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A tri-modal flocculation model coupled with TELEMAC for estuarine muds both in the laboratory and in the field

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Abstract

Estuarine and coastal regions are often characterized by a high variability of suspended sediment concentrations in their waters, which influences dredging projects, contaminant transport, aquaculture and fisheries. Although various three-dimensional open source software are available to model the hydrodynamics of coastal water with a sediment module, the prediction of the fate and transport of cohesive sediments is still far from satisfied due to the lack of an efficient and robust flocculation model to estimate the floc settling velocity and the deposition rate. Single-class and sometimes two-class flocculation models are oversimplified and fail to examine complicated floc size distributions, while quadrature-based or multi-class based flocculation models may be too complicated to be coupled with large scale estuarine or ocean models. Therefore, a three-class population balance model was developed to track the sizes and number concentrations of microflocs, macroflocs and megaflocs, respectively. With the assumption of a fixed size of microflocs and megaflocs, only four tracers are needed when coupled with the open-source TELEMAC system. It enables better settling flux estimates and better addresses the occurrence and concentration of

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larger megaflocs. This tri-modal flocculation model was validated with two experimental data sets: (1) 1-D settling column tests with the Ems mud and (2) in-situ measurements at the WZ Buoy station on the Belgian coast. Results show that the flocculation properties of cohesive sediments can be reasonably simulated in both environments. It is also found that the number of macroflocs created, when a larger macrofloc breaks up, is a statistical mean value and may not be an integer when applying the model in the field.

Keywords: Population balance equation; three classes; TELEMAC; cohesive sediments; settling column; Belgian coastal zones

1. Introduction

In aquatic science and engineering, sediment represents granular and particulate matter suspended in the water column or deposited on the bed (Winterwerp, 2012). Fine-grained Suspended Sediment Concentration (SSC) affects and controls turbidity, which is an important parameter to understand marine or fresh water ecosystems. Data on water clarity in coastal seas have shown significant changes caused by human activities and climate change (Capuzzo et al., 2015). These changes in SSC not only affect the ecosystems, but have further crucial impacts on sediment transport and the deposition in man-made environments such as fresh water reservoirs where the dam storage level reduces (e.g., Wisser et al., 2013) or estuaries and coastal areas where ports and navigational channels need frequent dredging in order to remain navigable (e.g., Song and Wang, 2013). Additionally, the transport of sediment controls the fate of pollutants and nutrients that tend to be adsorbed to fine particles. These impacts result in environmental and financial burdens due to the need for dredging and restoration works. Fine particles in suspension often attach with each other and form flocs or aggregates. A floc is an individual micro-ecosystem, composed of inorganic and organic particles, and water within or flowing through the pores, with various physical (e.g., turbulent shear), chemical (e.g., salinity) and biological (e.g., micro-organisms, exopolymers and fecal pellets) influences interacting with its aquatic surroundings or within the floc matrix (Droppo, 2001, 2003, 2006; Jago et al., 2007; Tan et al., 2012). The size and density of a floc significantly alter its settling velocity, and thus, the downward flux of sediments. Although flocs have lower densities, they settle faster than their constituent particles because of their larger size; therefore Droppo et al. (1998) pointed out that floc size is a crucial parameter to predict the settling velocity of the suspended particles. Natural particles, such as flocs, have irregular shapes and sizes, and generally have a Floc Size Distribution (FSD) with lognormal subordinates. As floc size increases, the effective density decreases; the settling velocity can

then be derived if a relationship between effective density and floc size is established. This can be achieved, e.g., by assuming a self-similarity between primary particles and flocs based on fractal theory (Kranenburg, 1994; Winterwerp, 1998) or by using density functions that describe the mass distribution over the FSD (Markussen and Andersen, 2013).

Numerical models have become an important tool for studying the hydrodynamic, sediment and associated contaminant transport, and morphology in aquatic regions. Various three-dimensional (3-D) large scale numerical models are available, such as DELFT3D (Lesser et al., 2000), ECOMSED (Estuarine Coastal and Ocean Modeling system with Sediment, see HydroQual, 2002), COHERENS (Luyten, 2011) and TELEMAC (Villaret et al., 2013). However, the predictions of sediment dynamics often are still poor, due to lack of advanced descriptions of flocculation kinetics. Since the 1990s it is known that models without flocculation will generate significant errors (Nicholas and Walling, 1996; Droppo et al., 1998). Nevertheless, an efficient flocculation model is still unavailable to account for appropriate corrections of the settling velocity and the deposition rate, since these parameters dynamically change with the turbulent shear, SSC and various chemical and biological effects. Flocculation models based on a single characteristic size (e.g., Winterwerp, 1998 and its variants), although including the description of aggregation and breakup processes, may lead to large errors when estimating the settling flux (Lee et al., 2012). Besides, one single median size may be biased to represent bimodal FSDs which nevertheless are commonly observed. Therefore, approaches that are able to simulate the FSDs with multiple groups are favorable, e.g., the Lattice Boltzmann Methods (LBMs) (Zhang and Zhang, 2011; Zhang et al., 2013) and the Population Balance Equations (PBEs) (McAnally and Mehta, 2002; Krishnappan and Marsalek, 2002; Maggi et al., 2007; Xu et al., 2008; Verney et al., 2011; Mietta et al., 2011; Shen and Maa, 2015, 2016a, 2016b; Shen, 2016; Cuthbertson et al., 2018). At the current stage, the LBMs are limited to study the particle micro-behavior such as the

1 collision efficiency of two approaching particles (Zhang et al., 2016). Thus, the PBEs are
2 paid increasing attention for the purpose to have the potential to model a relatively larger
3 study domain. For instance, McAnally and Mehta (2002) proposed a multi-class sediment
4 model with statistical collision efficiency for two flume experiments, despite with high
5 computational demands. Krishnappan and Marsalek (2002) employed multi-class PBE to
6 predict sediment transport of an on-stream stormwater detention pond, with the assumption of
7 spherical flocs settled following Stoke's equation. The idea of using an allocation functions to
8 distribute newly formed particles into different bins, was later applied by Cuthbertson et al.
9 (2018) to model the FSDs of clay-sand mixture. Also, Maggi et al. (2007) used eight size
10 classes to model the FSDs in a settling column experiment; nonetheless, their predictions of
11 mean sizes of FSDs are poor, and the model efficiency to be included in 1-D or 3-D models
12 have not been tested yet. Moreover, Verney et al. (2011)'s approach to include both fluid
13 shear and particle collision induced disaggregation, although recently has been included in
14 the ROMS (Regional Ocean Modeling System) model (Sherwood et al., 2018), might face the
15 problem of numerical diffusion towards larger sizes (Maerz et al., 2011). The models by Xu
16 et al. (2008) and Mietta et al. (2011) were similar as that by Verney et al. (2011), except that
17 the breakage due to particle collision was neglected. Furthermore, Shen and Maa (2015,
18 2016a, 2016b) used the quadrature method of moments to solve the PBE and applied it in a 1-
19 D longitudinal streamtube model (Shen and Maa, 2017). Their study reconstructed a
20 continuous FSD from their moments (which is mathematically solving a "finite moment
21 problem", e.g., see Chebyshev, 1961; John et al., 2007), and the conservation of floc volume
22 is guaranteed. Nevertheless, the classical quadrature method of moments is difficult to model
23 complicated FSDs with several peaks in biomass abounding tidal environments, unless using
24 additional heavy subroutines to better solve this "finite moment problem" (Lebaz et al., 2016).

