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Key Points:

- A new modeling framework incorporating flocculation for cohesive sediment transport in wave-bottom boundary layers is developed
- High-cohesion flocs may encourage the formation of a sharp negative concentration gradient and its displacement toward the bed
- Depth-averaged settling velocity scales well at low concentration, while Teeter's formulation promises to capture variabilities

Supporting Information:

Supporting Information may be found in the online version of this article.

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A Numerical Modeling Framework for Flocculation and Cohesive Sediment Transport in the Wave Bottom Boundary Layer

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Abstract Flocculation, a critical process in coastal and estuarine systems, plays a significant role in sediment transport, nutrient cycling, and ecological health. This study develops a cohesive sediment transport modeling framework tailored to the wave bottom boundary layer under dilute and equilibrium conditions, explicitly incorporating flocculation effects via a Population Balance Equation (PBE). Using Direct Numerical Simulation, six baseline cases, each with a distinct sediment concentration profile resulting from a constant settling velocity and critical erosion shear stress, are generated to drive the PBE flocculation model for given floc yield strength and stickiness. Results reveal that flocculation significantly influences sediment concentration profiles promoting three distinct stages, well-mixed, transition to lutocline, and well-developed lutocline. At low concentrations with well-mixed profiles, cohesive floc properties are less significant, and turbulence is a main flocculation driver. In contrast, as concentration increases, cohesive floc properties become crucial, facilitating lutocline formation. The analysis also highlights limitations of depth-averaged settling velocity as a parameterization. It is suitable for well-mixed and transitional profiles but fails in well-developed lutoclines, where empirical formulations that explicitly incorporate turbulent shear rate and sediment concentration better capture variability. This study underscores the necessity of incorporating flocculation effects into sediment transport models to enhance predictions of sediment dynamics in wave bottom boundary layers.

Plain Language Summary In coastal and estuarine waters, tiny sticky particles often clump together to form larger ones called flocs, a process known as flocculation. This process, driven by turbulence, particle concentration, and natural organic matter, strongly affects how sediments move, how nutrients cycle, and how healthy these ecosystems remain. In our study, we created a new model to better understand flocculation near the seabed, where waves stir up sediments. Using high-resolution computer simulations, we tested different sediment levels and found that at low concentrations, turbulence mainly controls flocculation, while at higher concentrations, the stickiness of the particles takes over, creating a dense sediment layer near the bottom (a lutocline). We also showed that a simple average method commonly used to predict how fast sediments settle only works under certain conditions, and empirical approaches that consider turbulence and sediment concentration are needed when lutoclines form. Overall, our work highlights the importance of including flocculation in sediment transport models to improve predictions of coastal and estuarine dynamics.

1. Introduction

Flocculation is a fundamental process in coastal and estuarine environments, influencing nutrient cycling, water quality, morphodynamics, and ecological stability. As freshwater meets saline conditions, flocculation causes fine particles and dissolved organic matter to aggregate, promoting the removal of nutrients and pollutants from the water column through rapid sedimentation (Jayaprakash et al., 2010; Karbassi et al., 2008). This nutrient trapping capability is essential for maintaining water quality, as it reduces nutrient concentrations that could otherwise contribute to eutrophication and harmful algal blooms (Asmala et al., 2014). From a morphodynamic perspective, flocculated particles settle faster, forming stable sediment layers in low-energy conditions that influence the

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topography and erosion patterns of salt marshes, tidal flats, and river deltas (O'Laughlin et al., 2014; Voulgaris & Meyers, 2004), which may contribute to coastal resilience against sea-level rise. Ecologically, flocculation plays a crucial role in shaping habitats, as the sediment layers formed provide essential substrates for microbial communities and vegetation, fostering biodiversity and supporting secondary production within these ecosystems (Poirier et al., 2017; A Wang et al., 2010). Additionally, the presence of vegetation further enhances flocculation by physically trapping particles, while the resulting stem-scale turbulence modifies floc properties, which in turn affects sediment stability and ecological interactions within salt marshes and intertidal flats (Choi et al., 2021). Thus, flocculation is not only a key mechanism in sediment transport but also an essential process that underpins water quality, landscape evolution, and ecological health in coastal systems.

