

**NUMERICAL MODELING OF FLOCCULATION  
AND COHESIVE SEDIMENT TRANSPORT IN BOTTOM BOUNDARY  
LAYER**

by

Jorge Alberto Penaloza Giraldo

A dissertation submitted to the Faculty of the University of Delaware in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Civil Engineering

Spring 2024

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## ACKNOWLEDGMENTS

I would like to begin by expressing my heartfelt gratitude to my family, who have supported me unconditionally throughout my doctoral training. My wife, Lorena, has been an unwavering pillar, always listening, advising, and sharing the challenges of this demanding process. She stood by my side through the highs and lows, making every moment count. To my son, Alejandro, whose infectious smile served as constant motivation, rejuvenating my energy, and urging me to give my best. I extend my thanks to my mother, Dignoria, who has consistently supported me in all my projects and dreams. Lastly, to my late grandmother, Emelina, a remarkable woman, and a source of inspiration. Her unexpected passing, while I was writing my second scientific article (Chapter 4 of this dissertation), deeply saddened me. I wish you could have seen me as a doctor. Each of you has played an important role in my journey, and I am profoundly grateful for your unwavering support and love.

I am profoundly grateful for the guidance and mentorship provided by my advisor, Tom. His patience, assistance, and generosity played an essential role in cultivating my critical and investigative thinking. Tom's unwavering commitment to my academic training always stood out, and I am thankful for the opportunities he offered to collaborate with esteemed researchers worldwide. A particularly memorable experience was my first visit to the Asian continent to share the progress of my research in South Korea. The best anecdote that I often recall is our first research meeting at the beginning of my second semester (spring 2019). Tom spoke about the reputation of the coastal lab, CACR. He mentioned that there is no ranking to measure its performance

on the internet, but for sure, CACR is like an MIT on coasts. He asked if I knew this, to which I replied "no." He was surprised and asked me why I applied to this program. My answer was, "Additionally, I liked your research in environmental fluid dynamics and sediment transport, ex-PhD students from Cornell University and former students of yours from UD said that you are a great person, and to me that is also important than rankings" After almost six years of working with Tom, I can confidently say that everything I heard was true. Tom is not only an exceptional researcher but also a remarkable person. Thanks, Tom, for being my role model in science.

I would like to thank my committee members, Dr. Tian-Jian (Tom) Hsu, Dr. James T. Kirby, Dr. Andreas Münchow, and Dr. Andrew Manning, for their guidance, suggestions, and scientific contributions. His guidance was indispensable for my academic and research training. I thank each of you for your time, dedication, and commitment.

I extend my heartfelt thanks to my lab classmates and friends in Newark, Delaware, for sharing unforgettable moments.

Finally, I want to say that this research was made possible by grants from the National Science Foundation (OCE-1924532, OCE-2242113). Numerical simulations presented in this study were carried out using the Caviness cluster at University of Delaware and Expanse cluster at SDSC via ACCESS.

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## ABSTRACT

Cohesive sediment transport significantly influences water quality, landforms, biogeochemical cycles, and the distribution of diverse substances in aquatic environments. Unlike non-cohesive sediment such as sand, cohesive sediment, having a primary particle diameter smaller than about  $63\ \mu\text{m}$ , exhibits a crucial physical property called flocculation. This process generates high porosity aggregates of cohesive mineral particles along with substances contained in them, which are called flocs. Through flocculation, a wide range of floc sizes exist due to the aggregation and fragmentation (breakup) induced by collisions driven by flow turbulence in the coastal environments. The presented dissertation explores the inter-relationship between flocculation dynamics and cohesive sediment transport within the bottom boundary layer. To address this, a novel modeling framework is developed in statistically steady (or quasi-steady states) and dilute condition with a variable settling velocity due to flocculation. The open-source Population Balance Equation (PBE) flocculation model (Verney et al., 2011) is employed to distribute initial turbulence-averaged sediment concentrations  $C$  into floc size distributions driven by turbulent shear rates  $S$  at the equilibrium state. The variable settling velocity is estimated from the resulting floc size distribution and incorporated into the mass balance equation to further calculate sediment distribution in the boundary layer. In this dissertation, the initial input of  $C$  and  $S$  profiles are generated by Direct Numerical Simulations with a constant settling velocity (no flocculation) to obtain accurate data representation in both current and wave bottom boundary layer.

Firstly, the key parameters in the PBE flocculation model are studied, namely the collisional efficiency, fragmentation rate, and fractal dimension via a comprehensive calibration process using laboratory measurements of temporal floc size statistics reported by Keyvani and Strom (2014) under a constant turbulent shear rate  $S$ . The results reveal that the median floc size statistic  $d_{50}$  is insufficient to constrain the model parameters, and extract time series such as  $d_{16}$  and  $d_{84}$  contributes to constrain the flocculation parameters with improved predictions. In addition, the clear correlation between the best calibrated fragmentation rate and floc size statistics provides a motivation to propose a two-value fragmentation rate approach, which shows a significantly improved agreement in matching the measured floc size statistics.

With a clear understanding of PBE flocculation model, the modeling framework is applied to a current bottom boundary layer. The findings illustrate that incorporating flocculation alters the concentration profile, stemming from changes in the floc size distribution and the consequent settling velocity. Flocs characterized by low cohesion exhibit smaller settling velocities and minimal settling velocity variability across the boundary layer, ultimately encouraging well-mixed vertical profiles. In contrast, when flocs possess high cohesion properties, more sediment is relocated near the bottom, increasing settling velocity magnitude and its variability. Moreover, the depth-averaged settling velocity emerges as a reliable approximation for calculating sediment profile in the current boundary layer, offering a practical tool with errors below 10%.

The modeling framework is further extended for wave (oscillatory) bottom boundary layer with an additional assumption that the time scale of the flocculation process is significantly larger than wave period. As a results, the variable settling velocity induced by flocculation is incorporated under wave-period-averaged condition.

In scenarios with low sediment availability, the turbulence shear rate ( $S$ ) takes precedence as the primary driving force of flocculation. Consequently, the inclusion of the flocculation effect yields well-mixed concentration profiles characterized by the generation of small flocs, which are notably insensitive to cohesive floc properties. In contrast, under high sediment availability, the cohesive properties of flocs become vital, emerging as a dominant factor governing the formation of lutoclines. Larger sediment concentration and cohesion sharpen the lutocline and lower its location in the wave bottom boundary layer. Particularly, when flocs exhibit high cohesion in conjunction with ample sediment availability, the lutocline essentially disappears, potentially inducing a laminarized wave bottom boundary layer. Furthermore, the implementation of depth-averaged settling velocity produces large discrepancies in modeling cohesive sediment transport in the wave bottom boundary layer.

The present study establishes a modeling framework to understand how flocculation influences the cohesive sediment transport in the bottom boundary layer. Future research in developing a modeling framework in nonequilibrium conditions is recommended. Additionally, measurements of temporal floc size distributions are needed for rigorous model validations.

## **Chapter 1**

### **INTRODUCTION**

#### **1.1 General**

Sediment transport in aquatic environments is an important earth surface process that shapes the landforms, affects water clarity, and delivers a variety of substances carried by sediment particles, to name a few. The transport of non-cohesive sediments, i.e., sand, mainly drives the morphological evolution (Sherwood et al., 2022). On the other hand, cohesive sediments exhibit a unique physical process called flocculation (e.g., Dyer, 1989; Mehta, 2013; Winterwerp and van Kesteren, 2004) that causes individual particles to stick together when two or more particles collide. Through flocculation, the transport of cohesive sediments in aquatic environments has a crucial impact on the ecosystem. Generally, when particulate concentrations in the water column are high, aquatic organisms face severe consequences due to the absence of photosynthesis, low levels of dissolved oxygen and depletion of energy sources (Jones et al., 2012; Vaz et al., 2019). Cohesive sediment transport also plays a critical role in shaping the morphology of estuaries and coastal areas (Edmonds and Slingerland, 2010) and controls the dynamics of estuarine turbidity maximum (ETM) (Burchard et al., 2018; Horemans et al., 2020). Similarly, floc formations are part of freshwater fluvial system processes when biological effect is active (Osborn et al., 2023).

Due to flocculation, the resulting flocs are formed as a porous mixture of minerals. This leads to two main consequences. Firstly, porous floc structures and pore water can encapsulate different substances (e.g., nutrients and organic matter).

Secondly, the porous floc structure also alters the settling velocity of cohesive sediment (Khelifa and Hill, 2006; Manning and Dyer, 1999). As results, cohesive sediments exert a fundamental control on the fate of nutrients and organic matter and, hence, alter the water quality (Asmala et al., 2022). Furthermore, low-density hydrophobic substances such as oil droplets can be deposited on the seafloor due to flocculation with suspended particulate matters and deteriorate benthic ecosystems (Daly et al., 2016; Ye et al., 2021).

Studying flocculation dynamics of cohesive sediment is an important and thriving research subject in aquatic science and engineering. In the following sections, flocculation dynamics, its effect on cohesive sediment transport, and their modeling are reviewed. Research gaps are then identified to motivate this study.

## **1.2 Flocculation**

Flocculation dynamics (or simply floc dynamics) is defined by two main processes that coexist simultaneously, aggregation, and fragmentation, also known as breakup (see Figure 1.1). Aggregation may take place when cations from dissolved salt in water create surface bridging around clay particles and decrease their repulsion force (Sutherland et al., 2015). Moreover, cohesion between particles can be significantly increased by bio-cohesion such as extra-cellular polymeric substance (EPS) (Malpezzi et al., 2013; Passow and Alldredge, 1995). For energetic aquatic systems, flow turbulence is considered as the dominant mechanism driving particle collision, which is quantified by the turbulent shear rate (Mhashhash et al., 2018; Spicer and Pratsinis, 1996). To study cohesive sediment transport in estuaries and continental shelves, turbulent shear rate is considered to be directly responsible for

floc formation and the growth of different floc sizes and their respective densities (porosity).

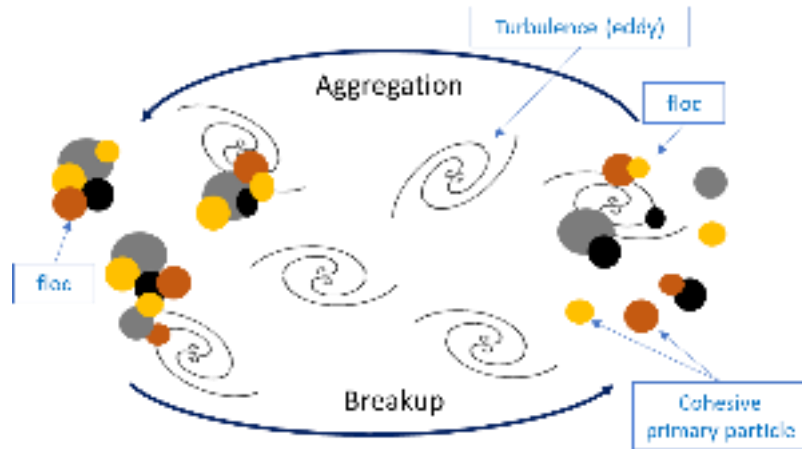


Figure 1.1 A schematic sketch of flocculation dynamics that include aggregation and breakup (fragmentation) driven by turbulence.