Recently, [Lee et al. \(2012\)](#) pointed out that a measured FSD generally can be decomposed into four lognormal FSDs to represent primary particles, microflocs, macroflocs and megaflocs, respectively. Primary particles have a size range of 0.25 – 4 μm which is the typical size range of clay. Microflocs in general have a size range of 4 – 20 μm and are relatively stable and compact; they can be treated as the building elements of flocs. The critical diameter (D_{sp}) to separate macroflocs and megaflocs (sometimes referred to as microflocs and macroflocs respectively in literature if only two classes are addressed) varies for different studies. For example, [Gratiot and Manning \(2002\)](#) determined $D_{sp} = 120 \mu\text{m}$ by roughly separating the two observed peaks of FSDs for Gironde and Tamar mud samples. [Mikkelsen et al. \(2006\)](#) selected D_{sp} as 133 μm since their instruments (LISST & floc digit camera) overlap in 133–500 μm . [Manning and Schoellhamer \(2013\)](#) recommended $D_{sp} = 160 \mu\text{m}$ in terms of the settling velocity and dry mass of each floc sub-population for a wide range of shear stress and suspended particulate matter concentration conditions. Macroflocs and megaflocs may also be demarcated as 200 μm at Belgian coast ([Lee et al., 2012](#)) due to automatic decomposition of observed FSDs. In order to model the observed multimodal FSDs with reduced size groups, [Lee et al. \(2014\)](#) developed a two-class PBE, solving with hydrodynamic and turbulence models, to identify the size-fixed microflocs (actually primary particles & microflocs) and the size-varying macroflocs (actually macroflocs & megaflocs) for matching a decomposed FSD. However, using two classes to represent the FSDs is sometimes oversimplified. On one hand, a single size-unfixed group of macroflocs is, however, not sufficient to represent the larger flocs that may be formed during algae blooms or periods with high biological activity. On the other hand, [Lee et al. \(2012\)](#) analyzed the FSD data collected from Belgian coast for shear-dependent and breakage-resistant flocculation conditions during normal and storm surge weather conditions. They used the FSDs of 32 classes from LISST instrument as a reference, and concluded that with two-class

the errors to estimate settling fluxes may be up to 10 %, while with an additional class the errors may be largely declined to 4 %.

Therefore, the main objective of this study is to improve [Lee et al. \(2011, 2014\)](#)'s model from a two-class to a three-class PBE to simulate the representative sizes and mass fractions of microflocs, macroflocs and megaflocs, respectively, for the purpose of better representing the FSDs and flocculation processes, and better estimating the settling velocities of fine-grained cohesive particles in aquatic environments. It assumes that only the inorganic components of the particles are explicitly considered before a more quantitative and comprehensive understanding of organic components is available. This flocculation model is further coupled with the open source code TELEMAC, suitable for large-scale applications, validated with experimental data from a settling column test and field data from the Belgian coastal zone. In a later stage, the model may be adapted for the application to the transport and dispersal of microplastic (MP) particles in coastal waters, accounting for the effects of weathering, biofouling and subsequent aggregation (including with sediment particles), in order to gain better insights into the 3-D pathways of MP particles in the aquatic environment from the water surface to the sea bottom ([Jahnke et al, 2017](#); [Ogonowski et al., 2018](#)).

2. Numerical models

2.1 Flocculation kinetics

The tri-modal PBE is developed to describe the flocculation processes, as an improvement of previous two-class PBE model (see [Lee et al., 2011, 2014](#)). For applications in a 1-D vertical water column, the governing equation without fluid advection can be simplified as:

$$\frac{\partial N_i}{\partial t} - \omega_{s,i} \frac{\partial N_i}{\partial z} = \frac{\partial}{\partial z} \left(D_z \frac{\partial N_i}{\partial z} \right) + (A_i + B_i) \quad i = P, F1, T1, T2 \quad (1)$$

where N_i is number concentration (in unit of m^{-3}), t is the time, ω_s is the settling velocity, z is the vertical coordinate, D_z is the eddy diffusivity, and A_i & B_i are aggregation and breakage source and sink terms. Eq.1 is actually a system of tracer transport equations that track (1) the number of microflocs and macroflocs in suspension per unit volume, with symbol N_P and N_{F1} respectively, (2) the total number of microflocs in all macroflocs (but not in megaflocs or in suspension) per unit volume N_{T1} , and (3) the total number of microflocs in all megaflocs (but not in macroflocs or in suspension) per unit volume N_{T2} .

In field measurements a large section of primary particles may be smaller than the lower size range of the measuring instrument (e.g., LISST-100X) and are thus not accurately measured. Further field data suggest that two populations of floc building blocks ($< 3 \mu\text{m}$ and microflocs of about $15 \mu\text{m}$) apparently coexist in situ (Fettweis et al., 2012). As a consequence, the relatively stable microflocs that consist of clusters of clay minerals are assumed to be the building elements of macroflocs and megaflocs. The average number of microflocs in one macrofloc per unit volume is $N_{C1} = N_{T1} / N_{F1}$; similarly, the average number of microflocs in one megafloc per unit volume is $N_{C2} = N_{T2} / N_{F2}$ (where N_{F2} is the total number of megaflocs in suspension). Thus, the sizes of microflocs and macroflocs can be determined as (Matsoukas and Friedlander, 1991)

$$D_{Fi} = D_P \cdot N_{Ci}^{1/\eta f_i} \quad i = 1, 2 \quad (2)$$

where ηf is the fractal dimension of flocs, and D_P , D_{F1} and D_{F2} are the characteristic sizes of microflocs, macroflocs and megaflocs, respectively. The size of microflocs D_P is assumed a constant (Lee et al., 2011, 2012, 2014), while D_{F1} , determined by N_{C1} (Eq.2) and thus by tracer N_{T1} and N_{F1} , is varying with time and space. In this study, D_{F2} is also assumed as a constant to reduce the number of tracers. This assumption can be supported by field data such as shown later in this study. In this sense, N_{C2} is fixed, and $N_{F2} = N_{T2}/N_{C2}$.

For microflocs D_P , macroflocs D_{F1} and megaflocs D_{F2} , the corresponding number concentrations are N_P , N_{F1} and N_{F2} , respectively. Their mass fractions can be computed as

$$M_i = \frac{N_i}{N_P + N_{T1} + N_{T2}} \quad i = P, T1, T2 \quad (3)$$

which can be used to construct the mass-based FSDs (as shown in Fig. 1).

The mechanisms included in this three-class PBE are summarized in Table 1, with five aggregation processes and two breakage processes. For the aggregation processes (Process 1 to Process 5), the fundamental assumption is that only two-body collision (i.e., two particles collide and attach to become one particle) are considered, with its creation rate proportional to their collision frequency β , collision efficiency α and their number concentrations. Inter-size collisions (Process 2, Process 3 and Process 5) are straightforward. If successfully attached, the collision of a microfloc and a macrofloc will create a larger particle classified in the group of macroflocs, the collision of a microfloc and a megafloc will produce a larger megafloc, and the collision of a macrofloc and a megafloc will also generate a larger megafloc. Intra-size collisions (Process 1 and Process 4) require additional assumptions. This is because, e.g., sorting a particle with two microflocs (as a result of two microflocs colliding together) as a macrofloc, is physically unreasonable when $N_{C1} \gg 2$. A practical way is distributing the particle based on its mass ratio (Jeong and Choi, 2003; Lee et al., 2011). Use Process 1 as an example. If the average microflocs in one macrofloc is $N_{C1} = 10$, the resulted one particle with 2 microflocs can be sorted as an 8/9 microfloc and a 1/9 macrofloc (totally still 1 particle). This is according to the ratio of the distance of this actual particle (with 2 microflocs) to the group of microflocs (with 1 microfloc) and macroflocs (with N_{C1} microflocs) are 1: 8. Therefore, the net result of a two-microfloc collision will lead to an increase of $1/(N_{C1}-1)$ macrofloc and a decrease of $2-(N_{C1}-2)/(N_{C1}-1) = N_{C1}/(N_{C1}-1)$ microfloc. A similar process is shown in Process 4. Note that the process which represents

1 the collision of two megaflocs creating a larger megafloc will not change the concentration of
 2 any tracers under the current assumptions.