Flocculation is governed by two simultaneous processes, aggregation and fragmentation (breakup). Aggregation occurs when cations from dissolved salts in water create surface bridging around clay particles, thereby reducing repulsive forces and forming flocs (Sutherland et al., 2015). Additionally, the presence of organic matter can significantly enhance aggregation by increasing floc stickiness, thereby influencing the floc size distribution (Mietta et al., 2009; Ye et al., 2021). In contrast, fragmentation reduces floc size when environmental forcing, such as turbulent shear, becomes sufficiently strong. Flocculation depends on collisions between cohesive particles or flocs, driven by three primary mechanisms, Brownian motion, differential settling velocity, and turbulent shear. In coastal environments, such as estuaries and continental shelves, turbulence predominates over the other mechanisms (J. C. Winterwerp, 2002). Therefore, it is very common to assume that turbulence is the main force driving the flocculation process via the turbulent shear rate $G = \sqrt{\varepsilon/\nu}$, where ε is the turbulent dissipation rate and ν is the kinematic fluid viscosity.

There are three main types of models used to simulate the flocculation process. The first is the single floc size method (J. C. Winterwerp, 1998), which is commonly employed to track the temporal evolution of the median floc size, d_{50}. The second model, known as the grain-resolved simulation, tracks individual cohesive particles with a fully resolved approach (Vowinckel et al., 2019). The third approach involves modeling the floc size distribution, either through distribution-based models with a fixed distribution (Maerz & Wirtz, 2009) or by using a Population Balance Equation (PBE), which quantifies the number of flocs in each size class while conserving mass (Mietta et al., 2011; Verney et al., 2011). Each of these methods has its limitations that must be carefully considered for a given study objective. For instance, the single floc size method does not represent the full complexity of floc size distributions. The grain-resolved approach is computationally expensive, making it impractical for many applications. The PBE-based approach, however, has gained popularity because it represents floc size distributions with reasonable computational efficiency.

This research utilizes the Population Balance Equation (PBE), as it avoids the limitations of predetermined distributions and captures bimodal floc behaviors commonly observed in aquatic systems (B. J. Lee et al., 2011; Manning & Dyer, 2007). The complexities associated with parameterizing the PBE-based size-class flocculation model have been widely studied and critical insights into its implementation challenges have been documented (Coufort et al., 2007; Jeldres et al., 2015; Mietta et al., 2011; Shen et al., 2018; Zhang et al., 2019). A key consideration in such model is the choice of maximum floc size and the number of floc size classes. If the maximum floc size class is specified insufficiently low under strong aggregation influence, sediment mass accumulates artificially in the largest size class, leading to unrealistic numerical errors. Conversely, an insufficient number of size classes can distort the temporal evolution of fine, medium, and coarse fractions during both growth and equilibrium phases. Penaloza-Giraldo et al. (2023) recommend performing a sensitivity analysis to determine the appropriate maximum floc size under strong aggregation regimes. As a result, they use 75 floc size classes in the size range of 4–300 μm to ensure accurate time series predictions. However, applying this recommendation in cohesive sediment transport models poses a significant computational challenge, as it requires solving the mass-conserving advection-diffusion equation for each floc class. Consequently, existing models that couple PBE with cohesive sediment transport typically limit the number of size classes. For example, the Regional Ocean Modeling System (ROMS v3.6) incorporates 15 classes (Sherwood et al., 2018) while a 3D Large Eddy Simulation (LES) model uses 27 (Liu et al., 2019). The model recently reported by Penaloza-Giraldo et al. (2025) implements 75 floc size classes within an equilibrium-based framework, but it is currently restricted to statistically steady unidirectional flow and excludes wave-induced cohesive sediment transport.

In general, the coupling between PBE and a cohesive sediment transport model consists of quantifying the evolution of floc size classes as a function of local sediment concentrations and turbulent shear rate G for given cohesive sediment properties. The settling velocities are directly quantified by floc size, typically calculated using Stokes' law with the floc density estimated by additional assumptions. The depositional flux of each size class is then calculated by the corresponding sediment mass and settling velocity. An illustrative example is the RIVFLOC model, which utilizes the advection-dispersion equation to simulate sediment concentration for each size fraction of the fine sediment. Subsequently, the flocculation model distributes these concentrations to predict floc size distribution based on a collision frequency parameter that includes flocculation mechanics in a single value (Droppo & Krishnappan, 2016). However, turbulence statistics can be estimated only rather empirically from the 1D Saint-Venant hydrodynamic model to drive the flocculation processes. The 3D coastal/ocean models, such as COAWST (Warner et al., 2010), address this limitation with a two-equation (e.g., $k - \varepsilon$) turbulence closure model since the local turbulent dissipation rate ε is more accurately modeled and used to calculate the turbulent shear rate G. Sherwood et al. (2018) incorporate the PBE-based size-class flocculation model of Verney et al. (2011) into the Coupled Ocean-Atmosphere-Wave-and-Sediment Transport modeling framework (COAWST). This modeling framework has gained traction in many applications such as tidal variations, consolidation process (Tarpley et al., 2019), wave-supported fluid mud (Zang et al., 2020) and oil-particle-aggregates (Cui et al., 2021). Nevertheless, since COAWST applications solve the wave-period-averaged Reynolds-Averaged Navier–Stokes (RANS) equations with limited vertical resolution, they are incapable of resolving bottom boundary layer processes accurately. Again, the modeling framework proposed by Penaloza-Giraldo et al. (2025) includes the bottom boundary layer by integrating fully-resolved turbulence data from a Direct Numerical Simulation (DNS) for a fully-developed channel flow.