Simultaneous with the aggregation process, the flocs can experience a fragmentation process (breakup) that decreases their size due to turbulent shear in energetic environments. Flocs can maintain their complex structures up to a specific size because of the floc strength maintained by inter-particle bonds (Bache et al., 1999; Jarvis et al., 2005). Flocs become more fragile as their size increases, and they can be broken up when a shear or tensile stress overcomes the floc strength (Yeung and Pelton, 1996). Unfortunately, quantifying the floc strength is not trivial due to difficulties in direct measurement, and a variety of factors, such as mineral types, zeta-potential, floc structures, turbulence intensity must be quantified (Jarvis et al., 2005; Sharp et al., 2006). Thus, most of the numerical models use a constant value of the floc strength for simplicity (Maggi et al., 2007; Verney et al., 2011; Winterwerp, 1998). In this study

(Chapter 3), we investigate the limitation of the constant floc yield strength assumption and begin to explore an alternative with satisfactory results.

The single floc size statistics method (Winterwerp, 1998) is usually implemented to track the temporal evolution of the median floc size  $d_{50}$  (or a representative floc size). Although this method has been used in many studies (Kuprenas et al., 2018; Son and Hsu, 2009), it is not designed to represent the complex floc size distribution. On the other hand, the most high-fidelity method is to simulate flocculation using a grain-resolved approach since it tracks all the individual cohesive particles in a fully-resolved turbulence field (Vowinckel et al., 2019). This allows to compute the floc strength and the fractal dimension by analyzing the bonds between the primary particles and the floc size/shape. The challenge lies in its limitation to represent practical flocculation problems due to its high computational cost. The middle-ground approaches are to model the floc size distributions. The distribution-based model (Maerz and Wirtz, 2009) requires the assumption of a fixed distribution, which constrains the bimodal floc behaviors observed in aquatic systems (Lee et al., 2011; Manning and Dyer, 2007). This limitation can be overcome by solving Population Balance Equations (PBE) that calculate the number of flocs in each given size class while maintaining the mass balance (Mietta et al., 2011; Verney et al., 2011). Many studies focus on calibrating multiple model parameters in the PBE-based size-class flocculation model using the equilibrium or temporal evolution of median floc size  $d_{50}$  (Jeldres et al., 2015; Shen et al., 2018b; Zhang et al., 2019), or floc size distribution at the equilibrium state (Coufort et al., 2007). A systematic PBE model calibration was carried out by Mietta et al. (2011) using temporal evolution of the median floc size  $d_{50}$  and the equilibrium floc size distribution for a wide variety of compositions (clay type,

salt type and different salinity). Importantly, using the temporal evolution of  $d_{50}$ , Mietta et al. (2011) showed an inverse proportionality between the collisional efficiency and the  $\zeta$ -potential. However, it is unclear if other model parameters can be well-constrained by these limited physical characteristics. The present study will further address this important modeling issue in Chapter 3.

### **1.3 Cohesive sediment transport**

Flocculation plays a crucial role in determining the physical characteristics of cohesive sediment and their transport dynamics in aquatic environments. Particularly, the settling velocity, a key variable in the deposition process of sediment, experiences dynamic changes due to flocculation (see Figure 1.2). As a result, the settling velocity not only depends on grain size, as observed in non-cohesive sediments, but is also affected by turbulent flow statistics, sediment concentration and the resulting floc structure (Kranenburg, 1994). Several modeling frameworks aim to integrate the flocculation process with cohesive sediment transport commonly utilize the turbulence shear rate ( $S$ ) to represent the effect of turbulent flow intensity. One approach employs a one-dimension-vertical (1DV) concentration balance equation coupled with a single floc size statistic flocculation model, driven by idealized isotropic turbulence (Manning and Dyer, 2002). While computationally efficient, this method falls short of capturing variations in floc size classes in turbulent environments. A more sophisticated alternative involves implementing a floc size distribution flocculation model (Maerz et al., 2011; Maerz and Wirtz, 2009; Verney et al., 2011) coupled with sediment transport models. The 1DV concentration balance equation in Reynolds-averaged formulations have been suggested to track each floc size class with a turbulent closure for the turbulent shear rate  $S$  (Krishnappan and Marsalek, 2002; Xu et al., 2008). Subsequently,

efforts to enhance models by increasing dimensionality to 2D in Reynolds-averaged formulations (Shen et al., 2018a; Sherwood et al., 2018; Xu et al., 2010) for estuarine applications or 3D large-eddy simulation for upper ocean mixed layers (Liu et al., 2019) have been proposed. However, challenges persist in accurately representing transitional turbulent flows in the bottom boundary layers, especially for wave bottom boundary layer processes. Additionally, due to high computation costs, models often limit the number of floc size classes to around 15 for turbulence-averaged modeling in Sherwood et al. (2018) or 28 for 3D large-eddy simulation in Liu et al. (2019). These numbers are significantly lower than the recommended value of 75 by Penaloza-Giraldo et al. (2023) (see also Chapter 3), who carried out a comprehensive PBE model study for numerical convergence of floc size distribution and to match the measured coarse, medium, and fine floc fractions obtained in the laboratory experiments of Keyvani and Strom (2023).

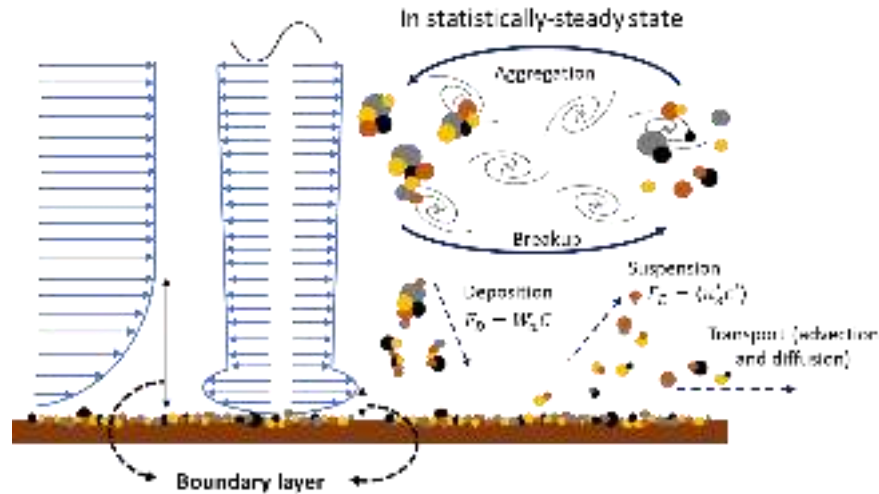


Figure 1.2. A schematic illustration of the interaction between the flocculation process and cohesive sediment transport in the bottom boundary layer.

A crucial aspect addressed in this dissertation is the investigation of cohesive sediment transport in the bottom boundary layer by explicitly considering the effect of flocculation (Chapter 4 and Chapter 5). In this region, current and waves interact with seafloor or riverbed, leading to erosion and the subsequent suspension of sediment into the water column (Grant and Madsen, 1986). However, given that the effects of the viscous sublayer and buffer layer are inherent in the boundary layer while wave boundary layers in most estuaries and continental shelves are only transitionally turbulent (Hara et al., 1983; Ozdemir et al., 2010), models relying on Reynolds-averaged formulations with an eddy viscosity can hardly be used due to the assumption of fully turbulent flow. Hence, turbulence-resolving models based on Direct Numerical Simulation (DNS) have emerged as valuable tools for studying fundamental sediment transport within the bottom boundary layer (e.g., Costamagna et al., 2003; Verzicco and Vittori, 1998). This approach has been applied to fine sediment transport with the assumption of constant settling velocity (ignoring flocculation dynamics) to study turbidity currents (Haddadian et al., 2021; Salinas et al., 2019a, 2019b), lutocline dynamics and density stratification (Ozdemir et al., 2010, 2011), erosion and deposition effects (Cheng et al., 2015), wave-current interaction (Nelson and Fringer, 2018), and wave-supported gravity flows (Yue et al., 2020). In particular, the formation of lutocline, a sharp negative sediment concentration in the wave bottom boundary layer, is known to play a critical role in determining the mode of cohesive sediment transport delivered by waves (Friedrichs and Wright, 2004; Traykovski et al., 2000), including well-mixed transport, two-layer-like transport with lutocline formation, and laminar-like condition, but their formation mechanism has been attributed to sediment-induced density stratification (Ozdemir et al., 2010a), hindered settling (Ross and Mehta,

1989), or even consolidation. Yet, the effect of flocculation in modifying the settling velocity has routinely been ignored. Indeed, the aforementioned modeling studies completely ignore flocculation dynamic and prescribe a constant settling velocity. It is unclear if the dynamic coupling between boundary layer flows, flocculation, variability of settling velocity, and sediment transport play an important role in altering our understanding of cohesive sediment transport in bottom boundary layers. This dissertation reports an effort to advance our understanding of this complex system in Chapter 5.

#### **1.4 Research questions**

This dissertation has the main purpose of understanding the inter-relationship between flocculation dynamics and cohesive sediment transport and their modeling. To fill the research gaps identified in the previous sections, this study will answer the following Research Questions:

1. What is the best practice to calibrate multiple model parameters in the population balance equation flocculation model?
2. Can a comprehensive model validation of flocculation with measured data reveal missing physics in the existing flocculation modeling?
3. What is the importance of flocculation dynamics in determining the settling velocity variability and sediment concentration distribution in the current bottom boundary layer?
4. What role does the flocculation process play in affecting the vertical structure of sediment concentration (e.g., the formation of lutocline) and transport modes in the wave bottom boundary layer?

## **1.5 Scope of this study**

This dissertation is dedicated to understanding the complexities of flocculation and its impact on cohesive sediment transport within the bottom boundary layer. A novel modeling framework is developed and presented in Chapter 2, outlining the implemented governing equations and different modules in the framework. Chapter 3 delves into a comprehensive exploration of the key parameters within the Population Balance Equation (PBE) flocculation model by comparing simulation results with a comprehensive experimental dataset to investigate Research Questions 1 and 2. The applications of the modeling framework to both current and wave bottom boundary layers are presented in Chapters 4 and 5 for investigating Research Questions 3 and 4, respectively. Finally, Chapter 6 summarizes the main findings, explicitly stating the contributions of this work, and outlining potential directions for future research.