3 For the breakage of macroflocs (Process 6) and megaflocs (Process 7), the creation
 4 rate is proportional to the breakage frequency a and their number concentrations. For the
 5 breakage of a parent macrofloc, it assumes that it will lead to number of K_1 smaller
 6 macroflocs with mass ratio $1-f_{P1}$ and several microflocs with mass ratio f_{P1} . Lee et al. (2011)
 7 assume $K_1 = 2$ in their study. For the breakage of a parent megafloc, it assumes that it will
 8 result in several microflocs with mass ratio f_{P2} , number of K_2 macroflocs with mass ratio
 9 $1-f_{P2}-f_{F2}$, and remained megafloc(s) with mass ratio f_{F2} .

10 Based on the above aggregation and breakage processes, the source and sink terms in
 11 Eq. 1 can be written as:

$$12 \quad (A_P + B_P) = -\frac{1}{2} \alpha \beta_{PP} N_P N_P \left(\frac{N_{C1}}{N_{C1} - 1} \right) - \alpha \beta_{PF1} N_P N_{F1} - \alpha \beta_{PF2} N_P N_{F2} + f_{P1} N_{C1} a_{F1} N_{F1} + f_{P2} N_{C2} a_{F2} N_{F2}$$

13 (4a)

$$14 \quad (A_{F1} + B_{F1}) = \frac{1}{2} \alpha \beta_{PP} N_P N_P \left(\frac{1}{N_{C1} - 1} \right) - \frac{1}{2} \alpha \beta_{F1F1} N_{F1} N_{F1} \left(\frac{N_{C2} / N_{C1}}{N_{C2} / N_{C1} - 1} \right) - \alpha \beta_{F1F2} N_{F1} N_{F2}$$

$$15 \quad + (K_1 - 1) a_{F1} N_{F1} + K_2 a_{F2} N_{F2}$$

16 (4b)

$$17 \quad (A_{T1} + B_{T1}) = \frac{1}{2} \alpha \beta_{PP} N_P N_P \left(\frac{N_{C1}}{N_{C1} - 1} \right) + \alpha \beta_{PF1} N_P N_{F1} - \frac{1}{2} \alpha \beta_{F1F1} N_{F1} N_{F1} \left(\frac{N_{C2}}{N_{C2} / N_{C1} - 1} \right)$$

$$18 \quad - N_{C1} \alpha \beta_{F1F2} N_{F1} N_{F2} - f_{P1} N_{C1} a_{F1} N_{F1} + (1 - f_{P2} - f_{F2}) N_{C2} a_{F2} N_{F2}$$

19 (4c)

$$19 \quad (A_{T2} + B_{T2}) = \alpha \beta_{PF2} N_P N_{F2} + \frac{1}{2} \alpha \beta_{F1F1} N_{F1} N_{F1} \left(\frac{N_{C2}}{N_{C2} / N_{C1} - 1} \right) + N_{C1} \alpha \beta_{F1F2} N_{F1} N_{F2} - (1 - f_{F2}) N_{C2} a_{F2} N_{F2}$$

20 (4d)

21 The collision efficiency α is a fitting parameter, and the collision frequency β can be
 22 expressed as (Thomas et al., 1999; Maggi, 2005)

$$\beta_{i,j} = \frac{1}{6}G(D_i + D_j)^3 + \frac{\pi}{4}(D_i + D_j)^2 \cdot |\omega_{s,i} - \omega_{s,j}| + \frac{2}{3} \frac{K_B T}{\mu} \frac{(D_i + D_j)^2}{D_i D_j} \quad (5)$$

where G is the shear rate, ω_s is the settling velocity, K_B is the Boltzmann constant, T is the absolute temperature and μ is the fluid dynamic viscosity. Eq. 5 assumes that the collision frequency is a linear combination of the effect of turbulent shear (first term in Eq. 5), differential settling (second term in Eq.5) and Brownian motion (third term in Eq. 5). It is important to note that the effect of turbulent shear is the main mechanism in natural environments (Winterwerp, 1998). The effect of differential settling is important during slack tide when turbulence is low (Lick et al., 1993), while the effect of Brownian motion is generally low for large particles (Winterwerp, 1998).

The breakup frequency a can be written as (Winterwerp, 1998)

$$a_i = E_b G \left(\frac{D_i - D_p}{D_p} \right)^{3-\eta_f} \cdot \left(\frac{\mu \cdot G}{F_y / D_i^2} \right)^{1/2} \quad (6)$$

where E_b is the breakage coefficient. The floc strength F_y , although not a constant (Kranenburg, 1999), is assumed as 10^{-10} Pa in this study (Maggi et al., 2007; Verney et al., 2011) before a thorough explanation of this parameter is available in the future.

The settling velocity is given by a fractal-corrected Stokes equation with hindered settling corrections (Winterwerp and van Kesteren, 2004):

$$\omega_{s,i} = \phi_{HS} \left(\frac{1}{18} \frac{(\rho_p - \rho_w)g}{\mu} D_p^{3-\eta_f} \cdot \frac{D_i^{\eta_f-1}}{1 + 0.15 Re_i^{0.687}} \right) \quad (7)$$

where ρ_w and ρ_p are the density of water and elementary particles respectively. The particle Reynolds number can be written as $Re_i = \omega_s \cdot D_i \cdot \rho_w / \mu$, and the correction factor for hindered settling is (Richardson and Zaki, 1954)

$$\phi_{HS} = (1 - \phi)^\gamma \quad (8)$$

where ϕ is the volume fraction of suspended particles, and γ is an empirical parameter and set as 4.65 for low Reynolds number condition when wall effects are neglected (Di Felice and Kehlenbeck, 2000). It is critical to note that the hindered settling factor described in Eq. 8 is only applicable for low solid volume fractions. At higher solid concentrations, the mud will form a network and exhibit a yield stress in both shear and compression. The maximal volume fraction is of the order 0.6 (cf. spherical particles, see Toorman, 1999). For flocs, it corresponds to the gelling concentration, i.e., corresponding to a typical density of fresh fluid mud which is typically 1100 kg/m³ for the North Sea area. If convert this in volumetric concentration of the particles, this corresponds to roughly 7 - 8 %, which is around 200 g/L. It further assumes that $\omega_{s,F1} = \omega_{s,T1}$ and $\omega_{s,F2} = \omega_{s,T2}$, since the microflocs within the macroflocs (or megaflocs) should settle as the same velocity as the macroflocs (or megaflocs) themselves.

The boundary conditions are specified as Eq. 9 (Lee et al., 2014)

$$\omega_{s,i} N_i - v_t \frac{\partial N_i}{\partial z} = 0 \quad \text{at } z = \eta \text{ (surface)} \quad (9a)$$

$$\omega_{s,i} N_i - v_t \frac{\partial N_i}{\partial z} = S_{D,i} - S_{E,i} \quad \text{at } z = z_b \text{ (bottom)} \quad (9b)$$

where η is the water surface and z_b is the reference elevation near bottom. Assuming only microflocs can erode but all particles can deposit (Lee et al., 2014), the erosion and deposition rate can be written as:

$$S_{E,P} = \frac{M}{(\pi/6) D_p^3 \rho_p} \left(\frac{\tau}{\tau_c} - 1 \right) \quad \text{if } \tau > \tau_c \quad (10a)$$

$$S_{D,i} = w_{s,i} \cdot N_i \quad (10b)$$

In Eq. 10a, M is the empirical erosion rate parameter, and τ and τ_c are the bottom shear stress and the critical bottom shear stress for erosion.

