**Technical Report**

**Two-Class Flocculation Model in COHERENS (TCPBE-COHERENS Model)**

**1. Model Description: Sediment Transport Model**

The sediment mass balance equation was used to simulate the 1-dimensional vertical transport of flocculi and flocs in the water column (Equation (1)). Size-fixed flocculi and size-varying flocs approximate a bimodal PSD varying in time and space (Figure 1) [*Lee et al.*, 2011]. To track the three time- and space-dependent variables, the number concentration of flocculi (*NP*) and the size and number concentration of floc (*DF* and *NF*), the sediment mass balance equation incorporate three differential equations for the time rate of change of: the number concentration of flocculi in suspension (*dNP/dt*), the number concentration of flocs in suspension (*dNF/dt*), and the number concentration of flocculi bound in flocs (*dNPF/dt*). On the right-hand side of Equation (2), the respective terms represent turbulence-mediated dispersion, gravity-driven sedimentation and flocculation kinetics. The flocculation kinetics (Ai + Bi) incorporates the two-class population balance equation (TCPBE) which is able to simulate bimodal flocculation (details in Section 2).

 (1)

In Equation (1), *Ni* = *Ni* (*z, t*) represents the number concentration, the subscript *i* represents flocculi and flocs in suspension (*NP* and *NF*) and flocculi bound in flocs (*NPF* = *NC* × *NF*), *NC* is a floc size index representing the number of flocculi bound in a floc, *C'μ* is a stability constant, (*Ai* + *Bi*) is the growth and decay rates of *Ni* by aggregation and breakage, and *ws,i* is the settling velocity of flocculi or flocs.

 

**Figure 1.** Schematic diagrams of (a) continuous particle size distributions and (b) discrete size groups of flocculi and flocs before and after flocculation, from (t0, x0) to (t1, x1). Figure 2(b) also represents the flocculation strategy of the TCPBE.

The Stokes equation, including the use of fractal theory for floc packing and shaping and the correction factor (Φ*HS*) for hindered settling in a highly concentrated near-bottom mud layer [*Winterwerp and van Kesteren*, 2004], was used to calculate the floc settling velocity (*ws,i*) (Equations (2), (3)). This settling equation is simply adopted from COHERENS, but will include some modifications for other purposes.

 (2)

 (3)

In Equations (2) and (3), *ρs* = particle density, *ρw* = fluid density, *g* = gravitational acceleration, *μ* = fluid viscosity, Φ*HS* = correction factor for hindered settling, *Φ*p = volumetric concentration of particles (m3 Particles / m3), *Φ* = volumetric concentration of flocs (m3 Flocs / m3), *Φ*\* = min{1, *Φ* }, and Re*i* = Reynolds number of a particle or floc (= *Di*·*ws,i*·*ρw*/*µ*).

The top boundaries of the number concentrations of flocculi in suspension, flocs in suspension and flocculi bound in flocs (*NP*, *NF* and *NPF*) were set to be a closed boundary, but the bottom boundaries were open for erosion and deposition, following formulation of shear-dependent erosion and continuous deposition (Equations (4), (5)) [*Ariathurai*, 1974; *Le Hir et al.*, 2011]. In the 1-DV TCPBE, both of flocculi and flocs are subject to deposition, but only flocculi are to erosion which may be referred to as entrainment or disruption [*Winterwerp and van Kesteren*, 2004].

 (4)

 (5)

In Equations (4), (5), the subscript *i* is *P*, *F* or *PF,* representing flocculi in suspension, flocs in suspension and flocculi bound in flocs, respectively. *M* is the empirical erosion parameter, *τ* is the bottom shear stress, *τc* is the critical shear stress for erosion. The denominator over *M* is used to convert the mass concentration to the number concentration. Erosion of flocculi (*EP*) is effective only when a pool of erodible sediments is available on the bottom (*B* > 0) and the bottom shear stress is over the critical shear stress (*τ* > *τc*), according to the Ariathurai-Partheniades equation [*Ariathurai*, 1974].

**2. Model Description: Two Class Flocculation Model Model**

The two-class PBE includes size-fixed flocculi and size-varying flocs as building blocks and buildings, respectively, in order to simulate bimodal flocculation (Figure 2). The number of flocculi bound in a floc (*NC*) is used as an index of floc size in the TCPBE. Because this new size index becomes one for flocculi (*NC* = 1), it gives the simplicity of the TCPBE. The TCPBE incorporates three coupled differential equations describing the time rate of change of: (1) the number concentration of microflocs (*dNP/dt*), (2) the number concentration of macroflocs (*dNF/dt*), and (3) the total number concentration of microflocs bound in macroflocs (*dNPF/dt*) (*NPF* = *NC* × *NF*) (Equation (6)), and they were incorporated to the growth and decay rates (*Ai* + *Bi*) of Equation (2). The TCPBE was explained in depth by [*Lee et al.*, 2011].

