Part IV
Behavior of Cohesive Sediment

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Analysis of Simulation Data for Cohesive Sediment Flocculation Using a Population Balance Model

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ABSTRACT

Cohesive sediments like mud, found in marine and river environments, are important for many aspects of water resource management and environmental engineering. These sediments consist of small particles that aggregate via cohesive forces and break apart under shear, a process called flocculation. Size-class-based population models, developed using experimental data, describe flocculation in a volume-averaged sense by considering mass conservation and the exchange of particles through breakup and aggregation. Although these models work well in controlled experimental conditions, more detailed data are needed for validation. Numerical simulations of sediment-laden flows allow for definition of particle properties and flow conditions to provide such data under precisely defined boundary conditions. This chapter applies a population balance equation (PBE) model to simulate results of flocculation in isotropic turbulence, resolving even the smallest turbulence scales in three dimensions. The positions and velocities of particles are tracked over time. Key PBE model parameters—fractal dimension, collision efficiency, and fragmentation rate—are compared with different primary particles used in the simulations. Results show that the PBE model can predict flocculation dynamics at moderate shear rates with sufficient particle cohesion. However, the analysis reveals limitations in modeling flocs with low aggregation tendencies.

9.1. INTRODUCTION

Fine cohesive sediments, commonly referred to as mud, are found almost everywhere on Earth and play an important role in a number of environmental processes. They can serve as carriers of organic and inorganic pollutants that can easily attach to the clay particles or organic material of sediment and thus be transported (Winterwerp, 2004). The most significant difference compared to noncohesive sediments is their ability to form larger aggregates. This ability results from their small grain size and thus large specific surface area, which allows surface forces to dominate over gravitational forces. The ability of cohesive sediments to form larger aggregates, however, makes it much more complicated to characterize and model the processes in which they are involved, because the aggregates formed have different properties than the primary particles: e.g., lower effective density, larger sizes, and possibly higher settling velocity (Krahl et al., 2022; Ye et al., 2023). In addition, the process is dynamic: aggregates formed can also disaggregate,

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and their properties depend on the flow conditions, which can vary greatly both spatially and temporally (Partheniades, 2009). The mechanisms of aggregation and disaggregation are referred to as *flocculation*, which is considered a key process in cohesive sediment dynamics. For modeling cohesive sediment transport, it is therefore essential to represent this process accurately (Sherwood et al., 2018).

Many experimental studies have dealt with the characteristics and influencing factors of flocculation (e.g., Li et al., 1999; Bouyer et al., 2004). The early pioneering work by von Smoluchowski (1917) provided the basis for a variety of numerical studies (e.g., Winterwerp, 2002; Maggi et al., 2007; Xu et al., 2008), in which the flocculation process is modeled using population balance equations (PBE). Following this approach, Verney et al. (2011) investigated flocculation behavior during an idealized tidal cycle, combining experimental data and numerical simulations. The authors developed the size-class-based population balance model FLOCMOD, which represents the complex three-dimensional behavior of flocs in a simplified way and provides averaged information about the flocculation process. More detailed insight into flocculation mechanisms can be obtained through sophisticated high-resolution numerical simulations that have recently become possible thanks to advances in computational power (e.g., Chen et al., 2019; Zhao et al., 2020; Zhao et al., 2021). Zhao et al. (2021) studied the dynamics of suspended cohesive particles in homogeneous isotropic turbulence on the basis of highly resolved numerical simulations. Unlike the previous studies, this study considers not only the early stages of flocculation but also the entire process until dynamic equilibrium is reached.

The objective of this chapter is to analyze the simulation results of Zhao et al. (2021) on the basis of the FLOCMOD numerical model developed by Verney et al. (2011). We attempt to reproduce the simulation results to investigate whether and to what extent the complex behavior of flocs can be represented by such a simplified model, and to gain an understanding of the calibration parameters of the FLOCMOD population balance model.