Resolving turbulence and sediment transport processes within the wave-bottom boundary layer (WBBL) is crucial because it directly governs sediment resuspension and subsequent transport, which significantly impact seabed evolution and fate of fine sediments (Nelson & Fringer, 2018; Traykovski et al., 2000; Yue et al., 2020). Since turbulence is a primary driver of flocculation, the near-bed turbulence generated by oscillatory flows is expected to dictate floc formation and vertical distribution of sediment, thereby influencing the development and evolution of lutoclines. WBBL in fine-sediment-rich environments typically exhibit transitional turbulence features between laminar and turbulent regimes (Ozdemir et al., 2014), which poses challenges when using classical turbulence closures within the Reynolds-Averaged Navier–Stokes (RANS) framework. Moreover, direct measurements within the WBBL are difficult due to its small vertical extent, typically on the order of millimeters (Trowbridge & Lentz, 2018). As a result, only a handful of studies report field measured sediment concentration and velocity profiles in the WBBL (Egan et al., 2020; Traykovski et al., 2000, 2007). In response to these limitations, laboratory experiments in an oscillating water tunnel have been conducted to study the effect of sediment-induced density stratification (Hooshmand et al., 2015) and bedforms (Han et al., 2021) on the wave-supported mud layer. Moreover, Direct Numerical Simulations (DNS) coupled with a fine sediment transport formulation have been applied to study turbulence attention by particle-induced density stratification (Ozdemier et al., 2010), lutocline dynamics (Ozdemir et al., 2011) and wave-supported gravity flows (Yue et al., 2020). However, none of the field experiments and laboratory experiments report flocculation dynamics in WBBL while all the numerical simulations studies have assumed a constant settling velocity for fine sediment, neglecting the flocculation process.

Recently, advances have been made to incorporate the flocculation effect on the settling velocity into sediment transport models. For instance, the wave boundary layer has been integrated into the Community Sediment Transport Modeling System (CSTMS) within the COAWST (Zang et al., 2020), introducing a transitional layer between the lowest water column and the seabed that accounts for wave-induced turbulence and its effects on sediment transport. Although COAWST has a PBE flocculation model (Sherwood et al., 2018) to quantify a variable settling velocity in the water column, it is not able to directly resolve the WBBL. Hence, Zang et al. (2020) opted to specify the settling velocity as a concentration-dependent equation based on Mehta (1996). While this development marks a significant step forward in representing the WBBL for regional-scale modeling, it still relies on depth-averaged properties and a linearized Chezy equation with a constant drag coefficient, limiting its ability to fully capture the vertical complexity of WBBL dynamics.

The primary goal of this study is to investigate the influence of flocculation-induced variable settling velocities on the structure of the concentration profiles within the WBBL under dilute and equilibrium conditions. Specifically, we test the hypothesis that certain floc properties dictate flocculation and the resulting settling velocity that may further control the formation and disappearance of lutoclines. The specific objectives are (a) to extend the modeling framework proposed by Penaloza-Giraldo et al. (2025) for wave-induced cohesive sediment transport in

