Two-class flocculation kinetic model: development and application to large-scale, multi-dimensional cohesive sediment transport

Lee Byung Joon[1], Qilong Bi[2], Erik Toorman[2], Michael Fettweis[3] and Holger Weilbeer[4]

[1] School of Construction and Environmental Engineering, Kyungpook National University
2559 Gyeongsang-daero, Sangju, Gyeongbuk, 742-711, South Korea
E-mail: bjlee@knu.ac.kr

[2] Hydraulic Laboratory, Civil Engineering Department, KU Leuven
Kasteelpark Arenberg 40, Heverlee, 3001, Belgium

[3] OD Natural Environment, Royal Belgian Institute of Natural Sciences
Gulledelle 100, 1200 Brussels, Belgium

[4] Federal Waterways Engineering and Research Institute (BAW)
Wedeler Landstr. 157, 22559 Hamburg, Germany

Introduction

Fluid mud layer, composed of cohesive sediments, has been a serious problem in many waterways, docks and harbours. For example, Zeebrugge Harbour in Belgium has been reported to build up one- or two-meter thick fluid mud layer. Flocculation is known to be a key process for developing such fluid mud layers. Flocculation is a combined process of (1) aggregation of small mud particles to large flocs and (2) breakage of large flocs, depending on a turbulent shear condition. Cohesive sediments remain small in an open water (e.g. river or ocean), due to breakage under high turbulent shear. When entering/traveling into a closed water (e.g. harbour or dock), cohesive sediments aggregate to large, settleable flocs under low turbulent shear and finally settle/deposit on the bottom.

Most of flocculation models assume an equilibrium (or pseudo-equilibrium) condition and a single floc size, thus disregarding the two important aspects, (1) flocculation kinetics in a time and space and (2) bimodal (or multimodal) floc size distributions of cohesive sediments. Flocculation is a relatively slow process, taking several to ten hours to reach an equilibrium condition in a river, estuarine or coastal environment. Therefore, an empirical, equilibrium flocculation model may cause errors, when involving a time or spatial transition. For example, the Deurganckdok study (WL | Delft Hydraulics, 2006) reported that an equilibrium flocculation model resulted in under- (or over-) estimation of flocculation and sedimentation in a dock next to a turbulent river (i.e. at a transition). Also, flocculation often develops bimodal floc size distributions. This bimodal behaviour cannot be simulated with a conventional single-size flocculation model.

To minimize such errors, we developed a new flocculation kinetic model, based on Two-Class Population Balance Equation (TCPBE) (Eqn. (1)) (Lee *et al.*, 2011). The two discrete size groups of flocculi and flocs, as building blocks and aggregates, were found to approximate a bimodal floc size distribution of cohesive sediments (Lee *et al.*, 2012, 2014). This observation led us to develop a new two class population balance equation (TCPBE), which can track the concentration of size-fixed flocculi and the size and concentration of size-varying flocs as an approximation of a multimodal PSD.

$$\left[\frac{\partial N_i}{\partial t}\right]+\left[\frac{\partial u_x N_i}{\partial x}+\frac{\partial u_y N_i}{\partial y}+\frac{\partial u_z N_i}{\partial z}\right]-\left[\frac{\partial}{\partial x}\left(\frac{0.09\rho_w k_e^2}{S_c \varepsilon}\frac{\partial N_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{0.09\rho_w k_e^2}{S_c \varepsilon}\frac{\partial N_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{0.09\rho_w k_e^2}{S_c \varepsilon}\frac{\partial N_i}{\partial z}\right)\right]=\pm(agg/break)_i - w_{s,i}\frac{\partial N_i}{\partial z}$$

$$(agg/break)_{N_P}=\frac{\partial N_P}{\partial t}=-\frac{1}{2}\alpha_{PP}\beta_{PP}N_P N_P\left(\frac{N_C}{N_C-1}\right)-\alpha_{PF}\beta_{PF}N_P N_F + fN_C a_F N_F$$

$$(agg/break)_{N_F}=\frac{\partial N_F}{\partial t}=+\frac{1}{2}\alpha_{PP}\beta_{PP}N_P N_P\left(\frac{1}{N_C-1}\right)-\frac{1}{2}\alpha_{FF}\beta_{FF}N_F N_F + a_F N_F$$

$$(agg/break)_{M_F}=\frac{\partial M_F}{\partial t}=+\frac{1}{2}\alpha_{PP}\beta_{PP}N_P N_P\left(\frac{N_C}{N_C-1}\right)+\alpha_{PF}\beta_{PF}N_P N_F - fN_C a_F N_F$$

$$w_{s,i}=\Phi_{HS}\left(\frac{1}{18}\frac{(\rho_s-\rho_w)g}{\mu}D_P^{3-n_f}\frac{D_F^{n_f-1}}{1+0.15Re_i^{0.687}}\right)$$

$$\Phi_{HS}=(1-\phi)^a$$

(1)

(Nomenclature)