2.2 Implementation of the flocculation module in TELEMAC

The general open source software TELEMAC developed by the LNHE (Laboratoire
 National d'Hydraulique et Environnement) of EDF (Electricité De France) consists of a
 complete processing chain for solving the water depth, velocity components, sediment
 motions and tracer transports. The earlier two-class version of the flocculation model (Lee et
 al., 2014) has been implemented into TELEMAC-3D by Ernst (2016), and has been extended
 here to three floc populations. The main idea for the implementation of this tri-modal PBE
 model is to create a new key word "PBE3C" in TELEMAC-3D to trigger the flocculation
 model and make minimum modifications to utilize most of the original source code. A
 detailed flow chart for coupling this flocculation model is summarized in Fig. 2. To
 successfully invoke the flocculation model, the key word "PBE3C" is added in the dictionary
 (*telemac3d.dico*) and the steering files (.cas) of TELEMAC-3D. This keyword can be
 declared as a Boolean or integer variable (*declarations_telemac3d.f*) and its value is
 recognized when the subroutine *lecdon_telemac3d.f* reads the steering file. The flocculation
 related variables, such as D_P , D_{F1} , D_{F2} , $\omega_{s,P}$, $\omega_{s,F1}$, $\omega_{s,F2}$, and the deposition and erosion flux
 of different size groups, are defined and allocated in the subroutine *declarations_telemac3d.f*
 and *point_telemac3d.f* respectively. The tracer transport equations are also in the form of
 advection-diffusion equations to be solved by subroutine *cvd3d.f*. The source and sink terms
 (Eq. 4) of the tracers are programmed in the subroutine *source_trac.f*, as well as the
 formulation of collision frequency (Eq. 5) and breakage frequency (Eq. 6). If the shear rate in
 Eq. 5 is imposed for a specific case (e.g., a constant for homogenous turbulence in the
 laboratory), it can be coded in any selected turbulence model such as *viscke.f*. The expression
 of settling velocities are expressed in terms of different size groups in the subroutine *vitchu.f*
 (Eq. 7), with hindered settling (Eq. 8) being considered. The boundary conditions (i.e., the
 erosion and deposition fluxes) for all the tracers are expressed in *clsedi.f* (Eq. 9), and can be
 adjusted for different assumptions (e.g., Eq. 10). After that, the mud bed evolution is

improved for three classes rather than two classes in the subroutine *fonvas.f*. In the main program *telemac3d.f*, code of initializing all the newly defined variables, adjusting any argument for modified subroutines, reading time series of input variables, and printing flocculation-related variables are required to make the program executable.

It is important to note that *telemac3d.dico*, *declarations_telemac3d.f* and *point_telemac3d.f* should be modified in the source code, while other changes can be included in a FORTRAN file with its name specified in the steering file and recognized by the program. Also, notice that the tracers N_P , N_{F1} , N_{T1} and N_{T2} are the number concentrations and thus usually a large value. To make it numerically friendly, these variables are “rescaled” by multiplication with the mass of one microfloc $m_P (= 1/6 \cdot \pi \cdot D_P^3 \cdot \rho_P)$. Therefore, rescaled number concentration $C_{P,S} (= N_P \cdot m_P)$, $C_{F1,S} (= N_{F1} \cdot m_P)$, $C_{T1,S} (= N_{T1} \cdot m_P)$ and $C_{T2,S} (= N_{T2} \cdot m_P)$ become the actual tracers in TELEMAC-3D. In fact, $C_{P,S}$, $C_{T1,S}$ and $C_{T2,S}$ are equivalent to the mass concentration of microflocs, macroflocs and megaflocs, respectively, while $C_{F1,S}$ does not have a specific physical meaning. This also means that the total sediment mass concentration C can be computed as $C = C_{P,S} + C_{T1,S} + C_{T2,S}$.

TELEMAC-3D in fact solves the 3-D Navier-Stokes equations with a free surface. Because of limited data and simplified environment both in the laboratory and in the field, TELEMAC-3D in this study is applied as a quasi-1D vertical case by de-activating the advection terms and focusing on the vertical profiles of the variables located at the geometry center of the cross section of the mesh column. The two-dimensional (2-D) mesh for the boundary of a simple square or circle is generated by the pre-processor BlueKenue, and the number of horizontal levels is specified for this quasi-1D case. It will not change the structures of the code, and can be tested for real 3-D cases in the estuaries if data from more stations are available.

3. Case studies

3.1 Case 1: Laboratory data validation

The settling column is one of the laboratory facilities to isolate complicated environments to emphasize the aggregation and breakage of cohesive flocs (van Leussen, 1994; Maggi, 2005; Tang, 2017), among which van Leussen's work has been utilized to validate the two-class PBE recently (Lee et al., 2011). Van Leussen's settling column has an internal diameter of 0.29 m and effective height of 4 m. An oscillating grid was placed inside the column to generate a reasonably homogenous and isotropic turbulence. The shear rate (G) and eddy diffusivity (D_z) are controlled by the oscillating frequency of the grid (σ), and can be computed as (van Leussen, 1994):

$$G = \sqrt{\frac{127 \cdot A_0^3 \cdot \sigma^3}{\nu}} \quad (11)$$

$$D_z = \alpha_g \cdot \sigma \cdot A_0^2 \quad (12)$$

where $\alpha_g = 0.19$ is a constant and $A_0 = 0.075$ m is the stroke distance. This relationship was calibrated by the relationship between the turbulence (measured by using a Laser Doppler Velocimeter) and the grid frequency, and should vary for different layouts of the grid bars.

The test case for Ems mud with grid frequency 0.1 Hz (i.e., shear rate $G = 7.31 \text{ s}^{-1}$ and eddy diffusivity $D_z = 1.07 \times 10^{-4} \text{ m}^2/\text{s}$) was addressed in this study, similar to the work by Lee et al. (2011). The Ems mud consists of 35% quartz, 20% illite, 15% chlorite, 4–13% organic matter, and a few other minerals such as kaolinite and smectite. The mud was passed through a 1 mm sieve and stored in a dark room with temperature 4–6 °C before being used in the settling column. Initially a homogenous sediment profile with concentration about 1 g/L was obtained by oscillating the grid at 4 Hz about 20 mins. At this point, the pump was stopped, the grid was controlled to the required frequency, and the time was marked as $t = 0$. Thus, it is reasonable to assume that large flocs are destroyed and all the particles are in the

form of stable microflocs at $t = 0$. Notice that since the FSDs are obtained through the cuvette by a Malvern 2600 particle sizer which might break up the flocs during sampling, the measured settling velocity at different height levels are instead used for comparison.

