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Modeling floc size distribution of suspended cohesive sediments using quadrature method of moments

Xiaoteng Shen *, Jerome P.-Y. Maa

Virginia Institute of Marine Science, College of William & Mary, P.O. Box 1346, Gloucester Point, VA 23062, USA

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ABSTRACT

An enhanced Quadrature Method Of Moments (QMOM) is employed to solve the population balance model (PBM) with a maximum of eight size classes for the purpose of describing the evolution of floc size distribution (FSD) of kaolinite suspension and colloidal montmorillonite. This approach can be used to estimate many representative sizes, e.g., d_{32} (Sauter mean size), d_{43} (De Broukere mean size), d_{60} (hydrodynamic mean size), and D_{50} (median size). The following three considerations are adopted to enhance the QMOM approach: (1) An adjustable factor, which is selected based on its ability to track up to eight size classes, is implemented; (2) moments higher than the third order are not necessarily simulated directly; (3) a restriction on the ratio between the minimum and maximum weights is used to exclude unreliable nodes. The above enhancements have been proposed by others, but are integrated for the first time in this study. Model results are verified by comparison with available experimental data. The results of this study suggest that the quadrature nodes and weights in the QMOM are the characteristic sizes and corresponding characteristic number densities to effectively predict the FSD of cohesive sediments. This study also demonstrates that the possible range of the correction factor (also sometimes referred to as "collision efficiency") for the Euclidean collision frequency could be larger than one because of both the difference in floc structure represented by fractal dimension as well as the impacts of organic matter.

1. Introduction

The prediction of transport and fate of fine-grained suspended cohesive sediments in estuaries and adjacent coastal waters is important for many scientific and engineering applications, e.g., siltation in navigation channels and harbors, water quality, and pollutant transport. An essential process of cohesive sediment dynamics is the flocculation that determines floc size, and thus, settling velocity. Flocculation is the result of simultaneous processes of aggregation and breakage. The challenge in modeling flocculation is that many factors can influence this process, e.g., the ambient turbulence intensity, local suspended sediment concentration, static electrical forces (i.e., due to salinity and other ions), and bio-activities such as the production of Extracellular Polymeric Substance (EPS), and thus, no accurate modeling experiment has been conducted yet.

Besides the chemical and biological factors, the most relevant mechanisms responsible for flocculation are Brownian motion (e.g., Eisma, 1986), differential settling (e.g., Lick et al., 1993; Zhang and Zhang, 2011), and fluid shear (e.g., Winterwerp, 1998; Mietta et al., 2008). It is well accepted that Brownian motion (also known as "perikinetic flocculation"), the random thermal moving of particles suspended in a fluid, only affects suspended particles less than 1–2 μm, so that it is negligible in natural estuarial waters where suspended sediment size is large and ambient turbulence is strong (Van Leussen, 1994; Winterwerp, 1998; Thomas et al., 1999; McAnally, 2000). Differential settling is a process that describes faster-falling particles overtaking slower ones. Fluid shear allows one particle to capture others more efficiently because of strong, random motions among particles. The relative importance of differential settling and fluid shear, however, depends on the applications. For example, Winterwerp (1998) and Maggi et al. (2007) showed fluid shear to be the dominant effect as the likelihood of a large (i.e., rapidly settling) particle colliding with a small (i.e., slowly falling) particle is small. This is because the trajectory of the small particle is deflected by strong hydrodynamic interactions with the larger particle. Here the hydrodynamic interaction describes the momentum transfer from a suspended particle to fluid molecules, and then from the fluid molecules to another particle (Ladd and Verberg, 2001). On the other hand, Lick et al. (1993) stated that differential settling may become the primary factor in open waters away from shore where turbulence is low. Zhang and Zhang (2011) also emphasized the effect of differential settling in their work.

In general, there are three kinds of flocculation models. The first kind of model is the simplified Lagrangian flocculation model (e.g., Winterwerp, 1998, 1999, 2002; Winterwerp and van Kesteren, 2004; Maggi, 2008; Son and Hsu, 2008; Maggi, 2009; Son, 2009; Son and Hsu, 2011a,b). Winterwerp (1998) first developed this kind of

* Corresponding author at: 1208 Greate Road, Gloucester Point, VA 23062, USA. Tel.: +1 8046847817.
E-mail address: xiaoteng@vims.edu (X. Shen).