## **Chapter 2**

### **METHODOLOGY**

Most existing cohesive sediment transport models for wave-current bottom boundary layers assume a constant sediment settling velocity by neglecting flocculation dynamics. Through flocculation, floc size and floc density are changed and so is the settling velocity. Locally, the settling velocity is a function of mineral characteristics (parameterized by for example, stickiness and floc yield strength), sediment concentration, and turbulent shear rate (or turbulent dissipation rate). In other words, the settling velocity in a wave-current bottom boundary layer is a variable while the sediment transport process is further controlled by the variability of settling velocity and turbulence. When sediment concentration is sufficiently large, sediment concentration distribution further modulates turbulence. Overall, flocculation, sediment transport, and turbulence in the bottom boundary layer constitute a coupled dynamic system. To begin to tackle this complex problem, we develop a weakly coupled cohesive sediment transport modeling framework for the bottom boundary layer. Section 2.1 discusses model assumptions and each component of the model framework. Section 2.2 is devoted to the model description of the PBE flocculation model adopted in this study. Section 2.3 introduces a Direct Numerical Simulation (DNS) model which produces the simulation data of bottom boundary layer and provides various turbulence statistics to be used by the present study.

To make a clear presentation of the mathematical model and assumptions, the model formulation is first presented for statistically-steady turbulent bottom boundary

layers in this Chapter. Later in Chapter 5, the model framework is extended for wave bottom boundary layer and additional averaging operation and model assumption will be discussed.

## 2.1 Modeling Framework

The model framework is driven by a turbulent shear rate profile (represented by  $S$ ) in a statistically steady (current). This approach combines flocculation modeling to determine the settling velocity of flocs followed by sediment transport calculations in dilute conditions. The turbulent shear rate is defined as

$$S = \sqrt{\frac{\varepsilon}{\nu}}, \quad (2.1)$$

where  $\varepsilon$  is the turbulence dissipation rate and  $\nu$  is the fluid viscosity. The model framework consists of the following solution procedures, as illustrated in the flowchart shown in Figure 2.1. The first step (Step I) is to provide a statistically (turbulence-) averaged shear rate  $S$  and sediment concentration  $C$  profiles in a bottom boundary layer by assuming a constant settling velocity  $w_s$ . Here, we define the coordinate  $x_3$  having its origin at the bottom and pointing vertically upward. These profiles are the input variables to the model framework, or they can be considered as the initial condition without considering flocculation dynamics. The PBE flocculation model is driven by these input profiles (Step II) to distribute sediment mass into different floc size classes at every vertical location (grid location) until each floc size class reaches the equilibrium state. The distributed floc properties from the flocculation model are used to calculate the weighted average settling velocity of the cohesive sediment  $W_a$  (see Step III in Figure 2.1). This new settling velocity, which includes the physics of flocculation, is

used to update the sediment concentration profile in the boundary layer via an iterative procedure (Step IV).

In a statistically-steady bottom boundary layer, turbulence-averaged sediment concentration  $C(x_3)$  must follow the (Reynolds-averaged) mass balance equation expressed as

$$K_s \frac{dC}{dx_3} + W_a C - \langle u'_3 c' \rangle = 0, \quad (2.2)$$

where  $K_s$  is the sediment diffusivity, and the bracket “ $\langle \rangle$ ” is the turbulence-averaging operator. The turbulent flux of sediment  $\langle u'_3 c' \rangle$  requires a closure model and we adopt the gradient transport model written as

$$-\langle u'_3 c' \rangle = K_t \frac{\partial C}{\partial x_3}. \quad (2.3)$$

where  $K_t$  is the turbulent diffusivity of the sediment. Substituting this approximation into the equation (2.2) leads to

$$\frac{dC}{dx_3} = - \frac{W_a C}{K_t + K_s}. \quad (2.4)$$

In a typical Reynolds-averaged models,  $K_t$  is estimated via the turbulent Schmidt number  $Sc_t$  and eddy viscosity  $\nu_t$  as  $K_t = \nu_t / Sc_t$ . In this study, we obtain eddy viscosity, turbulent sediment flux, and turbulent shear rate  $S$  from DNS data (see Section 2.3), which resolves all turbulent scales, and  $K_t$  is directly calculated via Equation (2.3). The relationship between eddy viscosity and turbulent diffusivity is also examined.

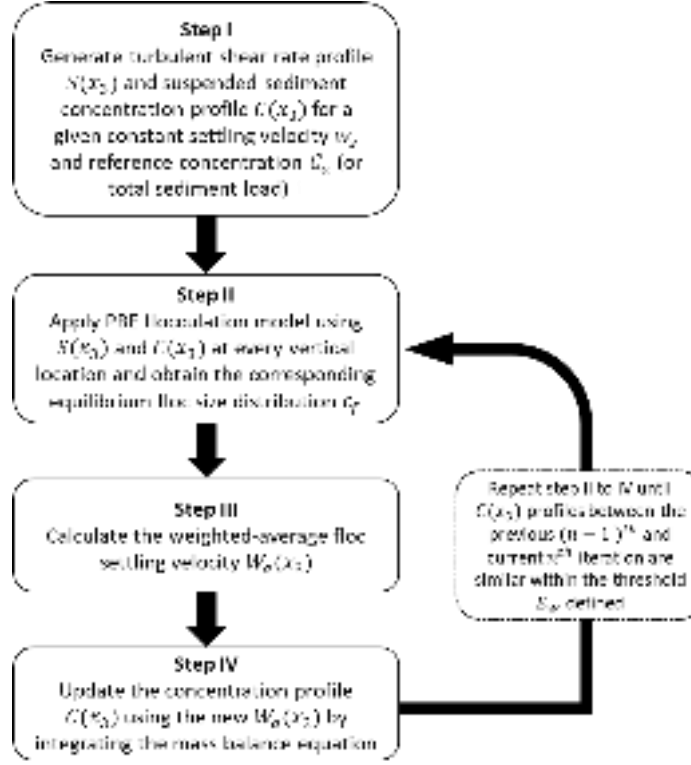


Figure 2.1 Flowchart for the cohesive sediment modeling framework with the flocculation dynamics.

## 2.2 Population Balance Equation (PBE) Flocculation model

### 2.2.1 Governing equations

The open-source PBE flocculation model FLOCMOD (Verney et al., 2011) is utilized in the present modeling framework to compute the floc size distribution due to the flocculation processes (see Step II in Figure 1). The PBEs describe the temporal evolution of the number concentration for each floc size class driven by a given local shear rate  $S$  and sediment mass concentration  $C$ , and they are written as

$$\frac{dn_f(k)}{dt} = G_{ag}(k) + G_{bs}(k) - L_{ag}(k) - L_{bs}(k), \quad (2.5)$$

where  $n_f(k)$  (units in  $m^{-3}$ ) is the floc number concentration for floc size class  $k$ . The terms  $G$  and  $L$  represent the gain and loss due to aggregation (subscript  $ag$ ) and breakup processes (subscript  $bs$ ) respectively. Since turbulent shear is the primary force driving flocculation in estuarine and coastal environments, other flocculation mechanisms such as Brownian motion and differential settling are neglected (Verney et al., 2011).

The gain  $G_{ag}$  and loss  $L_{ag}$  terms due to the aggregation can be defined as follows.

$$G_{ag}(k) = \frac{1}{2} \sum_{i+j=k} \alpha A(i, j) n_i n_j , \quad (2.6)$$

$$L_{ag}(k) = \sum_{i=1}^{N_f} \alpha A(i, k) n_i n_k , \quad (2.7)$$

where  $N_f$  is the total number of floc size classes, and  $\alpha$  is the collision efficiency, which parameterizes the sticking properties of the flocs. In this study, we assume that  $\alpha$  is a constant following Verney et al. (2011). In the following chapters, we calibrate its value with measured data and understand its effect in flocculation process. The floc collision is described by the collision probability function  $A$  for two colliding spherical particles driven by turbulent shear rate  $S$ , and it is written as

$$A(i, j) = \frac{1}{6} S (d_{f,i} + d_{f,j})^3 , \quad (2.8)$$

where  $d_f$  is the floc diameter for the  $i^{th}$  and  $j^{th}$  size class (McAnally and Mehta, 2000). The gain  $G_{bs}$  and loss  $L_{bs}$  due to turbulence are expressed as

$$G_{bs}(k) = \sum_{i=k+1} FDBS_{ki} B_i n_i , \quad (2.9)$$

$$L_{bs}(k) = B_k n_k , \quad (2.10)$$

where  $FDBS_{ki}$  refers to the distribution function of fragmented flocs, representing the process by which daughter flocs in the  $k$  size class are generated from larger  $i$  floc size classes. Following Verney et al. (2011), we specify a binary distribution, meaning that each breakup event divides a floc into two equal halves. The function  $B$  describes the rate of breakage of the flocs break due to the turbulent shear rate  $S$ , and it is written as

$$B_i(k) = \beta S^{3/2} d_{f,i} \left( \frac{d_{f,i} - d_p}{d_p} \right)^{3-f_d}, \quad (2.11)$$

where  $d_p$  is the primary particle diameter, and  $f_d$  is the fractal dimension for equivalent spheres (Kranenburg, 1994). The fragmentation rate  $\beta$  is dimensional (unit:  $s^{1/2} m^{-1}$ ) and it is defined as

$$\beta = E \left( \frac{\mu}{F_y} \right)^{1/2}, \quad (2.12)$$

where  $\mu$  (Pa·s) is the dynamic viscosity of water,  $E$  is an empirical (dimensionless) parameter and  $F_y$  (N) is the floc yield strength. Although  $\beta$  is a dimensional quantity, it is assumed to be an empirical constant in Verney et al. (2011). This inevitably presumes that the floc yield strength  $F_y$  is a constant, which is consistent with the fractal approach (Kranenburg, 1994). Because the direct measurement of floc yield strength is difficult, the assumption of a constant  $F_y$  is commonly adopted by many other studies (e.g., Maggi et al., 2007; Wang et al., 2013). In this study, the fragmentation rate  $\beta$  is treated as an empirical constant to be calibrated with measured data along with the collisional efficiency  $\alpha$ . However, in the second part of Chapter 3, we investigate the effect of a variable floc yield strength by specifying  $\beta$  as a variable.

