shear relative velocity increments, \( \Delta \dot{n} \) and \( \Delta \dot{s} \).

\[
\Delta D_n = -\eta_n \Delta \dot{n} , \quad \Delta D_s = -\eta_s \Delta \dot{s}
\]  

(6)

\[ \text{Fig. 1 The contact model of DEM} \]
The normal and tangential contact and damping forces at time $t$ are

$$
(F_n)_t = (F_n)_{t-1} + \Delta F_n, \quad (F_s)_t = (F_s)_{t-1} + \Delta F_s
$$  \hspace{1cm} (7)

$$
(D_n)_t = (D_n)_{t-1} + \Delta D_n, \quad (D_s)_t = (D_s)_{t-1} + \Delta D_s
$$  \hspace{1cm} (8)

The summation of these contact force components in each direction gives the resultant force.

The normal damping coefficient $\eta_n$, and the shear damping coefficient $\eta_s$ must satisfy the following relation, respectively.

$$
\eta_n = 2\sqrt{m_p k_n}, \quad \eta_s = 2\sqrt{m_p k_s}
$$  \hspace{1cm} (9)

### 2.2.3 Calculation of cohesive force using Van der Waals force

Van der Waals force was taken into consideration as the attraction and adhesion between particles. When the distance between the surfaces of particles approaches 0.1 $\mu$m or less, we calculate using the following equation.

$$
F_C = \frac{-AD_{pi}D_{pj}}{12(D_{pi} + D_{pj})Z_p^2}
$$  \hspace{1cm} (10)

$A$ in Eq. (10) is a Hamaker constant. When the distance between the particle surfaces was 4 $\AA$ or less, it was calculated by setting the value of distance to 4 $\AA$, and when particles contacted, it was calculated so that van der Waals force act as adhesion.

### 2.2.4 Calculation of drag force using the sphere equivalent diameter

The settling velocity of a particle cluster differs from the settling velocity of an isolated particle. In this calculation, when calculating the drag force between particle and fluid, we calculated using the sphere equivalent diameter of a particle cluster. The sphere equivalent diameter of a particle cluster is calculated from the volume of the composition particles of a particle cluster. The definition of the sphere equivalent diameter of the particles which consists of $N$ particles is shown by the following equation.

$$
(D_p)_{eq} = \left( \sum_{j=1}^{N} (D_{pi})^3 \right)^{1/3}
$$  \hspace{1cm} (11)

In this calculation, the equation of motion is solved not for particle clusters but for individual particles. Therefore, calculation of a drag force must be performed to individual particles which constitute a particle cluster. The drag force of particles calculated using the value which carried out dignity attachment of the sphere equivalent diameter obtained by Eq. (11) with the diameter of the particles which constitute a particle cluster. The diameter for calculating the drag force of the particles which constitute a particle cluster is shown by the following equation.

$$
(D_p)_{eq} = \frac{D_{pi}}{\sum_{j=1}^{N} (D_{pi})} (D_p)_{eq}
$$  \hspace{1cm} (12)
About the fluid velocity for calculating drag force, the value in the central point of each particle which calculated fluid velocity using proportional distribution was used.

3. CALCULATION CONDITIONS

The calculation conditions and the computational domain are shown in Table 1 and Figs. 2, respectively. The particles of two kinds of sizes (40 µm and 20 µm) were calculated in this calculation. The particles of the number of 5000 were calculated in total using the particles of the number of 2500, respectively. In this calculation, in order to calculate motions of particles and fluid, three-dimensional calculational domain was used. The size of the sedimentation container which is calculation space was made into horizontal length 1200 µm, depth length 480 µm, vertical length 1200 µm. When the particles of the number of 5000 were put in, the average void fraction in the container was set to 0.864. In this study, calculation in the flow state of two types, the case of still flow and the case of shear flow, was performed. In calculation of still flow, the no slip wall boundary condition was used for all walls. In calculation of shear flow, the periodic boundary condition was used for the wall of right-and-left both sides, and used the no slip wall boundary condition except it. Furthermore, in the case of shear flow, the flow velocity of X direction at the bottom was set to 0, and the flow velocity of X direction at the upper wall was given as fixed at the velocity of 6 times the terminal velocity of a large particle. And in the initial state, the flow velocity of the X direction in calculation space was set up so that the shear rate is fixed in the Z direction. Initial state of particles were formed to state of noncontact using a random number series. In this study, calculation was performed to use the physical properties of pure water for fluid and the physical properties of a glass bead for particles.