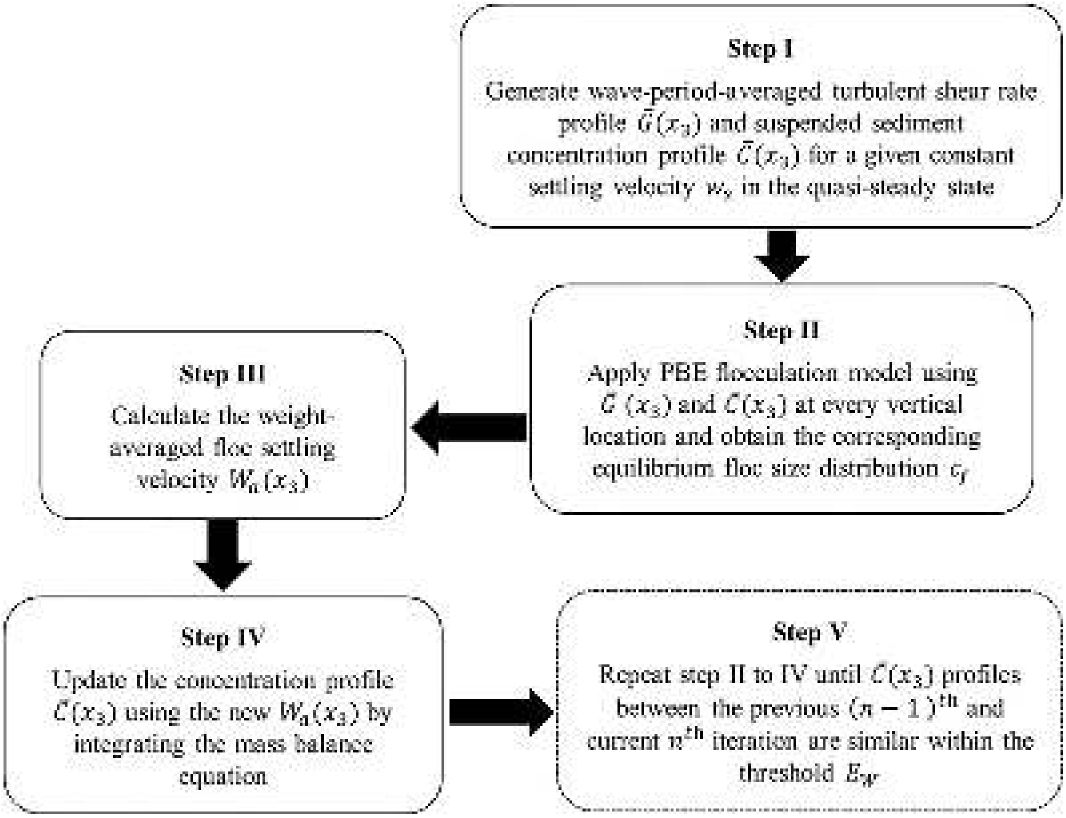

Figure 1. A flowchart for the cohesive sediment modeling framework considering flocculation dynamics in the wave-period-averaged wave bottom boundary layer.

the WBBL, (b) to evaluate how stickiness and yield strength of flocs control flocculation dynamics, settling velocity variabilities, and sediment concentration profiles, including changes in the vertical structure of sediment concentration (concentration gradient), and (c) to investigate effective parameterizations for flocculation-induced settling velocity, thereby highlighting the possibility of upscaling flocculation effects in modeling cohesive sediment in WBBL in regional scale models. The remainder of this paper is organized as follows. Section 2 presents a description of the modeling framework and data processing methods. Section 3 introduces the empirical formulations used to estimate settling velocities. Section 4 describes baseline cases using a constant settling velocity, which are used here as a reference for quantifying flocculation effects. Section 5 provides the major results to test the proposed hypothesis. Sections 6 and 7 cover the discussion and conclusions of the study, respectively.

2. Modeling Framework

The core modeling framework is based on the approach proposed by Penaloza-Giraldo et al. (2025), originally developed for statistically-steady, unidirectional flow with dilute sediment concentrations at the equilibrium flocculation state. To extend this framework to wave-induced cohesive sediment transport within the WBBL, a wave-period-averaged approach is implemented to model the coupling between flocculation processes and sediment transport in WBBL (Figure 1). The wave-period-average is justified by the fact that typical flocculation timescale for dilute flow (e.g., binary collision) is on the order of at least several minutes, significantly longer than typical wave period (J. C. Winterwerp, 2002). The model is initialized by two initial profiles as inputs (Step I). The first profile corresponds to the wave-period-averaged turbulent shear rate $\overline{G}$ while the second profile is the wave-period-averaged sediment concentration $\overline{C}$, where the overbar represents the wave-period-average. These two profiles represent dilute suspended sediment transport in quasi-steady state driven by a periodic wave forcing without considering flocculation (i.e., using a constant settling velocity w_s). Subsequently, the concentration $\overline{C}$ is distributed into a provided range of floc sizes by a PBE flocculation model controlled by the corresponding $\overline{G}$, the