### 2.2.2 Physical floc properties models

The fractal approach is adopted to model complex floc structures using a fractal dimension  $f_d$ . The floc density  $\rho_f$  of the  $k^{th}$  floc size class is calculated by the corresponding floc diameter  $d_f$  as (Kranenburg, 1994)

$$\rho_f(k) = \rho_w + (\rho_p - \rho_w) \left( \frac{d_p}{d_f(k)} \right)^{3-f_d}, \quad (2.13)$$

where  $\rho_p$  is the primary particle density. Following the same self-similarity concept, the sediment mass contained in each floc in size class  $k$  can be expressed as

$$m_f(k) = \rho_p \frac{\pi}{6} d_p^3 \left( \frac{d_f(k)}{d_p} \right)^{f_d}. \quad (2.14)$$

The floc settling velocity for each size class  $k$  is calculated by the Stokes' law using the corresponding flow density and diameter as

$$w_f(k) = \frac{(\rho_f(k) - \rho_w) g d_f^2(k)}{18\mu}. \quad (2.15)$$

By substituting Equation (2.13) into Equation (2.15), we obtain an explicit relationship between floc settling velocity and floc diameter for size class  $k$  as

$$w_f(k) = \frac{(\rho_p - \rho_w) g d_p^{3-f_d}}{18\mu} d_f^{f_d-1}(k). \quad (2.16)$$

It can be seen that for non-cohesive particle with  $f_d = 3$  and equation (2.16) recovers back to the well-known Stokes law without flocculation which shows that the settling velocity scales with the particle diameter quadratically. For flocs with  $f_d < 3$ , the dependency of settling velocity with respect to floc size is weaker than that of non-cohesive particles.

The resulting distributed floc properties from the PBE flocculation model applied at each vertical location  $x_3$  are used to calculate the weighted average quantities (see Step III in Figure 1), written as

$$\vartheta_a(x_3) = \sum_{k=1}^{N_f} \left( \frac{c_f(k)}{C(x_3)} \right) \vartheta_f(k), \quad (2.17)$$

where  $\vartheta_f$  is an arbitrary distributed floc property (such as  $d_f$ ,  $w_f$  or  $\rho_f$ ) and  $\vartheta_a$  is the corresponding weighted average quantity,  $c_f(k)$  is the mass concentration in floc size  $k$ , which is defined as  $c_f(k) = m_f(k) n_f(k)$ .

### 2.2.3 Population balance equation (PBE) at the equilibrium stage

A preliminary analysis is carried out to gain insight into the strategies to be used to effectively calibrate multiple model parameters in the flocculation model. By using the full PBE equations (2.5) and closures discussed previously, we obtain the governing equations by substituting the previous definitions from the equation (2.6) to (2.10) into the equation (2.5). The resulting expression can be written as follows.

$$\begin{aligned} \frac{dn_k}{dt} = & \frac{1}{2} \sum_{i+j=k} \alpha \frac{1}{6} S(d_i + d_j)^3 n_i n_j + \sum_{i=k+1} FDBS_{ki} \beta S^{3/2} d_i \left( \frac{d_i - d_p}{d_p} \right)^{3-f_d} n_i \\ & - \sum_{i=1}^N \alpha \frac{1}{6} S(d_i + d_j)^3 n_i n_k - \beta S^{\frac{3}{2}} d_k \left( \frac{d_k - d_p}{d_p} \right)^{3-f_d} n_k. \end{aligned} \quad (2.18)$$

During the initial stage of the flocculation (i.e. floc growth stage), the breakup terms can be neglected (second and fourth terms in equation 2.18) since the aggregation domains. This means that the calibration process should be carried out for  $\alpha$  essentially. However, once the flocculation is reaching equilibrium, the breakup terms become important as well because there must be a balance between these two processes. This agrees with the analysis presented in Winterwerp (1998) that mean equilibrium floc size

must depend on the ratio of  $r = \alpha/\beta$  and  $f_d$ . Therefore, both equilibrium stage and transient stage should be considered for a complete calibration procedure. In fact, this is consistent with the study of Mietta et al. (2011)

Further analysis can be found at the equilibrium stage ( $dn_k/dt = 0$ ) for the equation (2.18). Updating the previous equations, we obtain

$$n_k = \frac{\left[ \frac{1}{12} \frac{r}{S^{1/2}} \sum_{i+j=k} (d_i + d_j)^3 n_i n_j + \sum_{i=k+1} FDBS_{ki} d_i \left( \frac{d_i - d_p}{d_p} \right)^{3-f_d} n_i \right]}{\left[ \frac{1}{6} \frac{r}{S^{1/2}} \sum_{i=1}^N (d_i + d_j)^3 n_i + d_k \left( \frac{d_k - d_p}{d_p} \right)^{3-f_d} \right]}. \quad (2.19)$$

We notice that the parameters  $\alpha$ ,  $\beta$  and  $f_d$  are not unique parameters. The breakup distributions functions  $FDBS_{ki}$  is a complicated parameter, which must be considered since the flocculation model is based on the floc size classes. Nevertheless, focusing on very large floc fractions such as  $d_{84}$  (e.g. macrofloc), the gain due to breakup ( $G_{bs}$ ) and aggregation loss term ( $L_{ag}$ ) must be insignificant compared with the others. Hence, the above equations for large floc fractions reduces to

$$n_k = \frac{\left[ \frac{1}{12} \frac{r}{S^{1/2}} \sum_{i+j=k} (d_i + d_j)^3 n_i n_j \right]}{\left[ d_k \left( \frac{d_k - d_p}{d_p} \right)^{3-f_d} \right]}, \quad (2.20)$$

where the parameter  $FDBS_{ki}$  disappears allowing to focus the calibration process on the parameters  $\alpha$ ,  $\beta$  and  $f_d$ . On the other hand, the breakup distribution function  $FDBS_{ki}$  must be important for fine floc fraction such as  $d_{16}$ . Based on this analysis, we consider that calibrating different size class statistics is valuable, particularly on coarse floc fraction to avoid uncertainty in  $FDBS_{ki}$ .

### 2.3 Turbulence-resolving numerical model

The cohesive sediment transport model framework requires the input of turbulent shear rate shown in equation (2.1) and hence the turbulent dissipation rate  $\varepsilon$ . It is difficult to estimate turbulent dissipation rate directly from measured data as it requires the calculation of very high-resolution spatial gradient of turbulent velocity fluctuations. A key reason that we utilize DNS for the present flocculation and cohesive sediment transport study is because of its high-resolution temporal and spatial data that allows us to calculate turbulent dissipation rate accurately. However, we must emphasize that for the general use of the modeling framework presented in Chapter 2.1, other estimations of turbulent dissipation rate profile via semi-empirical theory combined with measured data, or a two-equation Reynolds-average closure, are applicable.

The open-source code TURBID reported by Yue et al. (2020) is implemented to generate the input turbulent shear rate  $S$  and sediment concentration  $C$  profiles for the model framework (see Step I in Figure 1), assuming a constant sediment settling velocity (no flocculation). This turbulence-resolving numerical model resolves all scales of turbulence and hence various turbulence statistics can be accurately calculated, such as the turbulent dissipation rate  $\varepsilon$  needed for flocculation modeling (see Equation (2.1)). Yue et al. (2020) simulated fine sediment transport in a computational domain defined as a rectangular prism with dimensions  $L_1 \times L_2 \times L_3$ , where the coordinate origin is located at the front of the bottom-left corner, pointing in the streamwise  $x_1$ , spanwise  $x_2$  and vertical  $x_3$  directions (see Figure 2.2). Periodic boundary conditions are implemented for 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 of the computational domain, respectively. The resulting current or

wave, driven by a prescribed streamwise constant or temporal-oscillatory pressure gradient, exerts a shear stress on the erodible cohesive sediment bed and suspends sediment into the computational domain if the bottom shear stress surpasses the critical shear stress, following the Partheniades-Ariathurai-type expression (Sanford and Maa, 2001). The sediment phase velocity is approximated by the flow velocity field, following the equilibrium Eulerian approximation (Balachandar and Eaton, 2009). Thus, the velocity field of sediment phase  $v_i$  is calculated from the velocity field of carrier flow (water)  $u_i$  and the constant particle settling velocity  $w_s$  as

$$v_i = u_i - w_s \delta_{i3} , \quad (2.21)$$

where the subscript  $i = 1, 2, 3$  corresponds to the streamwise  $x_1$ , spanwise  $x_2$  and vertical  $x_3$  directions, respectively. Again, the settling velocity  $w_s$  in the DNS is considered as constant to obtain the initial  $S$  and  $C$  profiles for the cohesive sediment transport model framework. Subsequently, the model framework updates the settling velocity as a variable via Equation (2.16) and (2.17) (see steps III and IV in Figure 2.1). Next, a more detailed discussion on the model formulation is given.

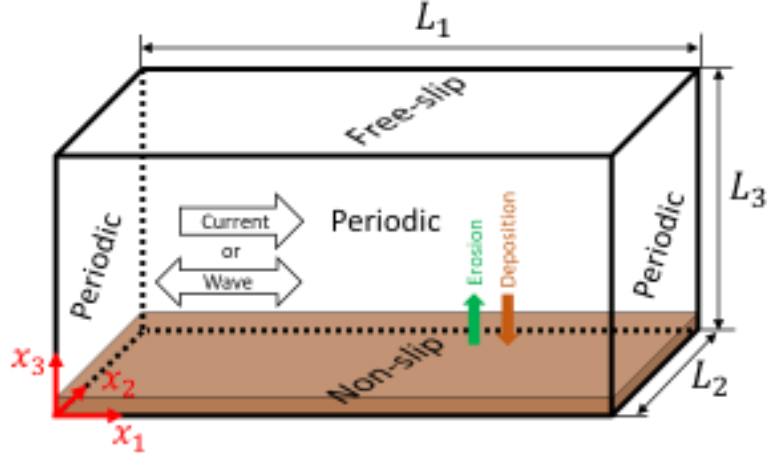


Figure 2.2. A sketch of the DNS computational domain and its boundary conditions

### 2.3.1 Fluid phase

The fluid mass and momentum equations are written as:

$$\frac{\partial u_i}{\partial x_i} = 0 , \quad (2.22)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_w} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + Rg\phi\delta_{i3} + S_i\delta_{i1} , \quad (2.23)$$

where  $\nu$  is the kinematic viscosity of the water,  $\rho_w$  is the water density,  $g$  is the gravitational acceleration,  $\phi$  denotes the volumetric concentration of sediment,  $p$  is the fluid pressure, and  $R = (\rho_p/\rho_w - 1) = 1.65$  is the submerged specific gravity of sediment where  $\rho_p$  is the primary sediment density. The third term on the right-hand side in the equation (2.23) is the buoyancy term, which models the coupling effects between fine sediment and carrier fluid flow. The last term  $S_i\delta_{i1}$  is the streamwise flow driving force that results from applying either constant or time-oscillatory pressure gradient. The time-oscillatory pressure gradient (i.e., to generate waves) is defined as

$$S_i = U_w \Omega_w \cos(\varphi) , \quad (2.24)$$

where  $U_w$  is the amplitude of free-stream velocity,  $\Omega_w = 2\pi/T_w$  is the wave angular frequency with a period  $T_w$ , and  $\varphi = \Omega_w t$  is the wave phase.