| Table 1 Calculation conditions |
|--------------------------------|
| **Particle diameter** $D_p$    | Large 40.0 µm | Small 20.0 µm |
| **Number of particles**        | Large 2500    | Small 2500    |
| **Terminal velocity of a single particle** | Large 1305 µm/s | Small 330 µm/s |
| **Particle density** $\rho_p$  | 2.5×10$^3$ kg/m$^3$ |
| **Fluid density** $\rho$       | 0.988×10$^3$ kg/m$^3$ |
| **Fluid viscosity** $\mu$      | 0.001 Pa·s    |
| **Averaged void fraction**     | 0.864         |
| **Computational cell sizes** $\Delta x \times \Delta y \times \Delta z$ | 120×120×120µm |
| **Numbers of cells**           | 10×4×10       |
| **Elastic coefficient** $E$     | 1.0×10$^5$ N/m$^2$ |
| **Friction coefficient**       | Particle 0.25 |
|                                | Wall 0.3      |
| **Poisson ratio** $\nu$        | 0.25          |
| **Time step** $\Delta t$       | 1.0×10$^{-6}$ sec |
| **Height of sedimentation vessel** $D$ | 1200 µm |
| **Hamaker constant** $A$        | 1.5×10$^{12}$ gcm$^2$ s$^{-2}$ |
| **Shear rate of fluid in the initial state** $\frac{du_x}{dz}$ | 6.53 s$^{-1}$ |
4. RESULTS

4.1 Settling velocity of particles
Fig. 3 shows the settling velocity of a certain large particle with time. Comparison of the result calculated using the sphere equivalent diameter and the result calculated without using it is shown. Furthermore, Fig. 4 shows the number of the particles adhering to the large particle shown in Fig. 3 with time. From these results, it is thought that the settling velocity according to a condensed state is calculable by using the sphere equivalent diameter. The theoretical terminal velocity of a large particle calculated from Stokes equation is 0.131 cm/sec, and in the case of isolated particle (i.e., when it calculates without using the sphere equivalent diameter), it sediments at the velocity almost equal to it. For example, the 5th data from the left of Figs. 3 and 4 are considered. The particle cluster consists of the three large particles and the one small particle, and the value which calculated theoretical terminal velocity using the sphere equivalent diameter is 0.279 cm/sec. It is shown that the settling velocity of this particle cluster in Fig. 3 is almost equal to the theoretical terminal velocity.

Fig. 5 shows the fluid mean velocity of the Z direction in the time for 0.1 sec, 0.2 sec, and 0.3 sec. A horizontal axis is non-dimension height, a vertical axis is fluid mean velocity, and fluid mean velocity is the value which averaged in each section of the Z direction. The direction of fluid flow is opposite to direction of particle settling. It is in the hindered settling state and the realistic phenomenon was shown in this calculation. It is thought that the fluid velocity near the bottom is large by 0.1sec is the influence which particles deposited on the bottom.

4.2 The snapshots of instantaneous particle configurations
Figs. 6 (a) - (f) show calculated snapshots of instantaneous particle configurations in the case of still flow. Figures are sectional view around the depth direction (Y-axis) central part, a vertical axis expresses the Z-axis and the horizontal axis expresses the X-axis. In these results, the state of particle settling and the state of forming the sediment near the bottom are shown. Since the settling velocity of large particles is 4 times of the settling velocity of small particles, particles contact in settling process and it forms a particle cluster. Since the particle clusters have higher settling velocity than the particles which exist independently, they sediment more quickly than independent particles. It is thought that these results are obtained since the sphere equivalent diameter is used for calculation of the settling velocity of the particle clusters.
Figs. 7 (a) - (f) show calculated snapshots of instantaneous particle configurations in the case of simple shear flow. Particles sediment moving to the right from the left by shear flow. From the result shown in Figs. 7, in the case of shear flow, many particle clusters are formed rather than the case of still flow. Since settling velocity becomes high by condensation of particles, particle cluster arrives early at the bottom, and the number of floating particles in the case of shear flow has become less than that in the case of still flow. In the case of shear flow, it is thought that the motion of particles becomes large by shear flow, and the contact opportunity of particles increase.

Fig. 3 Settling velocity of large particle in a particle cluster

Fig. 4 The number of the particles in a particle cluster

Fig. 5 The fluid mean velocity of Z direction
Figs. 6 Calculated instantaneous particle configurations in still flow

Figs. 7 Calculated instantaneous particle configurations in shear flow
4.3 The state of condensation and the fraction of particle clusters

Figs. 8(a), (b) show the number of particle clusters formed by 2 to 5 particles with time. The number of the particle clusters formed by 2 to 5 particles is shown in the vertical axis, and the particle cluster formed from 6 or more particles is not shown here. The number of particle clusters that consist of 2 particles increases rapidly at once when the calculation is started. Afterwards, the number of particle clusters that consist of 3 particles increases, and, in addition, the number of particle clusters that consist of 4 particles increases afterwards. The number of particles of the particle cluster increases by uniting it to other isolated particles or particle clusters. Therefore, the number of the particle clusters which consist of many particles increases with time. Oppositely, the number of the particle clusters which consist of few particles decreases as the particle cluster which consists of many particles increases. These results show that particle clusters are formed early in the case of shear flow.