9.2. SIMULATION DATA AND POPULATION BALANCE MODEL

9.2.1. Simulation Data of Flocculation

This analysis is based on the simulation data from the investigation of Zhao et al. (2021). In their study, the authors investigated the dynamics of suspended cohesive particles in homogeneous isotropic turbulence on the basis of one-way coupled direct numerical simulations. Every particle was tracked in space and time, and particles had the ability to collide and flocculate by cohesive forces, following the procedure of Vowinckel, Biegert, et al. (2019a) and Vowinckel, Withers, et al. (2019b). The collision and lubrication models between particles were validated by Biegert et al. (2017) up to Stokes number St = 152, and the cohesive model was introduced and validated by Vowinckel, Withers, et al. (2019b). The simulation approach used in Zhao et al. (2021) implies that the presence of particles does not sufficiently influence the flow velocity field. This is particularly relevant for globally dilute systems of particles that are smaller than the Kolmogorov length scale. Even considering the flocculation of primary particles, the influence of the floc on the velocity field can be considered negligible, because it was shown by Zhao et al. (2021) that the mean floc size is comparable to the Kolmogorov length scale and the density of the floc decreases with increasing size. Note that the drag model that acts on particles is suitable for simulating particles with small Stokes number values (Vowinckel, 2021), which is indeed the case here. The results of Zhao et al. (2021) confirmed that the flocculation process can be divided into an initial, transient flocculation stage followed by a statistically quasi-steady equilibrium stage. By investigating the temporal evolution of shape and floc-size distribution at the equilibrium stage, the authors were able to describe the governing influences on flocculation behavior during both stages. The authors conducted a total of 15 runs, where the effects of cohesiveness, turbulent shear rate, and particle inertia on the flocculation process were investigated.

Toward this end, Zhao et al. (2021) introduced 10,000 monodisperse primary particles with diameter $D_\mathrm{p} = 5\,\mu\mathrm{m}$ into a cubic, triple-periodic computational domain with edge length $L_0 = 125 D_\mathrm{p} = 6.25 \times 10^{-4}\,\mathrm{m}$. The fluid density was set to $\rho_\mathrm{f} = 1.0 \times 10^3\,\mathrm{kg/m^3}$ and the time scale of the random turbulent forcing process to $T_0 = 7.81 \times 10^{-5}\,\mathrm{s}$. From the characteristic time and length scale, the characteristic velocity scale becomes $U_0 = \frac{L_0}{T_0} = 8\,\mathrm{m/s}$. The authors used these scales to render the governing equations and parameters dimensionless. Based on these characteristic scales, the Reynolds number $\mathrm{Re} = U_0 L_0 \rho_\mathrm{f}/\mu$ was defined, where μ is the dynamic viscosity. In addition, cohesiveness was controlled by adjusting the cohesive number Co as the ratio of the maximum cohesive force to the particle inertia

$$\mathrm{Co} = \frac{\max\left(|F_{\mathrm{coh},ij}|\right)}{U^2 \eta^2 \rho_\mathrm{f}} = \frac{A_\mathrm{H} D_\mathrm{p}}{16 \lambda \zeta_0} \frac{1}{U_0^2 \eta^2 \rho_\mathrm{f}} \tag{9.1}$$

where A_H is the Hamaker constant as a function of particle and fluid properties, λ is the range of the cohesive forces, and ζ_0 is the size of microscopic surface roughness, which is typically on the order of a couple of nanometers. Furthermore, the particle inertia is governed by the characteristic fluid velocity $U = \left(\frac{\mu G}{\rho_\mathrm{f}}\right)^{1/2}$ and the Kolmogorov

Table 9.1 Physical Parameters of the Simulation Runs Used to Generate the Data of This Analysis

Case	Re (–)	μ (kg/(m s))	η (m)	A_H (J)	G (s^{-1})
Flo1	5.0×10^3	1.0×10^{-3}	1.65×10^{-3}	1.0×10^{-23}	3.673×10^3
Flo2	5.0×10^3	1.0×10^{-3}	1.65×10^{-3}	1.5×10^{-22}	3.673×10^3
Flo3	5.0×10^3	1.0×10^{-3}	1.65×10^{-3}	7.5×10^{-22}	3.673×10^3
Flo4	5.0×10^3	1.0×10^{-3}	1.65×10^{-3}	1.5×10^{-21}	3.673×10^3
Flo5	5.0×10^3	1.0×10^{-3}	1.65×10^{-3}	3.0×10^{-21}	3.673×10^3

Source: Adapted from Zhao et al. (2021).

length scale $\eta = \left(\frac{\mu}{G\rho_f}\right)^{1/2}$. Both quantities depend on the turbulent shear rate G. Details of the cohesive force model can be found in Vowinckel, Biegert, et al. (2019a) and Zhao et al. (2021).