Periodic boundary conditions are used in the streamwise and spanwise directions to solve the equations (2.22) and (2.23). Moreover, the implementation of the free-slip, rigid-lid boundary condition ensures a shear-free top boundary, and it is expressed as

$$\frac{\partial u_1}{\partial x_3} = 0, \quad \frac{\partial u_2}{\partial x_3} = 0, \quad u_3 = 0 \quad \text{at } x_3 = L_3. \quad (2.25)$$

As for the bottom of the computational domain, the no-slip boundary condition is imposed, and it can be read as

$$u_i = 0 \quad \text{at } x_3 = 0. \quad (2.26)$$

### 2.3.2 Sediment Phase

Since the equilibrium Eulerian approximation is applied, sediment volumetric concentration is solved by the law of mass conservation, and it is given by

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\phi v_j)}{\partial x_j} = K_s \frac{\partial^2 \phi}{\partial x_j \partial x_j} , \quad (2.27)$$

Sediment diffusivity  $K_s$  is similar to fluid viscosity  $\nu$ . The choice of sediment diffusivity is mainly for numerical stability and sub-grid diffusion effect (Ozdemir et al., 2010). For flow driven by a steady current, the sediment diffusivity  $K_s$  is set to be equal to fluid viscosity  $\nu$  following previous works (Ozdemir and Yu, 2018; Salinas et al., 2019b). For oscillatory flow, we set  $K_s = 2\nu$ , also follows previous studies (Cheng et al., 2015; Ozdemir et al., 2010; Ozdemir et al., 2011; Yue et al., 2020). The sediment phase velocity  $v_j$  is calculated according to equation (2.21).

To solve the equation (2.27), periodic boundary conditions are implemented as well in  $x_1$ - and  $x_2$ - directions. For the vertical direction, the zero net transport boundary condition is implemented at the top boundary, written as

$$\phi w_s \delta_{i3} - K_s \frac{\partial \phi}{\partial x_3} = 0 \text{ at } x_3 = L_3 \quad (2.28)$$

To model the exchange of sediment with the bed, the erodible/depositional boundary condition is specified at the bottom boundary, written as

$$\phi w_s \delta_{i3} - K_s \frac{\partial \phi}{\partial x_3} = q_e + q_d \text{ at } x_3 = 0, \quad (2.29)$$

where  $q_e$  and  $q_d$  are the sediment erosional and depositional fluxes, respectively. The depositional flux is modeled as  $q_d = \phi w_s \delta_{i3}$  following Sanford (2008) formulation. Regarding the erosional flux  $q_e$ , the Partheniades-Ariathurai-type expression (Sanford and Maa, 2001) is implemented as follows:

$$q_e = \begin{cases} m_e (|\tau_b|/\tau_c - 1) & \text{for } |\tau_b| \geq \tau_c \\ 0 & \text{for } |\tau_b| < \tau_c \end{cases}, \quad (2.30)$$

where  $m_e$  is an empirical erosion rate,  $\tau_c$  is the critical bottom shear rate,  $\tau_b$  is the bottom shear stress calculated in the present DNS model using the resolved velocity gradient at the bed as  $\tau_b = \rho \nu (\partial u_1 / \partial x_3)|_{x_3=0}$ . In the present simulation, the grid size near the bottom is less than 0.05 wall unit and the velocity gradient is well resolved.

### 2.3.3 Numerical Implementation

The governing equations are solved by a 3D pseudo-spectral scheme (Canuto, 1988) which is widely used in resolving turbulence and the full energy cascade process down to the Kolmogorov scales (Ozdemir et al., 2010; Salinas et al., 2019b, 2019a). The time-integration is solved by a third-order low-storage Runge-Kutta scheme

(Williamson, 1980). The numerical instabilities are controlled by Courant-Friedrichs-Lewy (CFL) criteria which limits the time step by specifying  $CFL=0.5$ . In streamwise and spanwise direction, the discretization is uniform and this 2D plane is approximated with the discrete Fourier transform (DFT) applying the periodic boundary conditions. On the other hand, the grid in vertical direction uses the Chebyshev-Gauss-Lobatto distribution having high resolution near the no-slip boundary. The advection terms in the equation (2.22) and (2.27) are discretized by Arakawa scheme, and the 3/2 rule is applied to remove the aliasing errors. The diffusion terms are approximated by the semi-implicit second-order Crank-Nicolson method. More details about the numerical solver can be found in Yue et al., (2019).

### **Chapter 3**

#### **THE IMPORTANCE OF TEMPORAL FLOC SIZE STATISTICS AND YIELD STRENGTH FOR POPULATION BALANCE EQUATION FLOCCULATION MODEL**

To investigate Research Question 1 and 2, the main goal of the study reported in this Chapter is to advance the understanding of several key model parameters of the PBE flocculation model and how they determine the resulting temporal evolution of floc size statistics driven by a constant turbulent shear rate. Motivated by the earlier studies on PBE modeling (Mietta et al., 2011; Verney et al., 2011) and floc yield strength (e.g., Jarvis et al., 2005), the specific objectives are to (1) confirm whether the median floc size statistics  $d_{50}$ , in terms of both the equilibrium floc size and the initial floc growth, is sufficient to constrain the model parameters, (2) investigate if the model parameters can be better constrained by using the temporal evolution of different floc size statistics, and (3) understand the importance of floc yield strength in the predicted floc size statistics. This Chapter is organized as follows. Section 3.1 introduces a laboratory dataset of flocculation reported by Keyvani and Strom (2014) to be used for model calibration, followed by a description of the PBE model setup. Section 3.2 focuses on extensive model investigations and error analyses for predicting the measured data. Section 3.3 is dedicated to investigating the floc yield strength in the flocculation model and Section 3.4 concludes this study. Major content reported in this Chapter has been published in Penaloza-Giraldo et al. (J A Penaloza-Giraldo et al., 2023).

### 3.1 Flocculation Model Configuration

#### 3.1.1 Experimental data

Keyvani and Strom (2014) report a flocculation experiment in a mixing tank using a mixture of kaolinite and montmorillonite clay. The flocculation experiment was performed for approximately 1800 *min* by using a total sediment mass concentration of  $C = 0.05 \text{ kg/m}^3$  and a turbulent shear rate  $S$  of  $35 \text{ s}^{-1}$ . In addition to the measured median floc diameter  $d_{50}$  at equilibrium, Keyvani and Strom (2014) also provide measured temporal evolutions of three different floc size statistics,  $d_{16}$ ,  $d_{50}$  and  $d_{84}$  (see Figure 3.1). This comprehensive dataset is selected to calibrate key empirical model parameters in the PBE-based size-class flocculation model of Verney et al. (2011). We simulate three important aspects in the measured time series, the equilibrium state ( $t \geq 700 \text{ min}$  in Figure 3.1), the initial floc growth stage ( $t \leq 200 \text{ min}$  in Figure 1), and the entire time series. In particular, matching the modeled initial floc growth stage with measured data allows us to evaluate the model's ability to predict the flocculation rate, which has been used by other studies to further quantify the stickiness of flocs (Ye et al., 2021). The abundance of measured data allows a deeper calibration of the model parameters.

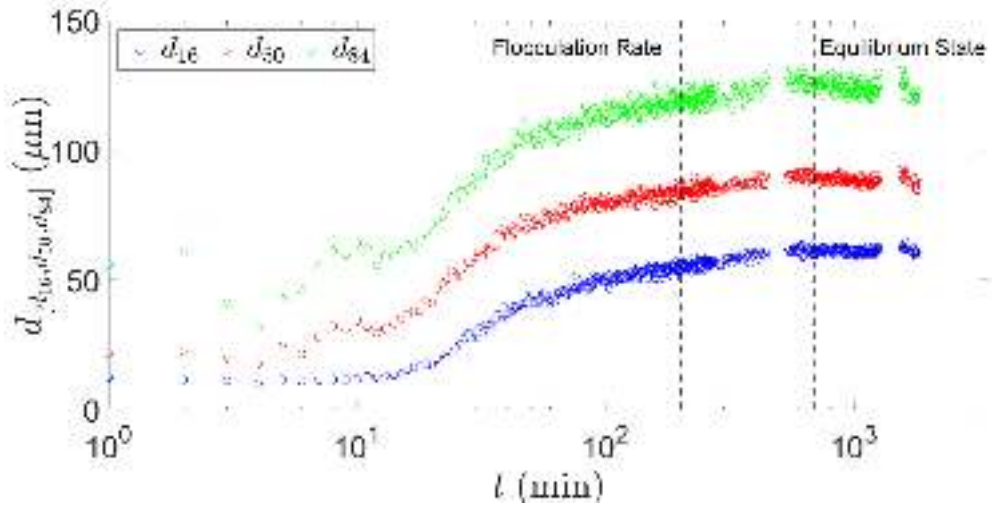


Figure 3.1. Measured data reported by Keyvani and Strom (2014) for the temporal evolution of three floc size statistics ( $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ). The analysis presented here further divides the time series into the initial floc growth stage (initial flocculation rate,  $t \leq 200$  min) and the equilibrium state ( $t \geq 700$  min in Figure 3.1).

### 3.1.2 Flocculation model setup

Following Keyvani and Strom (2014), the total mass concentration and turbulent shear rate from the experiment are prescribed accordingly in the flocculation model. The minimum floc size diameter is established as  $d_{\min} = 4 \mu m$ , which corresponds to the diameter of the primary particle typically used for flocculation modeling (Winterwerp, 1998). The maximum floc size is specified to be  $d_{\max} = 300 \mu m$  to ensure the modeled distribution is sufficiently wide and to avoid unrealistic fluctuations in the distributed mass concentration near and at the equilibrium state (see Figure 3.2). Since Keyvani and Strom (2014) do not discuss the initial floc size distribution, our exploratory numerical experiments show that using a log-normal distribution represents the experimental data better than punctual distribution especially at the early stage of floc growth (see Figure 3.3).