A simple 2-D mesh file (.slf) with the boundary condition file (.cli) were prepared by using BlueKenue for covering the cross section of the settling column with 195 nodes and 342 triangular elements. The nodes at the center of the circle along the vertical are used to represent the vertical profiles of this 1-D vertical column. The initial sediment concentrations for all tracers were specified in the steering file (.cas). The total mass concentration was selected as $C = 1.1$ g/L to better fit the experimental data (Lee et al., 2012), with concentration of microflocs $C_{P,S} = 1.07$ g/L (more than 97% of total mass) and seeded macroflocs and megaflocs $C_{T1,S} = 0.02$ g/L and $C_{T2,S} = 0.01$ g/L respectively. The size and density of microflocs are selected as $D_P = 12$ μm and $\rho_P = 1900$ kg/m³. Size-fixed megaflocs are set as $D_{F2} = 360$ μm to represent its size range of 200–500 μm . Seeded macroflocs are initially set as $D_{F1} = 80$ μm and will change with time. Also given the fractal dimension η_f valid for all particles, the initial concentration of $C_{F1,S}$ is computed by

$$C_{F1,S} = C_{T1,S} / (D_{F1} / D_P)^{\eta_f} \quad (13)$$

Erosion and deposition are further disabled in the steering file so that all deposited particles are assumed located in the bottom grid. A FORTRAN file should also be prepared to include all the modified subroutines such as *telemac3d.f*, *clsed.f*, *lecdon_telemac3d.f*, *source_trac.f*, *vitclu.f* and *viscke.f*. The model was finally implemented with 20 horizontal levels and time step 1 s. By trial-and-error, the model was operated with collision efficiency $\alpha = 0.2$, breakage coefficient $E_b = 1.0 \times 10^{-5}$ and an average fractal dimension $\eta_f = 2.4$. The model also assumes that the breakage of a macrofloc will result in microflocs with 10% mass and two equally smaller macroflocs, and the breakage of a larger megafloc will result in

microflocs with 5% mass, one macrofloc with 15% mass and one smaller megafloc with 80% mass. These selections were based on best fit of the SSC profiles and the settling velocities.

3.2 Case 2: Field data validation

The region of interest is the Belgian nearshore area (southern Bight of the North Sea). Field data are available at the station WZ Buoy, located about 2 km from the entrance of the harbor Zeebrugge (Fettweis et al., 2016). The WZ Buoy is located in the coastal turbidity maximum zone, and has similar characteristics as the nearby site MOW1 (Fettweis and Lee, 2017). This area is mainly controlled by semidiurnal tide with tidal amplitude about 4.5 m at spring tide and 2 m at neap tide. Slack water occurs around 3 hr before and after high water, and maximum flood around 1 hr before high water. Temperature and salinity are almost constant on inter- or intra-tidal timescales, with the temperature varying seasonally and salinity changing due to water mass advection. The waves generally have a period of 4 s, and the median significant wave height is around 0.6 m.

In this study, a period of three tidal cycles at Julian days around 321 to 322.5 (during spring tide in November) in the year 2013 is selected to validate the model. A 5 MHz ADV (Acoustic Doppler Velocimeter) Ocean, a LISST-100X (range 2.5 – 500 μm), two OBSs (Optical Backscatter Sensors) and an ADCP (Acoustic Doppler Current Profiler) were integrated in a tripod located at the bottom of the water column. The data were collected or averaged in 10 or 15 min intervals. The tidal range was 4.47 m, with the time series of water depth provided by both LISST and ADCP. The water depth H of three typical tidal cycles (marked as TC1, TC2 and TC3 in Fig. 3(a)) are selected, with each tidal cycle begins and ends with low slack.

The ADV measured the point mean velocities and their turbulent fluctuations (from which the turbulent kinetic energy k can be computed), at around 0.15 m above the bed

(hereafter referred to as τ). Therefore, the shear stress τ and shear velocity u_* can be estimated as (Schindler et al., 2013):

$$\tau = C \cdot (\rho_w \cdot k) \quad (14)$$

$$u_* = \sqrt{\tau / \rho_w} \quad (15)$$

The coefficient C is an empirical parameter and set to 0.19 according to the literature (e.g., Stapleton and Huntley, 1995; Verney et al., 2007; Schindler et al., 2013). The time series of u_* show the occurrence of high values around maximum flood and ebb flow and low values around slack tides (Fig. 3(b)). Note that since the water column is generally well-mixed because of strong tidal currents but low freshwater discharges (Fettweis et al., 2014, 2016), the turbulent kinetic energy k , turbulent dissipation rate ε and eddy viscosity ν_t along the vertical can be simply estimated by the following relationships:

$$k = \frac{u_*^2}{\sqrt{C_\mu}} \left(1 - \frac{z}{H} \right) \quad (16)$$

$$\varepsilon = \frac{u_*^3}{\kappa z} \left(1 - \frac{z}{H} \right) \quad (17)$$

$$\nu_t = \kappa z u_* \left(1 - \frac{z}{H} \right) \quad (18)$$

where z is the vertical coordinate, H is the water depth, $\kappa \approx 0.4$ is the von Karman constant and $C_\mu = 0.09$ is a constant widely used in any turbulence k - ε model. The reliability of the parabolic eddy viscosity profiles will be further discussed in Section 4.2. The eddy diffusivity D_z in Eq. 1 is assumed close to the eddy viscosity ν_t (i.e., with turbulent Prandtl number of 1) for simplicity. It is also interesting to notice that the empirical value 0.19 in Eq.14 was close to the coefficient $\sqrt{C_\mu}$ in the boundary condition of k (Eq. 16). Actually, C_μ may even decrease to 0.05 (with $\sqrt{C_\mu}$ closer to 0.19) if the shear rate is high (Shih et al., 1994).

Unfortunately, the two OBS used to measure the sediment mass concentration converted from the OBS voltage signals at 0.2 m and 2 m above bed failed during the selected period; however, data on sediment volume concentration are available. The LISST was mounted at 2 mab to measure the FSDs, the median floc size (D_{50}), as well as the Total Volume Concentration (TVC) and the optical transmission. The TVC shows high values close to maximum flood and maximum ebb and low values close to slack tides (Fig. 3(e)). The D_{50} and transmission show the opposite trend (Fig. 3(f) and Fig. 3(g)), with large flocs, low TVC and thus high water clarity due to high settling of the flocs during slack. As an example, hourly FSDs during tidal cycle 2 (Fig. 3(a)) are shown in Fig. 4. Large tails of small particles are presented close to high and low waters, while larger flocs appeared close to slack. It is important to notice that a stable peak with size around 360 μm was observed in the FSD curves, which partly supports the assumption of using a fixed size of megaflocs in this study.

The measured FSDs can also be decomposed into four lognormal distributions to represent the primary particles, microflocs, macroflocs and megaflocs, respectively, by using the software DistFit (Chimera Technologies, USA):

$$\frac{dV}{dD} = \sum_{i=1}^4 \frac{\bar{V}_i}{\sqrt{2\pi} \ln(\sigma_i)} \exp\left(-\frac{1}{2} \left(\frac{\ln(D/\bar{D}_i)}{\ln(\sigma_i)}\right)^2\right) \quad (19)$$

where V and D are the volumetric concentration and diameter of 32 size bins of FSDs from LISST, and $\bar{V}_i$, $\bar{D}_i$ and σ_i are the volumetric concentrations, geometric mean sizes and standard deviations of four log-normal distributions to identify primary particles, microflocs, macroflocs and megaflocs, respectively. The size of each class is set as 3, 15, 20–200 (Lee et al., 2012; Fettweis and Baeye, 2015) and 360 μm (Fig. 4) respectively, and the weighted size of primary particles and microflocs are combined in one class, i.e., microflocs, in the model. An example is shown in Fig. 5, with the representative sizes and volume fractions of four size groups extracted from a measured FSD.

An upward looking ADCP was mounted on the tripod at site WZ Buoy to record the vertical profiles of the horizontal velocities. These data can be used to validate any assumption on the eddy viscosity profiles to provide reliable hydrodynamic conditions for focusing on flocculation processes. During this period, the current was mostly alongshore, with about 1 m/s at 2 mab at the maximum flood and ebb (Fig. 3(c)). The wave effect is low, i.e., the significant wave H_s less than 0.4 m (Fig. 3(d)), and can be considered as “no wind” (Baeye et al., 2011) and thus is neglected in the model. The salinity was 31 and the water temperature was about 10 °C at the measuring point. Notice that the time series of water depth H and shear velocity u_* are used as model inputs, while other subfigures in Fig. 3 are used to show the environments during model setting.