 (6)

In Equation (6), *f* represents the fraction of flocculi generated by floc breakage. *α* is the collision efficiency factor, *β* is the collision frequency factor, and *a* is the breakage kinetic constant. The collision efficiency factor (*α*) is generally used as an application-specific fitting parameter and the collision frequency factor (*β*) is applied as a theoretical function correlated with Brownian motion, turbulent shear rate, and differential settling. Table 2 summarizes the aggregation and breakage kernels for the collision frequency factor (*β*) and the breakage kinetic constant(*a*) [*Burd and Jackson*, 2002; *Lee et al.*, 2011]. The aggregation kernels consist of the theoretical functions of Brownian motion, differential settling and turbulent shear, but the breakage kernel is composed only of the shear-dependent breakage kinetics function (Table 1).

**Table 2.** Aggregation and breakage kernels of the 1-DV TCPBE, from Lee et al. (2011).

|  |  |
| --- | --- |
| **Aggregation Kernel** | **Breakage Kernel** |
|  |  |
| *Di =* Diameter of a particle size class *i*  *βBR* = Collision frequency factor by Brownian motion  *βSH* = Collision frequency factor by fluid shear  *βDS* = Collision frequency factor by differential settling  *k =* Boltzmann’s constant  *T =* Absolute Temperature (K) | *p, q = Empirical parameters*  *μ = Absolute viscosity of the fluid*  *G = Fluid turbulent shear rate (/s)*  *wi = Sedimentation velocity of size class i*  *Eb = Breakage efficiency factor*  *Fy = Yield strength of flocs (10-10 Pa)* |

**3. Numerical Method: Discretization and Adoption of TCPBE in COHERENS**

Finite difference method was used to solve TCPBE, adopting explicit discretization for time stepping. A preliminary numerical test indicated that both the explicit and implicit time discretization methods produced almost identical results with a short time step size (e.g. 12 seconds in this test), and thus the explicit discretization method will be as good as the implicit method with less computational cost for simulating a large-scale and multi-dimensional coastal and estuarine system with relatively small computational cost (Equation (7)). Note that sedimentation is a fast process taking minutes to cross over a computational cell, while flocculation is a relatively slow process taking hours to reach a steady state in a cell. Thus, as long as a numerical model adopts a short time step size for sedimentation, the explicit discretization method will be good enough for flocculation to obtain the same quality simulation as the implicit discretization method does.

 (7)

The subroutine "twoclass\_flocculation" was developed for solving the discretized TCPBE (Equations (7)). It was implemented under the subroutine "sediment\_equations", replacing the subroutine "settling\_velocity". The main program calls "twoclass\_flocculation", when calling "settling\_velocity". In the subroutine "twoclass\_flocculation", the volume concentrations (*CV,P* and *CV,T*; Global variables) are firstly converted to the number concentrations (*NP* and *NT*; Local variables). However, the number concentration of flocs (*NF*) keeps the same format throughout the program, representing information about floc size (*DF* = ƒ(*NF*, *NT*)). Then, the discretized TCPBE (Equation (7)) updates the number concentrations (*NP*, *NF* and *NT*), the size and settling velocity of flocs (*DF* and *ws,F*). The number concentrations (*NP* and *NT*) are finally converted back to the volume concentrations (*CV,P* and *CV,T*) for the main COHERENS program.

**4. User Manual of TCPBE with COHERENS**

*X*- and *Y*-components of pressure gradient, which users can find and change in the subroutine "usrdef\_1dsur\_data" in the subroutine "usrdef\_model", are the main flow-driving force. This simulation applied a cyclic pressure gradient function to induce flood-ebb tidal flow (Equation 8). This method was improvised to use the measured data of friction velocity. However, note that other pressure gradient terms can be used in simulation [*Burchard*, 1999; *Luyten et al.*, 2002].