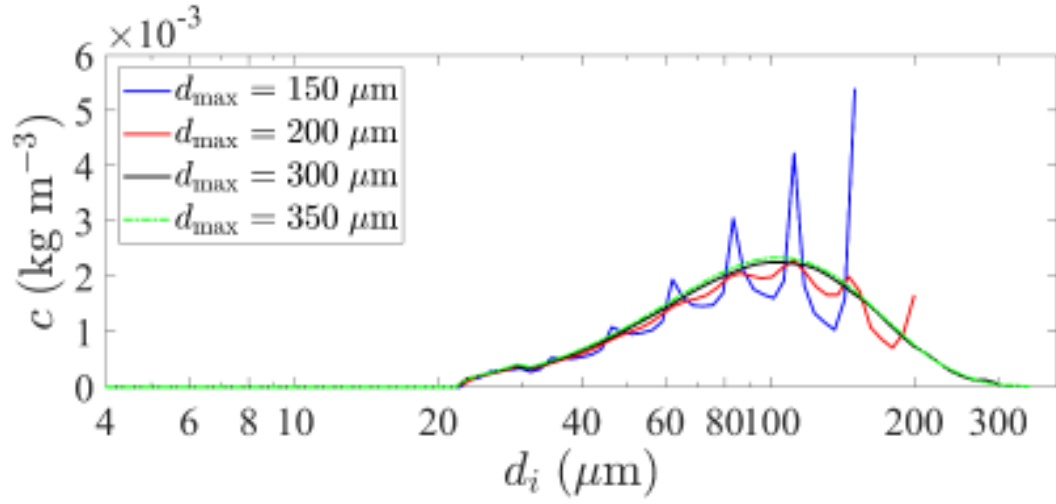


Figure 3.2. Equilibrium mass concentration distribution as a function of floc size for simulations using different maximum floc diameter  $d_{\max}$ .

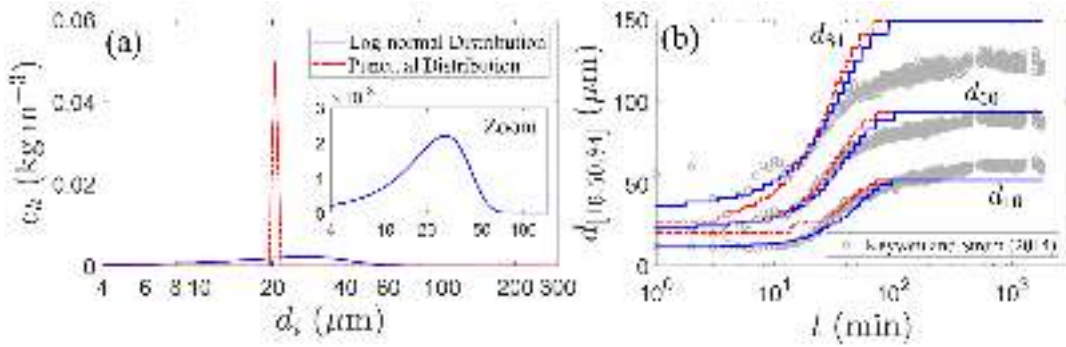


Figure 3.3. Sensitivity analysis on the prescribed initial mass concentration distribution as a function of floc size for (a) the Log-normal distribution vs the Punctual distribution, and (b) the resulting temporal evolution of floc size statistics.

The flocculation model of Verney et al. (2011) requires the use of many classes to discretize the floc diameter distribution. Therefore, establishing the minimum number needed for an accurate numerical solution of the size distribution is an important step. The evaluation is carried out with different numbers of size class  $N_c$  to discretize the distribution. Verney et al. (2011) recommended  $N_c = 15$  to be sufficient based on calibrating the median floc size  $d_{50}$  at the equilibrium state. However, our results suggest that even at  $N_c = 25$ , the low resolution negatively affects the predicted temporal evolution and, hence, the flocculation rate (see the first 80 minutes of floc growth in Figure 3.4a) for fine, median, and coarse fractions. Another issue is the pronounced step-like feature during the floc growth when  $N_c$  is small. Careful examination of the model results indicates that the step-like feature is due to coarse numerical discretization of the floc size distribution, but not the time step, (the absence of certain size classes causes a jump in modeled size statistics during floc growth). A converged solution can be obtained when  $N_c \geq 75$ . In Figure 3.4b, we evaluate this convergence by using the Root-Mean-Square-Error  $RMSEc$  from the target solution using  $N_c = 200$ . Large errors are observed when  $N_c = 15$  especially for the coarse fraction ( $RMSEc_{d_{84}} > 40 \mu m$ ). By increasing the  $N_c$  to 25 and 50, the errors decrease significantly. In this study, we use  $N_c = 75$  to maintain an affordable computational time (around 20 minutes per simulation in workstation) with  $RMSEc_{d_{[16,50,84]}} \leq 0.5 \sim 3 \mu m$ .

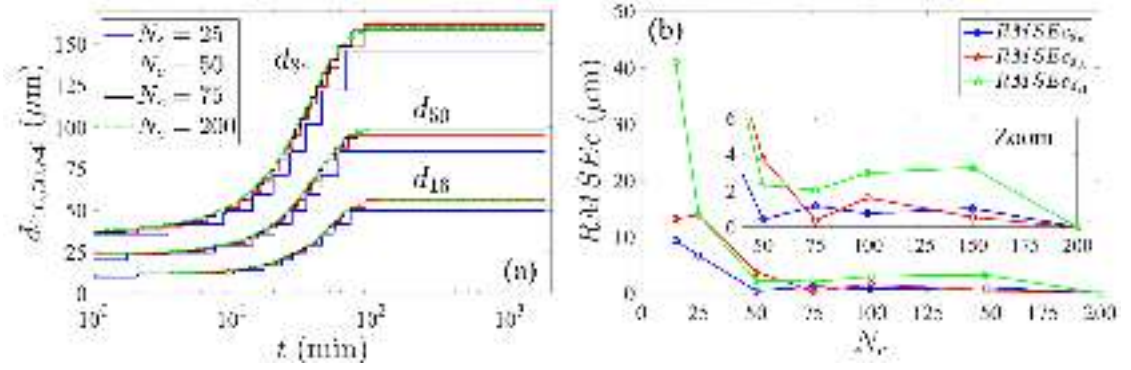


Figure 3.4 Convergence analysis for different  $N_c$ . (a) Temporal evolution of floc size statistics  $d_{[16,50,84]}$  with different number of classes  $N_c$ . (b) Root-Mean-Square-Error  $RMSEc$  for different  $N_c$ .

### 3.2 Results

Motivated by the previous study of Verney et al. (2011), we concurrently calibrate  $\alpha$  and  $\beta$  to match measured data and evaluate if the resulting fractal dimension  $f_d$  falls within the expected range. 6,400 simulations were carried out using  $\alpha = 5 \times 10^{-2} \sim 80 \times 10^{-2}$  with an interval of  $5 \times 10^{-2}$ , and  $\beta = 2 \times 10^{-3} \sim 80 \times 10^{-3}$  with an interval of  $2 \times 10^{-3}$  for ten different fractal dimension values in the range of 1.7 to 2.9. All simulations use a computational time of 1800 min, and an explicit integrator is implemented to solve the PBEs (Equation 2.5) with an initial time step equal to 1 s. If this value is insufficient to preserve the mass concentration within a threshold, the time step is decreased until the criterion is satisfied. Using the measured data (Keyvani and Strom, 2014), three different RMSE are computed to evaluate the model performance at the equilibrium state  $RMSE_{eq}$  ( $t \geq 700 \text{ min}$ ), the growth stage of flocculation  $RMSE_{fr}$  ( $t \leq 200 \text{ min}$ ), and the entire flocculation time series  $RMSE_{fp}$  for the tri-temporal floc size statistics  $d_{16}$ ,  $d_{50}$  and  $d_{84}$  (see Figures S3~S5 in the Supplemental Material). In Section 3.2.1 and 3.2.2, the search for the optimized

parameters  $\alpha$ ,  $\beta$  and  $f_d$  is carried out exclusively to match measured  $d_{50}$  by these three criteria, namely, minimizing the errors at the equilibrium state  $\min(RMSEeq_{d_{50}})$ , at the initial growth stage of flocculation  $\min(RMSEfr_{d_{50}})$ , and for the entire time series  $\min(RMSEfp_{d_{50}})$ . In Section 3.2.3, two more criteria are imposed (objective functions) by matching measured fine and coarse fractions, i.e.,  $\min(RMSEfp_{d_{16}})$  and  $\min(RMSEfp_{d_{84}})$ .

### 3.2.1 Temporal evolution of median floc size $d_{50}$

The median floc size  $d_{50}$  is the most widely reported quantity in laboratory experiments and field observations. We analyze the model's capability to represent the flocculation process using exclusively  $d_{50}$  with constraints of the parameters  $\alpha$ ,  $\beta$  and  $f_d$ . Moreover, since many studies only report the median floc size in the equilibrium state, it is important to investigate if the model can reproduce the entire measured time series by solely calibrating model parameters using the equilibrium median floc size.

Using the measured data from Keyvani and Strom (2014), the RSME at the equilibrium state  $RMSEeq_{d_{50}}$  ( $t \geq 700 \text{ min}$ ) is calculated for the 6,400 simulations and results are summarized in Figure 3.5 for all combinations of the parameters  $\alpha$ ,  $\beta$  for any given  $f_d$ . Each interaction between these parameters is examined in a simulation with the error magnitudes demarcated by a hot colormap. The dark-red color represents excellent agreement with measured  $d_{50}$  in the equilibrium state. Importantly, all the fractal dimensions ( $f_d = 1.7 \sim 2.9$ ) show multiple choices of  $\alpha$  and  $\beta$  that are in very good agreement ( $RMSEeq_{d_{50}} = 1.72 \mu m$ , the finite value of  $1.72 \mu m$  reflects the variabilities in the measured data) with the measured  $d_{50}$  at the equilibrium state. Clearly, low error values cluster around a line with a constant slope for each fractal dimension indicating that the best agreement is obtained at a nearly constant  $\alpha/\beta$  ratio,

regardless of the individual  $\alpha$  and  $\beta$  values. This finding is consistent with that reported by Verney et al. (2011). In addition to the multiple choices of the  $\alpha$  and  $\beta$  pair, another important limitation of using only the equilibrium  $d_{50}$  data to calibrate the flocculation model is that excellent agreement can be found for very large (e.g.,  $f_d = 2.9$ ) or very low (e.g.,  $f_d = 1.7$ ) fractal dimension values outside the typical range for mud. As we will discuss next, despite the multiple options for  $\alpha$  and  $\beta$  pairs to match the equilibrium  $d_{50}$ , the predicted time series of  $d_{50}$  for some of the options are not acceptable (see Figure 3.6). At this point, we can conclude that sole measurement of  $d_{50}$  in the equilibrium state is insufficient to narrow the values of  $\alpha$ ,  $\beta$  and  $f_d$ . Additional characteristics of the flocculation statistics should be considered for an improved model calibration.