4. Results and discussion

4.1 Ems muds in the settling column experiment

The predicted and measured SSCs are reasonably matched at $t = 450, 900, 1350, 1800, 3600$ and 7200 s (Fig. 6(a)). The errors (E_c) of SSC profiles can be estimated by

$$E_r = \frac{1}{n_M} \sum_i |C_{S,i} - C_{M,i}| \quad (20)$$

in which C_S and C_M are the simulated and observed SSCs, and n_M is the number of measurements from surface to 0.5 m above bed for each SSC profile. Compared with previous two-class PBE (Ernst, 2016, see double dot dashed lines in Fig. 6(a)) with $E_r = 0.036\text{--}0.084$, the simulated SSC profiles by this three-class PBE (with $E_r = 0.025\text{--}0.062$) better match the measured profiles, especially for longer simulating time. At $t = 0$, a well-mixed profile is assumed due to high frequency of the oscillating grid. After the grid was set to the specified frequency, particles were flocculated and settled, leading to low SSC at the upper water column and high SSC near the bottom. The surface SSC was lower than 0.1 g/L after 3600 s, while the SSC close to the bottom exceeded 2 g/L. The predicted settling

velocities for microflocs, macroflocs and megaflocs are mass-weighted to compare with the
 measured settling velocities at different height levels (Fig. 7). Stable particles at different
 height levels started with size of microflocs (which was the initial condition), gradually
 aggregated until maximum value after half an hour, and decreased again because of the
 created large floppy flocs breaking up. It was also shown that the settling velocities close to
 the surface (e.g., $Z = 3.475$ m) are lower than that close to the bottom (e.g., $Z = 1.475$ m),
 which proves the occurrence of flocculation. The time series of predicted maximum settling
 velocity for $Z = 3.475$ m match excellently with the measurements, with $w_{s,\max} \approx 0.8$ mm/s.
 Both the predictions of $w_{s,\max}$ $Z = 1.475$ m and $Z = 2.475$ m at $t = 30$ mins were about 10 %
 higher than the measurements. The simulated w_s for $Z = 1.475$ m after 3 hrs are higher than
 the measured w_{ss} , which implies that less large flocs were expected on the lower water column
 at that time. These deviations may be explained by insufficient understanding of the
 flocculation processes or a variation of the measuring location where the data were obtained.
 The largest settling velocity under current grid frequency was about 1 mm/s. Lager values of
 w_s can be obtained by reducing the grid oscillating frequency.

In order to obtain the best quality simulation results, various parameters were selected
 based on previous studies or treated as fitting parameters to match the observed SSC profiles
 and the settling velocities such as the collision efficiency α , breakage coefficient E_b , fractal
 dimension n_f and the parameters describing the fragmentation distribution of macroflocs or
 megaflocs (Processes (7) and (8) in Table 1). Higher collision efficiency α and lower
 breakage coefficient E_b enhanced flocculation and moved the SSC profiles downward, while
 the SSC profiles shift upward (i.e., less flocculated) for a smaller α or larger E_b (Fig. 6(b)). If
 initially most of the flocs were destroyed to their elementary particles, the collision efficiency
 α dominated the growth phase at the beginning while the breakage coefficient E_b controlled
 the unrealistic infinite particle growth by breaking up large macroflocs or megaflocs. With a

1 larger fractal dimension (n_f) the SSC curves tended downward (Fig. 6(b)) with the dominant
2 effects of an increase in floc size according to Eq. 2, and vice versa. Although n_f was
3 assumed globally a constant in this case (also see Lee et al., 2011, 2014), it was sometimes
4 modelled as a function of size to better describe the fact that larger flocs have lower fractal
5 dimensions, and thus lower densities but higher settling velocities (Khelifa and Hill, 2006).
6 The relationship between the fractal dimension and the floc size, however, needed careful
7 calibration and the fitting coefficients may differ under different nutrient or biomass
8 environments (e.g., Tang, 2017). A recent study pointed out that even for a given floc size,
9 the fractal dimension is not a single value but distributed (Xu and Dong, 2017). Since flocs
10 are not self-similar, the floc density may be easier to understand to describe the floc fractal
11 properties (Toorman, 2000). Model results were also sensitive with the selection of
12 fragmentation distribution functions (Mietta et al., 2008; Shen and Maa, 2016b). Until now,
13 there are no effective measuring techniques to directly observe how a parent floc breaks up
14 without disturbing the in-situ flocs. Thus, the possible fragmentation distribution function
15 was only selected by data fitting from the assumptions of binary breakup, ternary breakup,
16 binominal breakup and so on. In this study, it followed Lee et al. (2011) assuming that a large
17 floc may separate into several smaller flocs and a few elementary particles. For example, for
18 the megaflocs, a daughter megafloc with 80% mass of the parent megafloc remains after the
19 destroying of the parent megafloc. It is consistent with the assumption by Prat and Ducoste
20 (2006) that at least one daughter particle with 80% of the parent particle is formed after
21 breaking up, which is based on the experimental observations by Kusters (1991). For the
22 macroflocs, however, we assumed that two equal daughter macroflocs and 10% elementary
23 microflocs are formed after a parent macrofloc breaking up. This assumption can be treated
24 as the condition of binary breakup with surface erosion of elementary particles. This part may
25 be enhanced in the future by a micro-behavior model.

4.2 In-situ suspended sediments in the Belgian coast

By comparison with the measured three-class FSDs, the best quality simulations were obtained by fitting the aggregation and breakage coefficients (α and E_b), floc structures (ηf), and erosion and deposition constants (τ_{ce} and M). All the parameters used in the best quality fitting are provided in Table 2. Notice that the fractal dimension of macroflocs and megaflocs are selected as 2.3 and 2.0 respectively. The initial SSC is set as 0.3 g/L, close to that given by Lee et al. (2014) also in the Belgian coastal zone. The initial mass percentages of three classes are based on measurements. It is critical to note that the number of created macroflocs when a larger macrofloc splits is fitted as 1.7, is not an integer. This follows from the fact that the fragmentation distribution after a parent particle breaks up is a statistically averaged parameter. Thus, a $K_p = 1.7$ for the breakage of macroflocs means that the probability is 70% that one smaller macrofloc occurs while the probability is 30% for the occurrence of two smaller macroflocs. At present, this hypothesis can only indirectly be validated by comparison with the resulting FSDs and should be improved in the future.

With an input time series of measured water depth and derived shear velocity (Fig. 3(a)(b)), the hydrodynamics, SSCs and FSDs can be addressed by this PBE enabled TELEMAC system. One tidal cycle (TC2) was selected to focus on in detail (Fig. 8(a)) with five snapshots. As shown in Fig. 8(b), the bell-shaped eddy viscosity ν_t reaches its maximum $\sim 0.05 \text{ m}^2/\text{s}$ around $t = 2.33 \text{ hr}$ at peak flow. It decreases until smaller than $0.02 \text{ m}^2/\text{s}$ at slack tide, and increases again until its second maximum at $t = 7.83 \text{ hr}$ around low water. Particles from the bed will be resuspended in the water column during periods of peak flow with high turbulence, whereas slack water periods with low turbulence will promote aggregation kinetics and lead to floc size growth. The simulated SSCs tend to be more uniformly distributed around peak flows (e.g., $t = 2.33$ and 7.83 hr), in contrast with higher sediment