$N_i = N_P$, N_F, or M_F $w_{s,i}$ = Floc Settling Velocity D_P, D_F = Diameter of Flocculi and Floc
N_C = Number of Flocculi in a Floc n_f = Fractal Dimension
$M_F = N_F \times N_C$ Φ_{HS} = Factor for Hindered Settling
f = Flocculi Fraction Generated by Breakage Φ = Factor for Hindered Settling

Model development and application: large-scale, multi-dimensional TCPBE-TELEMAC model.
For application to large-scale cohesive sediment transport, TCPBE is implemented to an open-source hydrodynamic and sediment transport model (TELEMAC in this study). We modify the original code of TELEMAC, adopting shear rate ($G = (\mathcal{E}/v)^{0.5}$) and settling velocity (w_s) as two key factors for controlling flocculation kinetics and sediment transport. At each time step in computation, TELEMAC calculates shear rates (G), which then control flocculation kinetics of TCPBE. On the other hand, TCPBE calculates floc settling velocities (w_s), which then determine floc sedimentation/deposition (i.e. sink) rates.

The combined TCPBE-TELEMAC model is applied to simulate cohesive sediment transport in Belgian near-shore area and Elbe Estuary in Germany. The results show that the TCPBE-TELEMAC model can more realistically simulate cohesive sediment processes (i.e. flocculation, advection, dispersion, sedimentation and deposition) than the equilibrium flocculation model. For example, the TCPBE-TELEMAC model can simulate a lag phase of flocculation at a time and spatial transition (e.g. from slack to peak flow; from an open ocean to a harbour), because it takes into account "kinetics". The conventional equilibrium flocculation model however does not consider kinetics nor the lag phase, so that it often develops steep gradient (or discontinuity) of flocculation at a time and spatial transition. In addition, because the TCPBE-TELEMAC model takes into account the bimodality with the two groups of flocculi and flocs, it can simulate background turbidity floating around in the water column. The single-class equilibrium flocculation model often develops zero turbidity, which is not real, because it does not differentiate turbidity-causing flocculi from flocs.

Further remarks: biologically-mediated TCPBE
The TCPBE model is theoretical but not empirical. This implies that the TCPBE model can easily add on other physical, chemical and biological processes without breaking the physics of flocculation. Thus, in future studies, the TCPBE model will be used as a generic model to adopt biologically-mediated flocculation. Especially, Extracellular Polymeric Substances (EPS) are known to scavenge and assemble biomass and sediment particles into large flocs (Engel *et al.*, 2004). Thus, the biologically-mediated TCPBE will include: (1) EPS formation kinetics controlled by microbial population dynamics and (2) particle aggregation and breakage kinetics between different particles species (i.e. EPS, biomass and minerals) (Fig. 1).

Heterogeneous Floc

Flocculi (P)

TEP

Biomass (BM)

$$\rho_{Floc} = (1-e)(x_{TEP}\rho_{TEP} + x_{BM}\rho_{BM} + x_P\rho_P) + e\rho_{Water}$$

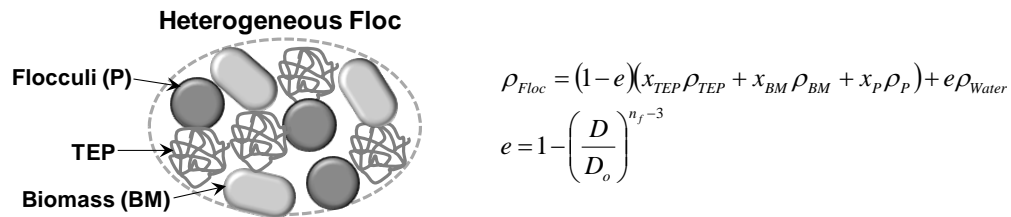$$e = 1 - \left(\frac{D}{D_o}\right)^{n_f - 3}$$

Fig. 1. A schematic diagram of a biomass-sediment floc with heterogeneous composition and mathematical formula for calculating the density of a heterogeneous floc. x is the volume fraction of TEP, biomass or flocculi in a floc, e is the void fraction, D is the size of a floc and D_o is the size of a primary particle.

References
Engel A., S. Thoms, U. Riebesell, E. Rochelle-Newall and I. Zondervan. 2004. Polysaccharide aggregation as a potential sink of marine dissolved organic carbon. Nature 428:929-932.
Lee B.J., E. Toorman and M. Fettweis. 2014. Multimodal particle size distributions of fine-grained sediments: mathematical modeling and field investigation. Ocean Dynamics 64(3):429-441.
Lee B.J., M. Fettweis, E. Toorman and F. Molz. 2012. Multimodality of a particle size distribution of cohesive suspended particulate matters in a coastal zone. Journal of Geophysical Research 117. C03014.
Lee B.J., E. Toorman, F.J. Molz and J. Wang. 2011. A two-class population balance equation yielding bimodal flocculation of marine or estuarine sediments. Water Research 45(5):2131–2145.
WL | Delft Hydraulics. 2006. 3D slibtransport model Zeeschelde - Scenario 4: effect CDW op sedimentatie Deurganckdok, nieuw instrumentarium.