For this analysis, we use all parameters of interest in their dimensional sense. Toward this end, the dynamic viscosity is defined as $\mu = L_0 U_0/\mathrm{Re}$, and the dimensional Kolmogorov length scale is given by $\eta = D_p \eta'/D_p'$, where the prime indicates dimensionless quantities. From these considerations, the dimensional shear rate can be obtained as $G = \mu/(\rho_f \eta^2)$. Table 9.1 summarizes the relevant physical parameters of those cases that were investigated in this chapter. For reasons that we discuss in section 9.4, we limit our analysis to the campaign that focused on the impact of cohesiveness on the flocculation (Flo1–5). The particle density can therefore be set constant to $\rho_p = 2{,}650$ kg/m^3 according to the density of silica materials. The initial number of particles in the computational domain can be expressed as the initial concentration $c_0 = N V_p \rho_p / L_0^3 = 7.104\,\mathrm{kg/m^3}$, where V_p is the volume of the spherical primary particles. It is noticeable that the shear rates obtained from these numerical simulations are very high. Even in the event of high turbulence due to breaking waves, the energy dissipation rate would only be as high as $O(10^{-3} \sim 10^{-2})$, which corresponds to a shear rate of $G = 100 \sim 200$/s (Vowinckel et al., 2022). Zhao et al. (2021), on the other hand, reported shear rates one order of magnitude above those reference values (i.e., $G \sim 10^3$/s).

9.2.2. Population Balance Equation Model

The PBE model used here is based on the derivation of the FLOCMOD model by Verney et al. (2011) and later disseminated as a MATLAB implementation by Sherwood et al. (2018). This model is meant to reproduce experimental results of flocculation in terms of characteristic sizes as well as floc-size distribution as a function of time. FLOCMOD is a 0D size-class-based model: i.e., an isotropic environment is assumed, and the floc distribution is represented in discrete size classes. Like many other models, FLOCMOD is based on the Smoluchowski equation (von Smoluchowski, 1917), which describes the temporal evolution of a floc population, partitioned into N classes, by number concentration. A sufficiently large number of size classes is needed to accurately model the flocculation processes (Penaloza-Giraldo et al., 2023). The size classes are logarithmically distributed from the primary particle diameter D_p to a maximum floc size D_{max}. The range and number of size classes can be adjusted as needed. The authors of the model follow the assumption of a fractal behavior of the flocs. This allows us to establish the following relations between the primary characteristics of a floc in each class i:

$$m_i = \rho_p \frac{\pi}{6} D_p^3 \left(\frac{D_i}{D_p}\right)^{n_f}, \tag{9.2}$$

$$\rho_i = \rho_f + (\rho_p - \rho_f)\left(\frac{D_p}{D_i}\right)^{3-n_f}, \tag{9.3}$$

where m_i, D_i and ρ_i are the mass, diameter, and density of a floc in class i and n_f is the fractal dimension.

The generic equation for the flocculation process is composed of the aggregation, shear breakup, and collision breakup terms, and n_k denotes the number concentration in class k. For a new floc to form, at least one existing floc must give up its identity (to ensure mass continuity), so each of these terms exists as a gain (G) and loss (L) term. The generic equation can therefore be written as

$$\frac{\partial n_k}{\partial t} = G_{ag}(k) + G_{br,sh}(k) - L_{ag}(k) - L_{br,sh}(k). \tag{9.4}$$

For aggregation to occur, two flocs must come into contact, and the attractive forces must dominate over the repulsive ones. Therefore, the two aggregation terms (G_{ag} and L_{ag}) are each a function of the collision probability function $A(i,j)$ and the collision efficiency α:

$$G_{ag}(k) = \frac{1}{2} \sum_{i+j=k} \alpha_{i,j} A(i,j) n_i n_j, \tag{9.5}$$

$$L_{ag}(k) = \frac{1}{2} \sum_{i} \alpha_{i,k} A(i,k) n_i n_k. \tag{9.6}$$

The collision probability function is a binary function governed by the shear rate G and the floc diameters D_i and D_j:

$$A(i,j) = \frac{1}{6} G(D_i + D_j)^3. \tag{9.7}$$

The collision efficiency α parameterizes the cohesiveness of the flocs. Typically, α is set as a constant value and used as an optimization parameter. Turbulent shear is assumed to be the driving mechanism for flocculation. At the same time, if turbulent shear becomes too strong, it may also lead to the fragmentation of flocs. This is expressed via the gain and loss terms of shear breakup:

$$G_{\mathrm{br,sh}} = \sum_{i+j=k} \Pi_{ki} B_i n_i, \tag{9.8}$$

$$L_{\mathrm{br,sh}} = B_k n_k. \tag{9.9}$$

The turbulent shear and its yield strength determine the probability of breakup of a k-class floc. The fragmentation probability function is written as

$$B_i = \beta G^{3/2} D_i \left(\frac{D_i - D_\mathrm{p}}{D_\mathrm{p}} \right)^{3-n_\mathrm{f}}, \tag{9.10}$$

where B_i is a function of the shear rate G and the fragmentation rate β. The latter represents the yield strength of the flocs, which, like cohesiveness, depends on their composition. Therefore, β is often set as a constant value similar to α and used as an optimization parameter. The breakup function Π_{ki} characterizes different breakup scenarios. Here, we choose the default of a binary distribution: i.e., a floc of mass m_i fragments into two flocs of equal mass $m_j = m_i/2$. Moreover, a suitable time step must be selected to ensure mass continuity and avoid processing more flocs than are present in each class. FLOCMOD offers the option of a variable time step. A check is performed in each time step to see whether a class has a negative mass. In such a case, the time step is recomputed with a new time step half the size of the previous one. If all classes have positive masses, a new time step is chosen that is twice as large until at least one class has a negative mass or a maximum time step size is reached, which is set to be 60 s. Based on these capabilities, the varying time step method is used in this study, and the initial time step is set to $\Delta t = 3T_0$.

9.3. POST-PROCESSING OF THE FLOCCULATION DATA

9.3.1. Transient Behavior

The simulation data contain information about the number of flocs and the number of particles in each of these flocs for each time step. By grouping the flocs into five size classes based on the number of primary particles per floc, N_p, and plotting the temporal evolution of these size classes, a first insight into the simulation results is obtained in Figure 9.1. The boundaries between the five size classes were logarithmically distributed between a floc consisting of only a single primary particle and the maximum number of particles in a floc observed in this data group. Therefore, each size class comprises a different number of floc sizes.

Figure 9.1 shows the distinct temporal behaviors for the cases Flo1–5 that vary in terms of cohesive forces. The two phases of transient flocculation and statistically quasi-steady equilibrium, as described by Zhao et al. (2021), are readily apparent. The floc with the largest number of particles formed in this group during the simulations consisted of 432 primary particles. The effect of the variable cohesive number is also clearly visible. For the case Flo1 ($A_\mathrm{H} = 3 \times 10^{-23}$ J), the size class containing flocs with only one or two primary particles (blue line) dominates with a total number of flocs of $O(10^3 \sim 10^4)$, which was at all times one order of magnitude larger than the next larger size class. At the same time, the number of flocs of the size class describing the largest flocs ($101 \leq N_\mathrm{p} \leq 432$) was very small. Often, no floc of this size existed. In contrast, in the Flo5 case ($A_\mathrm{H} = 3 \times 10^{-21}$ J), the number of flocs in the size class containing flocs with only one or two primary particles decreased steadily, whereas the size class containing the largest flocs with more than 100 particles increased until it reached a quasi-steady state that was established until the end of the simulation (brown line).

Zhao et al. (2021) furthermore computed the floc size in their simulations as the characteristic Feret diameter defined as

$$D_\mathrm{f} = 2 \max\left(\|x_{\mathrm{p},i} - x_\mathrm{c}\|\right) + D_\mathrm{p}, 1 \leq i \leq N_\mathrm{p}, \tag{9.11}$$

in which $x_{\mathrm{p},i}$ indicates the center of the primary particle i and x_c describes the floc's center of mass, determined as $x_\mathrm{c} = \sum_{i=1}^{N_\mathrm{p}} x_{\mathrm{p},i}/N_\mathrm{p}$. In what follows, the temporal evolution is smoothed by a moving average with an average window of 0.085 s to filter out the fluctuations of the highly resolved simulation data.

9.3.2. Equilibrium Stage

To interpret the flocculation results of Zhao et al. (2021) in terms of their floc-size distributions at the equilibrium stage, we present normalized histograms to properly represent the likelihood of flocs forming with a certain number of particles. Representing the equilibrium stage, the histograms show the floc-size distribution recorded at the end of the simulation time.