concentration occurring near the bottom during slack tide (e.g., $t = 0, 5$ and 12.17 hr) (Fig. 8(c)). This is because low turbulence at slack tide could enhance aggregation, and thus increase the settling velocities and make the SSC curves increase stronger towards downward. In contrast, a high turbulence during peak flow could break up large flocs, and thus create more microflocs and decrease transmissivity (Fig. 3(g)). The macrofloc size D_{F1} profiles at 2 mab match excellently with the observed values at $t = 0, 2.33, 7.83$ and 12.17 hr, and follow a trend where the smaller macroflocs are found near the bed (due to significantly higher turbulent shear rate near bed) and slightly increasing upward (Fig. 8(d)). At $t = 5$ hr (close to high water slack), the simulated D_{F1} is smaller than the measured value, which might be because of the megafloc size derived from the measurements is possibly overestimated. The predicted three-class FSDs also reasonably agree with the measured ones (Fig. 8(e)), with the mass fraction of macroflocs dominating the suspended flocs. Also, more microflocs, but less megaflocs, occur during peak flow, since high shear destroys the large megaflocs and resuspends small microflocs from the bed. This trend can be shown more clearly by tracking time series of the size and mass percentage of FSDs (Fig. 9(a)). It is also shown that the predicted mass fractions of microflocs are smaller than the measured values around maximum flood. This is probably because of the assumption of using a constant critical shear stress for erosion, which should also vary with time and could be improved in the future. Smaller sizes of suspended macroflocs with D_{F1} around $50\text{ }\mu\text{m}$ appear around peak flows, while larger macroflocs with D_{F1} around $100\text{ }\mu\text{m}$ are expected around slack tides (Fig. 9(b)). A few points of measured D_{F1} around maximum flood are even larger than $150\text{ }\mu\text{m}$, which could be improved by better understanding the flocculation processes during that period.

During the deployments, various acoustic (such as ADV and ADCP) and optical (such as OBS and LISST) instruments are integrated in a tripod to capture the hydro- and sediment dynamics at station WZ Buoy. It is clear that the instruments itself are associated with

1 uncertainties that should be taken into account when using field data for model calibration.
2 Acoustic sensors are widely accepted as an excellent instrument for measuring the three-
3 dimensional velocities using Doppler effect. The corresponding turbulent flow parameters,
4 such as the ADV derived turbulent kinetic energy, might be sensitive to different de-spiking
5 selections at high turbulence regions. Although ADV has been used to measure the SSCs and
6 settling velocities based on its backscatter signals (Maa and Kwon, 2007; Cartwright, 2013),
7 the interaction of sound with aggregated cohesive particles still lack a clear quantitative
8 inversion formulation. Optical instruments are instead often used to measure SSCs and FSDs,
9 although changes in inherent optical properties of the particles, which are difficult to quantify
10 during long term deployments, will influence the FSD and the OBS signal (Fettweis et al.,
11 2012; Schwarz et al., 2017). The combination of LISST and OBS could also be used to
12 estimate the settling velocities of suspended flocs (e.g., Fettweis and Baeye, 2015). LISST
13 uses laser diffraction as well as the available beam transmission to measure the volume
14 concentrations and the size spectra (Agrawal and Pottsmith, 2000). The uncertainties and
15 limitations of the LISST detector are related to the size and shape of the particles and flocs
16 (Mikkelsen et al., 2006), and to the measuring principle itself (Goossens, 2008). For example,
17 particles smaller than the size range results not only in a rising tail in the lowest size classes
18 but may affect the entire FSD (Andrews et al., 2010; Graham et al., 2012). A rising tail in the
19 lowest size classes of the LISST is frequently observed in our data. Particles exceeding the
20 LISST size range of 500 μm also contaminate the FSD in multiple size classes in the range
21 between 250 and 400 μm and to a lesser extend in the smaller size classes (Davies et al.
22 2012). These biases may further enhance or influence the separation between the peaks of
23 primary particles, microflocs, macroflocs and megaflocs in our analysis.

24 It is also essential to notice that for a well-mixed water column such as the Belgian
25 coastal zone, a parabolic eddy viscosity is assumed and imposed in TELEMAC in this section.

This assumption is based on the mixing length theory with logarithmic velocity profiles expressed by the law of the wall. This selection can simplify the turbulence condition to focus on the flocculation processes. To evaluate this hypothesis, an additional vertical 1-D model developed by Shao et al. (2017) was used to check the velocity profiles as well as to simulate the eddy viscosity profiles at maximum flood and ebb. This model has previously been successfully used to mimic the hydrodynamics in Chicago Sanitary and Ship Canal (U.S.A.), Menai Strait (U.K.), and Yangtze (Changjiang) River estuary (China) for both steady and tidal flows. This application used time series of water depth as model inputs, with a constant salinity 31 and a constant temperature 10 °C. The shear velocity u_* was obtained from a high vertical resolution (2 cm) of the simulated velocities in the bottom 1 m (Maa and Kim, 2002). The driving force was the surface pressure gradient $\partial\eta/\partial x$ (which can be related to $\partial\eta/\partial t$, see Shao et al., 2017). Thus, even without additional adjustments of the phase lag (which is related to the tidal amplitude attenuation) and the background pressure gradient (which represents freshwater discharge and baroclinic effect), the velocity profiles $u(z)$ at maximum flood (~ 1.4 m/s) and ebb (~ 1.1 m/s) agree well with the ADCP measurements (Fig. 10). The corresponding eddy viscosity profiles also reasonably match the parabolic model. It adds our confidence to use parabolic eddy viscosity profiles for non-stratified, quasi-steady (tidal) turbulent flows, such as in the Belgian coastal region. At later stage, a $k-\epsilon$ turbulence model will be tested to account for more physics, such as the advection of turbulence.

5. Conclusions

A tri-modal PBE was developed to track the sizes and mass fractions of microflocs, macroflocs and megaflocs, respectively. This model was validated by comparisons with vertical suspended sediment profiles, settling velocities at selected water levels, or FSDs for the comprehensive floc groups. It draws the following specific conclusions:

(1) By introducing an additional size groups of megaflocs, the three-class PBE model has the potential of better predicting the settling and deposition properties of cohesive sediments, and better addressing the large flocs that occur in estuarine and coastal waters, compared to the previous two-class PBE model. This is in agreement with the expectations based on field data analysis by Lee et al. (2012), justifying the additional computational effort.

(2) With the assumption of size-fixed microflocs and megaflocs, only four tracers are monitored in the tri-modal PBE model. It keeps the efficiency by only adding one tracer than two-class PBE, while better representing the FSDs by an additional size class.

(3) This three-class PBE was also coupled with open TELEMAC to address the FSDs of estuarine muds. With this contribution, any progress regarding to the mechanisms and processes of cohesive sediment flocculation can be easily coded in TELEMAC for further testing.

(4) The number of generated macroflocs when a larger macrofloc destroying may not necessarily be an integer. That is, the fragmentation distribution function of flocs may need to be expressed by a micro-behavior model to represent its statistical property.

(5) Although the PBE enabled TELEMAC-3D is used in this study for testing a 1-D case, the code itself is a 3-D code. The model can be used to test in-situ 3-D case by regenerating the mesh for a real bathymetry, imposing different boundary conditions and adding appropriate driving forces.

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Figure Captions

Fig. 1 Schematic diagram of the FSDs before and after flocculation. At time $t = 0$, all particles are concentrated on microflocs. With time, macroflocs and megaflocs have appeared because of aggregation and breakage processes.

Fig. 2 Flow chart of implementing the tri-modal population balance model in the open TELEMAC.

Fig. 3 Times series of (a) water depth H , (b) shear velocity u_* , (c) alongshore and cross-shore current velocities at 2 m above bed (mab), (d) significant wave H_s , (e) total sediment volumetric concentration at 2 mab, (f) median sizes D_{50} at 2 mab and (g) optical transmission at 2 mab during the time around Julian Day 320.9–322.5 in the year 2013. Dots are measurements and the lines are smoothed results. Notice that (a) and (b) are model inputs, while other subfigures show the environmental parameters during the measuring period.