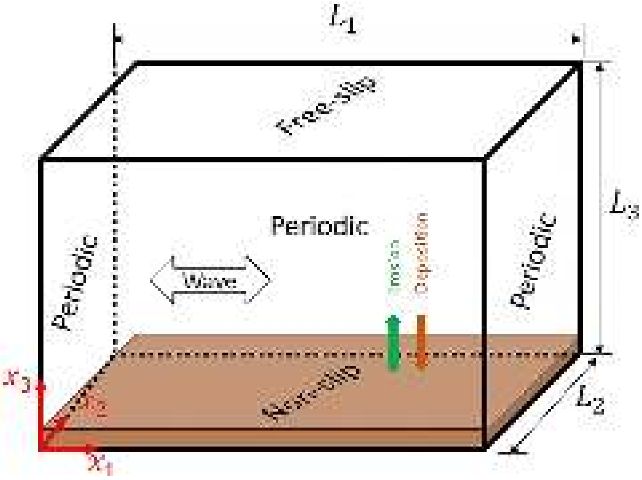

Figure 2. Sketch of the DNS computational domain including its boundary conditions.

number density of flocs in each size class, the assumed floc structure (fractal dimension in this study), and the floc cohesion/breakup properties (Step II). The resulting distributed concentration is used to estimate a new settling velocity profile (Step III), which is then incorporated into a wave-period-averaged mass balance formulation in the bottom boundary layer to update the concentration profile (Step IV). In Step V, we calculate the difference between the newly obtained settling velocity profile and the initial settling velocity profile. We continue the procedure with an iterative scheme by repeating Steps II to V utilizing the newly updated sediment concentration profile, along with the given $\overline{G}$ profile, to drive the PBE flocculation model and provide updated settling velocity and concentration profiles. The iteration is continued until convergence is achieved in the settling velocity profile. In the following subsections, the five steps of the modeling frameworks (see Figure 1) are explained in detail.

2.1. Direct Numerical Simulation Data (Step I)

One of the quantities needed to drive the model framework is the wave-period-averaged turbulent shear rate $\overline{G}$, which requires information on the turbulent dissipation rate ε in the bottom boundary layer. However, directly estimating the turbulent dissipation rate from measured data for wave (oscillatory) bottom boundary layers is challenging due to the need for very high-resolution spatial gradients of turbulent velocity fluctuations close to the bed. A viable alternative is the implementation of DNS, which provides high-resolution temporal and spatial data of turbulent velocity flow fields, enabling accurate calculation of ε in the oscillatory bottom boundary layer. In this study, the open-source code TURBID developed by Yue et al. (2020) is implemented to simulate dilute fine sediment transport for a prescribed constant settling velocity in an oscillatory boundary layer and provide input data of $\overline{G}$ and $\overline{C}$ to the cohesive sediment modeling framework.

The DNS computational domain is shaped as a rectangular prism with dimensions $[L_1 \times L_2 \times L_3]$, where the coordinate origin is located at the bottom-left-front corner, oriented in the streamwise x_1, spanwise x_2 and vertical x_3 directions. The carrier flow velocities u_i and pressure p are solved by the Navier–Stokes equations for incompressible flow, considering the buoyancy term for the coupling effects from the fine sediment. For this carrier flow phase (water), periodic boundary conditions are imposed in the statistically-homogeneous streamwise (x_1) and spanwise (x_2) directions, while no-slip and free-slip boundary conditions are imposed at the bottom and top boundaries as illustrated in Figure 2. In addition, the streamwise flow driving force is established by a temporal-oscillatory pressure gradient to generate an oscillatory flow similar to that in an oscillating water tunnel (U-Tube) to approximate the near-bed flow driven by surface waves. As discussed in more detail in Yue et al. (2020), this configuration neglects the vertical velocity induced by surface waves and the corresponding surface wave induced boundary layer streaming. However, main turbulent wave bottom boundary layer features associated with streamwise periodic motion are retained.

The volumetric concentration of the sediment ϕ is computed by the advection-diffusion-settling equation with periodic boundary conditions specified in the x_1 and x_2 directions as well. The exchange of sediment with the bed is modeled by an erodible/depositional boundary condition at the bottom boundary. If the resulting flow exerts a shear stress on the erodible fine sediment bed that surpasses the established critical shear stress τ_c, fine sediment is suspended into the computational domain, following the Partheniades-Ariathurai-type expression (Sanford & Maa, 2001). Finally, the sediment phase velocity is approximated by the flow velocity field plus a constant particle settling velocity w_s. Further details about the numerical model can be found in Yue et al. (2020).

Once the DNS model generates the instantaneous sediment concentration $\phi(x_1, x_2, x_3, t)$ and velocity $u_i(x_1, x_2, x_3, t)$ fields, these data can be processed to calculate the wave-period-averaged turbulent shear rate $\overline{G}(x_3)$ and concentration $\overline{C}(x_3)$ profiles as input data for the modeling framework (step I in Figure 1). Several averaging operations used in this study are defined here.

To identify the quasi-steady state in the sediment-laden oscillatory bottom boundary layer, the volume-averaged concentration $\langle\phi\rangle_{123}$ field is computed as