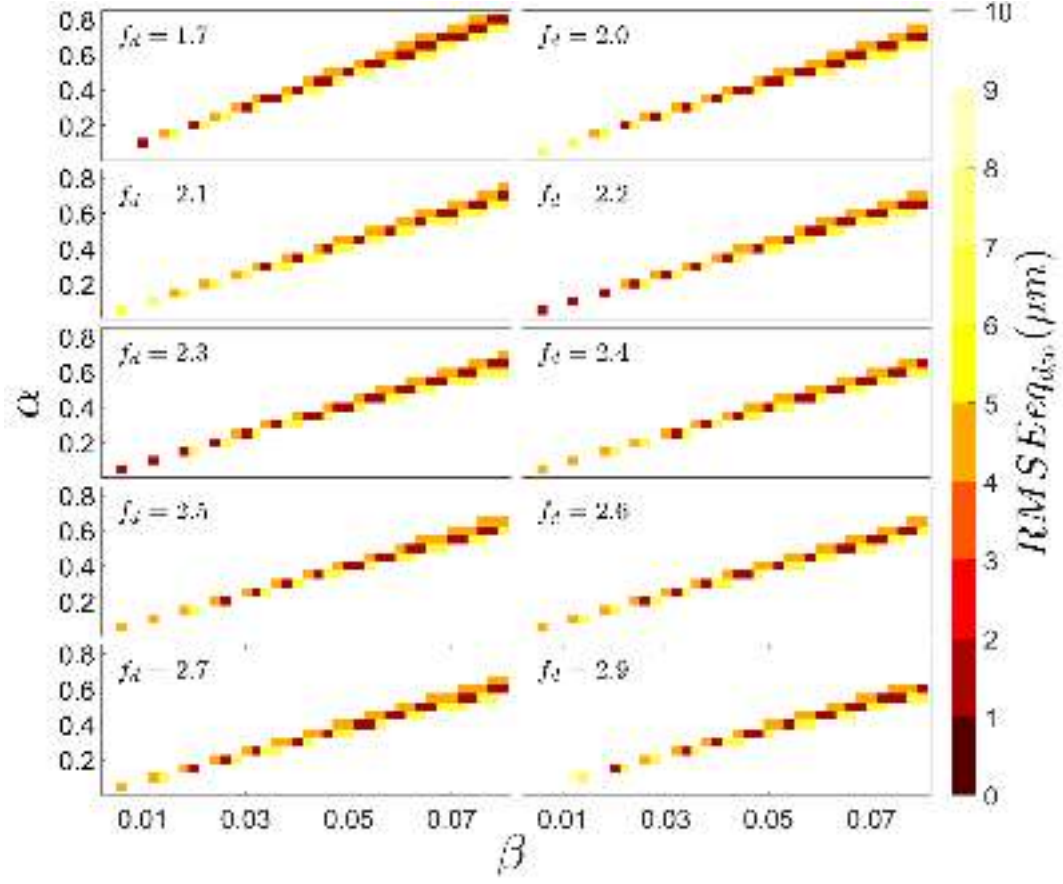


Figure 3.5 Root-Mean-Square-Error matrix for the median floc size  $d_{50}$  at the equilibrium state for different combinations of collisional efficiency  $\alpha$  and fragmentation rate  $\beta$  at fractal dimension  $f_d$  from 1.7 to 2.9.

Since there are multiple pairs of  $\alpha, \beta$  values that satisfy minimizing errors in the equilibrium state with  $\min(RMSEeq_{d_{50}}) = 1.72 \mu m$ , we sequentially applied the second criterion of minimizing the error values at the initial stage of the flocculation ( $t \leq 200$  min)  $\min(RMSEfr_{d_{50}})$ . The predicted time series associated with the best and the worst agreement with measured data for the initial stage of flocculation ( $RMSEfr_{d_{50}}$ ) are presented for the fractal dimension in the range of  $f_d = 1.9 \sim 2.9$  (see Figure 3.6). The calibrated parameter values and respective minimum errors at a given

fractal dimension are detailed in Table 3.1. The predicted time series using the pair of  $\alpha, \beta$  that matches the equilibrium  $d_{50}$  but having large error of  $RMSEfr_{d_{50}}$  are clearly far from satisfactory (see red lines in Figure 3.6). This confirms that using solely the first criterion of minimizing the equilibrium median floc size errors is insufficient to predict the entire time series of median floc size evolution. However, applying first the criterion of  $\min(RMSEeq_{d_{50}})$  followed by the second criterion of  $\min(RMSEfr_{d_{50}})$  yields generally good agreement with the measured data for the entire time series when  $f_d = 2.2 \sim 2.7$  (see blue lines in Figure 3.6c~3.6i) with a  $RMSEfp_{d_{50}} \leq 2.8 \mu m$  (see “best” in Table 1). Further analysis confirmed that the same results can be obtained by simply minimizing the errors of the entire flocculation time series, i.e., using the objective function  $\min(RMSEfp_{d_{50}})$ . Nevertheless, we emphasize our main point that one should proceed with caution when utilizing the equilibrium data as the only model calibration criterion. Applying these two criteria sequentially (or minimizing the error for the entire time series) also significantly narrows the options for fractal dimension, with the three lowest errors occurring at the fractal dimensions  $f_d = 2.4, 2.6$  and  $2.7$ .

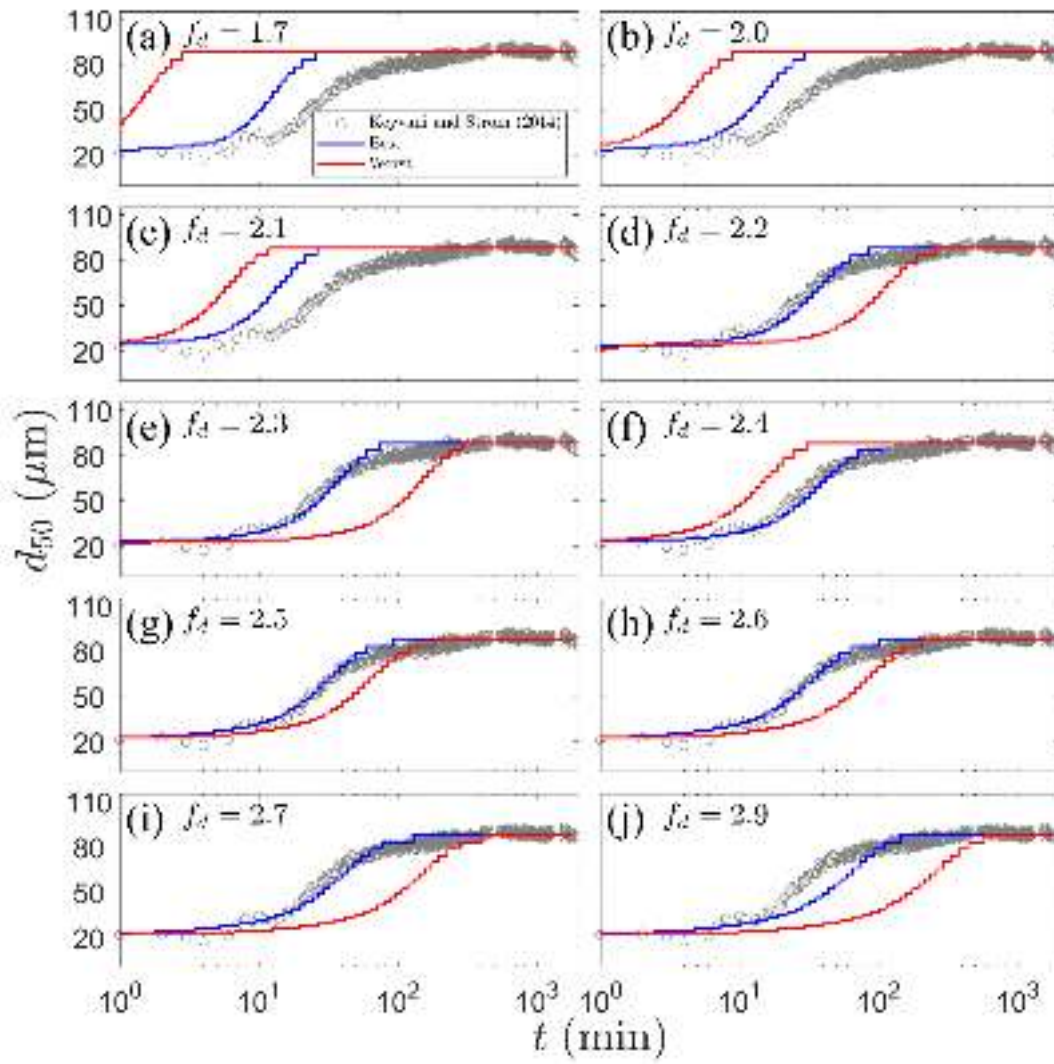


Figure 3.6 Temporal evolution of the median floc size  $d_{50}$  for different fractal dimension applying the condition  $\min(RMSEeq_{d_{50}}) \rightarrow \min(RMSEfr_{d_{50}})$  (blue line, best agreement and red line, worst agreement).