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model for a constant fractal dimension to describe the floc shape. Later, Son and Hsu (2008) extended this model for a variable fractal dimension. An advantage of this kind of model is that it can track the evolution of a characteristic size (usually the median size) with reasonable computing efficiency, and it is easy to couple with hydrodynamic models, turbulence models, and sediment transport models (Winterwerp, 2002). A weakness is that only one characteristic size (i.e., the median floc size) is addressed. Other properties, notably the floc size distribution (FSD) and detailed evolution processes of particle number and volume, cannot be resolved by this kind of model.

The second kind of model is the extended Lattice Boltzmann Model (LBM) (e.g., Zhang and Zhang, 2011; Zhang et al., 2013). The traditional LBM is a mesoscopic hydrodynamic model (not a flocculation model) that is mapped onto the incompressible Navier–Stokes equations (Ladd and Verberg, 2001). Ladd (1994a,b) extended the LBM by adding the motion of solid particles in suspension. They treated the solid particles as imposing moving boundary conditions on the fluid. This method was further extended to explore the flocculation of cohesive sediments due to deferential settling (Zhang and Zhang, 2011) and turbulent shear (Zhang et al., 2013). This latest approach provides more information, including FSD and floc settling velocities, than the first kind of model, and allows collision behaviors to be studied directly through statistical analyses of model results. However, prohibitive computational costs and memory requirements for simulating a larger study domain limit the use of this approach to only studying the process itself, e.g., determining the collision efficiency (also called correction factor in this study).

The third kind of model is the Population Balance Model (PBM) (e.g., Maggi, 2005; Prat and Ducoste, 2006; Maggi et al., 2007; Prat and Ducoste, 2007; Mietta et al., 2008; Xu et al., 2008; Lee et al., 2011; Mietta et al., 2011; Verney et al., 2011; Furukawa and Watkins, 2012), which is the model type used in this study. PBM is essentially a transport equation that tracks number density of flocs of certain size at any location and at any time in a system. A thorough review of the origins and derivation of PBM can be found in Sporleder et al. (2012), and a summary of various methods for solving a PBM is presented in Su et al. (2009).

Among all the available methods for solving PBM, the Quadrature Method Of Moments (QMOM) is the most efficient one (Marchisio et al., 2003c; Prat and Ducoste, 2006, 2007). QMOM transfers PBM to a set of moment transport equations (McGraw, 1997), so that the lower-order moments of FSD are tracked with high accuracy with a low computational cost (see "Section 4" for more details). In addition, their mean sizes (e.g., arithmetic mean size, Sauter mean diameter, and De Broukere mean diameter) are recorded with high accuracy. However, conventional QMOM usually fails when tracking more than four size classes, and thus, it is difficult to construct the FSD from the conventional QMOM. Su et al. (2007) employed adjustable factors assigned to different processes to track the moments of FSD with lower computational demands than that from the standard QMOM. Since the purpose of their work did not entail tracking additional size classes to find the FSD, they only used three size classes and did not report any FSD in their results.

The objective of this study is to investigate the temporal evolution of FSD, including the aggregation and breakage behaviors of cohesive sediments. To achieve this goal, the adjustable QMOM approach that solves the PBM is modified to track changes of particle density for a maximum of eight size classes. Data from two available laboratory experiments (one with suspended kaolinite and the other with colloidal montmorillonite) are simulated. Detailed information, such as the FSD itself, its mode, mean, and median size, and the processes of birth and death of floc number and floc volume, are monitored.

This paper is organized as follows. Methods are described in Section 2. Section 2.1 reviews the PBM model and standard QMOM approach. Section 2.2 presents QMOM with an adjustable factor and illustrates how to apply this approach. Section 2.3 explains the selection of appropriate aggregation and breakage functions, i.e., the collision frequency, the correction factor, the breakup frequency, and the fragmentation distribution function. Section 3 sets up this flocculation model. The model is calibrated and verified by comparison with available data reported by Mietta et al. (2008) and Furukawa and Watkins (2012) for kaolinite suspension and colloidal montmorillonite, respectively. Results and discussions are included in Section 4, and concluding remarks are delivered in Section 5.