 (8)

A lot of model parameters are used in TCPBE (see Table 3), but those parameters are not equally important in simulation. Thus, I recommend users to change several flocculation kinetic parameters for model validation and test-case simulation. For example, users may change only collision and breakage efficiency factors (*α* and *Eb*) and fractal dimension (*nf*) (highlighted in Table 3). All the parameters of TCPBE can be found and changed in the new subroutine "twoclass\_flocculation". Later, these parameters will be placed in user-defined subroutine "usrdef\_sediment" (in progression). Besides flocculation, erosion and deposition controls cohesive sediment transport. Thus, users have to pay attention to select the best empirical erosion parameter (*M*) and critical shear stress for erosion (*τc*), in case of applying the Ariathurai-Partheniades equation [*Ariathurai*, 1974]. These erosion-controlling parameters can be found and changed in subroutine "usrdef\_sediment".

**Table 3.** Parameters and initial conditions of the 1-DV TCPBE for the best-quality simulation.

|  |  |  |  |
| --- | --- | --- | --- |
| **Kinetic Parameters and Physicochemical Constants** | | | |
| **Classification** | **Symbol** | **Default** | **Description** |
| Flocculation  Kinetics | *α* | 0.1 | Collision efficiency factor [-] |
| *Eb* | 2.0e-5 | Breakage efficiency factor [s0.5/m] |
| *nf* | 2.2 | Fractal dimension of flocs [-] |
| *f* | 1.0 | Fraction of flocculi by floc breakage [-] |
| *Fy* | 1.0e-10 | Yield strength of flocs [Pa] |
| a *p* | 1.0 | Empirical parameter of breakage kinetics |
| Erosion  Deposition | *M* | 1.0e-3 | Empirical erosion parameter [kg/m2/s] |
| *τc* | 1.5 | Critical shear stress for erosion [pa] |
| Sediment  Property | *ρP* | 1800 | Density of flocculi [kg/m3] |
| *ρw* | 1050 | Density of sea water [kg/m3] |
| *DP* | 15.0 | Diameter of flocculi [μm] |
| **Initial Conditions (at t = 0)** | | | |
| Sediment Concentration | *C*V,P | 16.02e-5 | **Volume** conc. of Flocculi [m3/m3] |
| *C*n,F | 2.015e+8 | **Number** conc. of Flocs [m3/m3] |
| *C*V,T | 1.78e-5 | **Volume** conc. of Flocculi bound in Flocs [m3/m3] |
| a *p* was set as 1.0 to narrow FSDs' width, instead of 0.5 of Winterwerp and van Kasteren (2004). | | | |

**6. Model Validation: TCPBE-COHERENS versus in-house TCPBE**

Flocculation and transport of cohesive sediments was simulated in 1-dimensional vertical water column during flood-ebb tidal cycles. Both of TCPBE-COHERENS and In-house TCPBE were tested and compared to each other. In the time series plots of model variables (Figure 3), TCPBE-COHERENS has a similar up-and-down trend to In-house TCPBE, but it has smaller floc size but higher solid concentration near slack water. TCPBE-COHERENS and In-house TCPBE adopt different turbulence closures, *k-ε* equations and analytical equations, respectively. This difference might cause the gap near slack water.



**Figure 3.** Time series plots of model variables.

The depth profiles of TCPBE-COHERENS and In-house TCPBE seem similar to each other as shown in Figure 4. However, their differences are found around peak flow and slack water. Around peak flow (e.g. t = 27 hr), TCPBE-COHERENS has higher eddy viscosities throughout the water column but lower solid concentrations than In-house TCPBE. Around slack water (e.g. t - 30 hr), TCPBE-COHERENS has smaller floc size than In-house TCPBE. These differences around peak flow and slack water might also be caused by the different turbulence closures of the two models. Despite the differences described above, TCPBE-COHERENS is overall proven to be capable of producing the same (or better) quality simulations as In-house TCPBE does.

 

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**Figure 4.** Depth profiles of model variables.

**7. Conclusion and Recommendation**

The combined TCPBE-COHERENS model is now ready for users to simulate flocculation and transport in 1-dimensional water column during flood-ebb tidal cycles. The TCPBE-COHERENS model, unlike other empirical flocculation models, is a good mechanistic model, based on flocculation theories. Thus, the TCPBE-COHERENS model allows scientists and engineers to investigate cohesive sediment flocculation in a more systematic, based on with theoretical backgrounds. Moreover, the TCPBE-COHERENS model is capable of easily adopting other bio-physico-chemical processes because of its mechanistic nature [*Lee et al.*, 2012]. In short, the TCPBE-COHERENS model is promising and ready for many scientists or engineers to investigate flocculation-involving bio-physico-chemical processes in a marine and coastal environment.

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