![Graphs showing the number of particle clusters formed by 2 to 5 particles with time for still flow and shear flow.](image)

Fig. 8 The number of particle clusters formed by 2 to 5 particles

Fig. 9 shows the fraction of the particle clusters in all particles with time. The fraction of the particle clusters increases rapidly immediately after starting settling, and the slope is loose after passing over about 0.1 sec. The tendency of graphs is nearly equal in both. On the whole, the fraction of particle clusters in the case of shear flow is higher than that in the case of still flow.

Fig. 10 shows the fraction of particle clusters in the floating particles with time. Here, the number of the floating particles is sum total of the number of the floating particle clusters and the number of the floating isorated particles. The value in the case of shear flow is small in time after 0.15 sec. It is thought that the particle cluster arrives at the bottom early since the settling velocity of particle clusters is large, and the number of the floating particle clusters decrease.

Fig. 11 shows the distribution of void fraction in the sediment made at the bottom. Table 2 shows the average value, max value, min value of the data in Fig. 11. It was obtained from the result after all particles sediment. The value averaged in the depth direction (Y direction) is shown. Under the conditions of this study, there was no difference clearly made into the average value of void fraction. Moreover, the void fraction became an almost fixed value in the X direction.
5. CONCLUSION

The numerical simulation of particle settling process in the case of still flow and the case of shear flow was performed. In order to calculate the contact force of particles, DEM was used, and in order to calculate the adhesion between particles, van der Waals force was used. Moreover, in order to calculate the settling velocity of particle clusters, the sphere equivalent diameter was used. The following conclusion was obtained from the calculation results.

Simulation results well describe various phenomena, such as particle condensation, particle dispersion and the hindered settling state.

|                        | Average | Max  | Min  |
|------------------------|---------|------|------|
| still flow             | 0.400   | 0.437| 0.390|
| shear flow             | 0.393   | 0.409| 0.383|

Fig. 9 Fraction of Particle clusters

Fig. 10 Fraction of particle clusters in the floating particle

Fig. 11 Distribution of void fraction at the bottom
The settling velocity according to the condensed state of particles was obtained by using a sphere equivalent diameter. The settling velocity of this simulation result is almost equal to the theoretical terminal velocity.

Comparison of the results in the case of still flow and the results in the case of shear flow, the fraction of particle clusters in the case of shear flow is higher than that in the case of still flow.

The difference of void fraction in a sediment did not appear clearly.

**NOMENCLATURE**

- **A**  
  Hamaker constant  
  [J]

- **D**  
  height of sedimentation vessel  
  [m]

- **D_j**  
  damping force at contact point j  
  [N]

- **D_p**  
  particle diameter  
  [m]

- **(D_p)_eq**  
  sphere equivalent diameter  
  [m]

- **(D_p)_d,eq**  
  diameter of dignity attachment of **(D_p)_eq**  
  [m]

- **F_{Cj}**  
  cohesive force at contact point j  
  [N]

- **F_j**  
  dispersion force at contact point j  
  [N]

- **g**  
  gravitation acceleration  
  [m/s²]

- **k**  
  stiffness  
  [N/m]

- **m_p**  
  particle mass  
  [kg]

- **N**  
  particle number of cluster  
  [-]

- **n**  
  number of particles per unit volume  
  [-]

- **\Delta n, \Delta s**  
  increments of normal and shear relative displacement  
  [m]

- **\Delta \dot{n}, \Delta \dot{s}**  
  increments of normal and shear relative velocities  
  [m]

- **P**  
  pressure  
  [Pa]

- **Re**  
  Reynolds number  
  [-]

- **Re_p**  
  particle Reynolds number  
  [-]

- **Sp**  
  interaction term due to fluid drag force  
  [-]

- **t**  
  time  
  [sec]

- **U_0**  
  terminal velocity of a large particle  
  [m/s]

- **u**  
  fluid velocity vector (= \((u, v, w)\))  
  [m/s]

- **u_p**  
  particle velocity vector (= \((u_p, v_p, w_p)\))  
  [m/s]

- **X, Y, Z**  
  coordinates  
  [-]

- **\Delta X, \Delta Y, \Delta Z**  
  computational cell sizes  
  [-]

- **Z_p**  
  Distance between the particle surfaces  
  [m]

- **\nabla**  
  non-dimensional nabla operator  
  [-]
Greek Letters

$\varepsilon$ void fraction  
$\eta$ damping coefficient  
$\mu$ fluid viscosity  
$\rho$ fluid density  
$\rho_p$ particle density  
$\tau$ molecular viscous stress tensor

Subscripts

$i$ particle $i$  
$j$ particle $j$  
$n$ normal direction  
$s$ tangential direction

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