2. Model description and numerical methods

2.1. Population balance modeling and quadrature method of moments

The length-based PBM describes the change of number density for flocs with size L. A PBM box model, which is simplified by eliminating the advection, diffusion, and settling terms (see Eq. 1 in Marchisio et al., 2003b), is selected as the first effort in this study. This simplification is also convenient for calibration and verification using published data from Mietta et al. (2008) and Furukawa and Watkins (2012). Inclusion of these omitted terms will be restored in a future study. The simplified PBM model can be represented as

$$\frac{\partial n(L;t)}{\partial t}=\frac{L^2}{2}\int_0^L\left[\frac{\beta\left(\left(L^3-\lambda^3\right)^{1/3},\lambda\right)\cdot\alpha\left(\left(L^3-\lambda^3\right)^{1/3},\lambda\right)}{\left(L^3-\lambda^3\right)^{2/3}}\cdot n\left(\left(L^3-\lambda^3\right)^{1/3};t\right)\cdot n(\lambda;t)\right]d\lambda$$
$$-n(L;t)\int_0^\infty\beta(L,\lambda)\alpha(L,\lambda)n(\lambda;t)d\lambda+\int_L^\infty a(\lambda)\cdot b(L|\lambda)\cdot n(\lambda;t)d\lambda-a(L)\cdot n(L;t) \tag{1}$$

where λ is the integral variable with the same dimension of floc size L, $n(L;\,t)$ is the number density function defined by floc size L at time t, $\beta(L,\lambda)$ is the Euclidean collision frequency function that describes the frequency of two spheres with size L and λ colliding to form a particle with size $(L^3+\lambda^3)^{1/3}$, $\alpha(L,\lambda)$ is the correction factor (also called collision efficiency) that includes effects of particle geometry, contact efficiency, and sticking probability, $a(L)$ is a breakup frequency function that denotes the frequency of disruption for particles with size L, and $b(L|\lambda)$ is a fragmentation distribution function that represents particles with size L produced by the breakup of a particle with size λ. The first term on the right hand side of Eq. (1) is the birth of flocs with size L due to aggregation of smaller particles with size $(L^3\text{-}\lambda^3)^{1/3}$ and λ. The second term on the right hand side is the death of flocs with size L due to aggregation with other particles. The third term is the birth of flocs with size L due to fragmentation of bigger particles λ, and the last term is the death of flocs with size L due to breakup into smaller particles.

The moment transfer (Hulburt and Katz, 1964; McGraw and Saunders, 1984) is applied to Eq. (1) using the following definition:

$$m_k=\int_0^\infty L^k n(L;t)dL \tag{2}$$

in which m_k is the kth order moment. Notice that the size class L varies from zero to infinity in the transformation.

After applying the transformation to Eq. (1) with $k = 0, 1,\ldots, K$, the PBM becomes a set of moment equations (Eq. (3)) that are essentially a system of non-linear integro-differential equations (Kariwala et al., 2012)

$$\begin{aligned}\frac{\partial m_k}{\partial t}=&\frac{1}{2}\int_0^\infty n(\lambda;t)\int_0^\infty\beta(L,\lambda)\cdot\alpha(L,\lambda)\cdot\left(L^3+\lambda^3\right)^{k/3}\cdot n(L;t)dLd\lambda\\&-\int_0^\infty L^k n(L;t)\int_0^\infty\beta(L,\lambda)\alpha(L,\lambda)n(\lambda;t)d\lambda dL\\&+\int_0^\infty L^k\int_0^\infty a(\lambda)\cdot b(L|\lambda)\cdot n(\lambda;t)d\lambda dL-\int_0^\infty L^k a(L)\cdot n(L;t)dL\end{aligned} \tag{3}$$

Eq. (3), however, cannot be solved, either numerically or analytically, because the integrations terms have not been expressed in term of the