Fig. 4 Hourly measured FSDs during a typical tidal cycle (marked as “TC2” in Fig. 3(a)) at the station WZ Buoy.

Fig. 5 An example of measured and decomposed FSDs at 2 hrs after low slack during TC2. The bars are the measured FSDs by LISST, and the dashed and solid lines are the four subordinate lognormal FSDs and the total FSD processed by the software DistFit. The triangles are the representative sizes and volume fractions of microflocs, macroflocs and megaflocs, respectively.

(a) Measured (symbols) and simulated (solid lines) SSC profiles for the Ems mud in the settling column experiment (van Leussen, 1994), with oscillating grid frequency 0.1 Hz and initially well-mixed solid concentration 1 g/L. Predictions using two-class population balance equation (Ernst, 2016, see double dot dashed lines) are represented for comparison. (b) Sensitivities of the SSC profiles with different selections of collision efficiency α , breakage coefficient E_b and fractal dimension n_f at time $t = 450, 900, 1350, 1800, 3600$ and 7200 s.

Fig. 7 Measured (symbols) and simulated (solid lines) time evolution of settling velocities in different column heights $Z = 1.475, 2.475$ and 3.475 m for the same case described in the caption of Fig. 6.

Fig. 8 (a) The water surface of selected tidal cycle TC2, and the simulated (b) eddy viscosity profiles, (c) SSC profiles, (d) D_{F1} profiles and (e) the FSDs at selected times. In subfigure (d), circles are measurements. In subfigure (e), grey lines and cycles are the measured 32-class and three-class FSDs respectively, while the black diamonds are modeled three-class FSDs.

1

2 Fig. 9 Comparison of time series of measured (symbols) and simulated (lines) FSDs. In
3 subfigure (a), the mass fractions of (i) microflocs and (ii) microflocs & macroflocs are
4 represented; in subfigure (b), the sizes of macroflocs D_{F1} are displayed.

5

6 Fig. 10 Comparison between the simulated (solid lines) and measured (symbols) velocity
7 profiles at the maximum flood and ebb by using an additional vertical 1-D model, with the
8 corresponding eddy viscosity (ν_t) profiles plotted with parabolic ν_t profiles.

Highlights

- The sizes of flocs are dynamically altered because of particle aggregation and breakage.
- A three-class population balance flocculation model was developed.
- This flocculation model has been successfully implemented in the open source TELEMACH.
- Four tracer variables, representing the floc size distributions, were included in TELEMACH.
- The model was validated with settling column tests and field measurements.

Table 1 Aggregation and breakage processes of suspended particles with three size groups.

Processes (<i>j</i>) ↓	Description	Components (<i>i</i>) →			Creation Rate
		N_p	N_{F1}	N_{F2}	
(1) Aggregation Microflocs & Microflocs		$-\frac{1}{2} \left(\frac{N_{C1}}{N_{C1}-1} \right)$	$\frac{1}{2} \left(\frac{1}{N_{C1}-1} \right)$	$\frac{1}{2} \left(\frac{N_{C1}}{N_{C1}-1} \right)$	$\alpha \beta_{pp} N_p N_p$
(2) Aggregation Microflocs & Macroflocs		-1	0	+1	$\alpha \beta_{pF1} N_p N_{F1}$
(3) Aggregation Microflocs & Megaflocs		-1	0	+1	$\alpha \beta_{pF2} N_p N_{F2}$
(4) Aggregation Macroflocs & Macroflocs		0	$-\frac{1}{2} \left(\frac{N_{C2}/N_{C1}}{N_{C2}/N_{C1}-1} \right)$	$-\frac{1}{2} \left(\frac{N_{C2}}{N_{C2}/N_{C1}-1} \right)$	$\alpha \beta_{F1F1} N_{F1} N_{F1}$
(5) Aggregation Macroflocs & Megaflocs		0	-1	N_{C1}	$\alpha \beta_{F1F2} N_{F1} N_{F2}$
(6) Breakage Macroflocs		$f_{p1} \cdot N_{C1}$	$-f_{p1} \cdot N_{C1}$	0	$a_{F1} N_{F1}$
(7) Breakage Megaflocs		$f_{p2} \cdot N_{C2}$	$(1-f_{p2}-f_{F2}) \cdot \frac{N_{C2}}{N_{C2}}$	$-(1-f_{F2}) \cdot N_{C2}$	$a_{F2} N_{F2}$

Nomenclature: N_p = number of microflocs in suspension per unit volume; N_{F1} = number of macroflocs in suspension per unit volume; N_{F2} = number of microflocs in macroflocs per unit volume; N_{C1} = number of microflocs in megaflocs per unit volume; N_{C2} = number of microflocs in one macrofloc; $N_{C1} = N_{F1} / N_{F1}$; $N_{C2} =$

number of microflocs in one megafloc, $N_{C2} = N_{T2} / N_{F2}^{\dagger}$; f_{P1} = mass fraction of created microflocs when a macrofloc breaks up; f_{P2} = mass fraction of produced microflocs when a megafloc breaks up; f_{F2} = mass fraction of the remaining megafloc when a larger megafloc breaks up; K_1 = number of created macroflocs when a larger macrofloc breaks up; K_2 = number of generated macroflocs when a megafloc breaks up; α = collision efficiency; β_{PP} = collision frequency between two microflocs; β_{PF1} = collision frequency between a microfloc and a macrofloc; β_{PF2} = collision frequency between a microfloc and a megafloc; β_{F1F1} = collision frequency between two macroflocs; β_{F1F2} = collision frequency between a macrofloc and a megafloc; β_{F2F2} = collision frequency between two megaflocs; a_{F1} = breakup frequency of a macrofloc; a_{F2} = breakup frequency of a megafloc.

[†] N_{F2} = number of megaflocs in suspension per unit volume. For fixed size of megaflocs, N_{C2} is a constant, and thus $N_{F2} = N_{T2} / N_{C2}$.

Table 2 Summary of parameters used in the best quality simulation at station WZ Buoy.

Flocculation Kinetics	Value	Description
α	0.2	Collision efficiency
E_b	1.0×10^{-4}	Breakup fitting parameter
F_y	1.0×10^{-10}	Floc strength (Pa)
f_{P1}	0.7	Mass fraction of produced microflocs when a macrofloc breaks up
f_{P2}	0	Mass fraction of created microflocs when a megafloc breaks up
f_{F2}	0	Mass fraction of the remaining megafloc when a larger megafloc breaks up
K_1	1.7	Number of generated macroflocs when a larger macrofloc breaks up
K_2	2	Number of produced macroflocs when a megafloc breaks up
nf_1	2.3	Fractal dimension of macroflocs
nf_2	2.0	Fractal dimension of megaflocs
K_B	1.38×10^{-23}	Boltzmann constant (J/K)
T	283.0	Temperature (K)
Initial Condition ($t = 0$)	Value	Description
c	0.3	Sediment mass concentration (g/L)
D_{F1}	100	Size-varying macroflocs (μm)
Ψ_P	15	Mass percentage of microflocs (%)
Ψ_{F1}	75	Mass percentage of macroflocs (%)
Ψ_{F2}	10	Mass percentage of megaflocs (%)
Other parameters	Value	Description
Δt	2	Time step (s)
n_z	13	Number of horizontal levels
τ_{ce}	0.6	Critical shear stress for erosion (Pa)
D_P	14	Size-fixed microflocs (μm)
D_{F2}	360	Size-fixed megaflocs (μm)
M	1.0×10^{-4}	Empirical erosion parameter ($\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$)
ρ_P	2600	Microfloc density ($\text{kg} \cdot \text{m}^{-3}$)
ρ_w	1024	Sea water density ($\text{kg} \cdot \text{m}^{-3}$)