Table 3.1. Root-Mean-Square-Errors (in  $\mu m$ ) and flocculation parameters of the median floc size statistics  $d_{50}$  obtained in Figure 3.6.

| $f_d$ | Option | $RMSEeq_{d_{50}}$<br>( $\mu m$ ) | $RMSEfr_{d_{50}}$<br>( $\mu m$ ) | $RMSEfp_{d_{50}}$<br>( $\mu m$ ) | $\alpha$ | $\beta$ | $r = \alpha/\beta$ |
|-------|--------|----------------------------------|----------------------------------|----------------------------------|----------|---------|--------------------|
| 1.7   | best   | 1.72                             | 14.58                            | 5.18                             | 0.10     | 0.010   | 10.00              |
|       | worst  | 1.72                             | 21.71                            | 7.45                             | 0.80     | 0.078   | 10.25              |
| 2.0   | best   | 1.72                             | 13.36                            | 4.81                             | 0.20     | 0.022   | 9.091              |
|       | worst  | 1.72                             | 19.85                            | 6.85                             | 0.70     | 0.078   | 8.974              |
| 2.1   | best   | 1.72                             | 14.28                            | 5.09                             | 0.30     | 0.034   | 8.824              |
|       | worst  | 1.72                             | 18.93                            | 6.56                             | 0.70     | 0.080   | 8.750              |
| 2.2   | best   | 1.72                             | 5.98                             | 2.7                              | 0.15     | 0.018   | 8.333              |
|       | worst  | 1.72                             | 21.74                            | 7.44                             | 0.05     | 0.006   | 8.333              |
| 2.3   | best   | 1.72                             | 6.38                             | 2.80                             | 0.20     | 0.024   | 8.333              |
|       | worst  | 1.72                             | 27.47                            | 9.35                             | 0.05     | 0.006   | 8.333              |
| 2.4   | best   | 1.72                             | 5.27                             | 2.54                             | 0.25     | 0.032   | 7.813              |
|       | worst  | 1.72                             | 13.58                            | 4.88                             | 0.65     | 0.080   | 8.125              |
| 2.5   | best   | 1.72                             | 5.76                             | 2.65                             | 0.40     | 0.052   | 7.692              |
|       | worst  | 1.72                             | 10.22                            | 3.86                             | 0.20     | 0.026   | 7.692              |
| 2.6   | best   | 1.72                             | 5.34                             | 2.55                             | 0.50     | 0.066   | 7.576              |
|       | worst  | 1.72                             | 14.80                            | 5.25                             | 0.20     | 0.026   | 7.692              |
| 2.7   | best   | 1.72                             | 4.71                             | 2.41                             | 0.55     | 0.074   | 7.432              |
|       | worst  | 1.72                             | 26.72                            | 9.25                             | 0.15     | 0.020   | 7.500              |
| 2.9   | best   | 1.72                             | 9.13                             | 3.55                             | 0.60     | 0.080   | 7.500              |
|       | worst  | 1.72                             | 36.35                            | 13.97                            | 0.15     | 0.020   | 7.500              |

We further explore the benefits of simply minimizing the errors present at the initial floc growth stage. The best calibrated model parameters and error values can be found in Table 3.2. As expected, this approach decreases the errors in the predicted flocculation rate (cf.  $RMSEfr_{d_{50}}$  in Table 3.1 and Table 3.2). The equilibrium state is affected negatively ( $RMSEeq_{d_{50}}$  values increase from  $1.72 \mu m$  to  $6.06 \mu m$  for fractal dimension  $f_d = 2.2 \sim 2.7$ ) but only slightly. Figure 3.7 illustrates visually these consequences where the floc growth stage is predicted well but the agreement in the equilibrium value is slightly reduced. This approach also allows us to narrow down the

choice of fractal dimension, based on the best three  $\min(RMSEfr_{d_{50}})$ , to be  $f_d = [2.4, 2.5, 2.6]$ . When evaluating the agreement for the entire time series, we observe that  $RMSEfp_{d_{50}}$  is around  $5.7 \mu m$  for  $f_d = [2.4, 2.6]$ . This is considered a good agreement as only one criterion of  $\min(RMSEfr_{d_{50}})$  is adopted. We can also conclude that the PBE-based size class flocculation model has a good capability of predicting equilibrium median floc size once the key model parameters are calibrated for predicting the initial growth of flocculation (i.e., the flocculation rate).

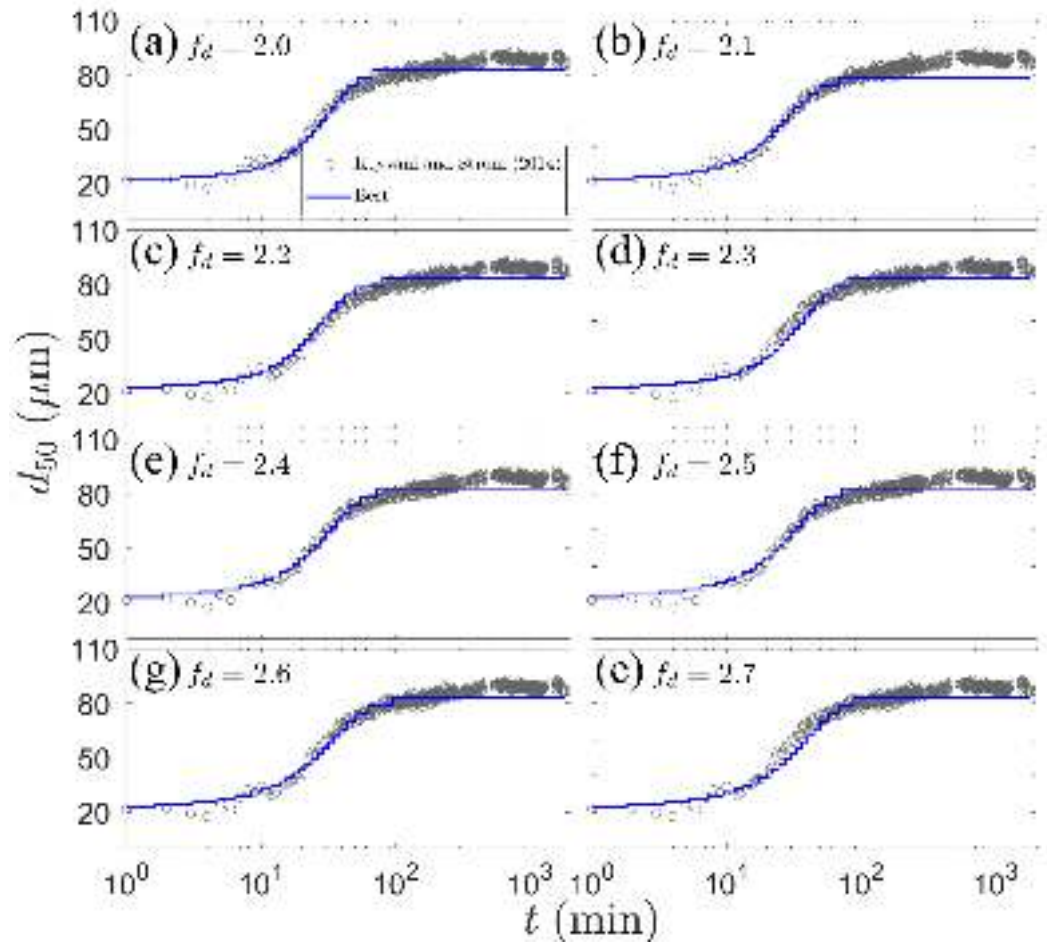


Figure 3.7 Temporal evolution of the median floc size statistics  $d_{50}$  for different fractal dimension applying the criteria  $\min(RMSEfr_{d_{50}})$ .

Table 3.2. Root-Mean-Square-Errors (in  $\mu m$ ) and flocculation parameters of the median floc size statistics  $d_{50}$  obtained in Figure 3.7.

| $f_d$ | $RMSEeq_{d_{50}}$<br>( $\mu m$ ) | $RMSEfr_{d_{50}}$<br>( $\mu m$ ) | $RMSEfp_{d_{50}}$<br>( $\mu m$ ) | $\alpha$ | $\beta$ | $r = \alpha/\beta$ |
|-------|----------------------------------|----------------------------------|----------------------------------|----------|---------|--------------------|
| 1.7   | 15.11                            | 6.36                             | 14.25                            | 0.05     | 0.006   | 8.33               |
| 2.0   | 6.06                             | 3.16                             | 5.72                             | 0.10     | 0.010   | 8.33               |
| 2.1   | 10.70                            | 3.31                             | 10.00                            | 0.15     | 0.020   | 7.50               |
| 2.2   | 6.06                             | 2.99                             | 5.71                             | 0.20     | 0.030   | 7.69               |
| 2.3   | 6.06                             | 3.25                             | 5.72                             | 0.20     | 0.030   | 7.69               |
| 2.4   | 6.06                             | 2.85                             | 5.70                             | 0.30     | 0.040   | 7.50               |
| 2.5   | 6.06                             | 2.93                             | 5.70                             | 0.40     | 0.050   | 7.41               |
| 2.6   | 6.06                             | 2.49                             | 5.68                             | 0.50     | 0.070   | 7.14               |
| 2.7   | 6.06                             | 3.55                             | 5.74                             | 0.55     | 0.080   | 7.24               |
| 2.9   | 4.64                             | 8.99                             | 5.50                             | 0.60     | 0.078   | 7.69               |

### 3.2.2 Tri-temporal floc size statistics $d_{16}$ , $d_{50}$ and $d_{84}$ with $\min(RMSEfp_{d_{50}})$

Since the best calibrated cases that match the measured temporal evolution of median floc size are obtained for a wide range of fractal dimension  $f_d = 2.2 \sim 2.7$  (see Figure 3.6,  $RMSEfp_{d_{50}} \leq 2.8 \mu m$ ), the selection of a unique set of  $\alpha, \beta$  parameters is not yet conclusive. Fortunately, Keyvani and Strom (2014) provide two more measured floc size statistics of  $d_{16}$  and  $d_{84}$  and these are added to the model calibration to evaluate the possibility of further constraining the model parameters. Figure 3.8 illustrates the predicted tri-temporal floc size statistics ( $d_{50}$ ,  $d_{16}$  and  $d_{84}$ ) at the six fractal dimension values  $f_d = 2.2 \sim 2.7$  using the  $\alpha, \beta$  parameters that achieve the best agreement for the temporal evolution of the median floc size  $d_{50}$  (recall Figure 3.6). At the floc growth stage ( $t < 30 \text{ min}$ ), good agreement can be seen for both the fine  $d_{16}$  and coarse  $d_{84}$  fractions (Figure 3.8). However, larger discrepancies arise before reaching the equilibrium stage ( $30 \text{ min} < t < 200 \text{ min}$ ). It becomes clear that by minimizing the

error for the median floc size  $d_{50}$ , the equilibrium floc statistics for the finer fraction  $d_{16}$  is under-predicted by the model while the coarse fraction  $d_{84}$  is over-predicted.

Identifying the best parameters hierarchically to represent the tri-temporal floc size statistics from Figure 3.8 can be difficult based on its similar trend across the fractal dimension values. Therefore, we evaluate the error values during the initial growth stage of the flocculation ( $RMSEfr$ ) and the entire flocculation time series ( $RMSEfp$ ) in a wider range of fractal dimension  $f_d = 1.7 \sim 2.9$  (see Figure 3.9). The  $RMSEfr$  confirms the discrimination process for the lowest ( $f_d \leq 2.1$ ) and highest ( $f_d = 2.9$ ) fractal dimension since their errors increase considerably. Regarding the fractal dimensions  $f_d = 2.2 \sim 2.7$ , the  $RMSEfr$  for the median floc size statistics  $d_{50}$  behaves in a quasi-stable way. However, the error values for  $d_{16}$  and  $d_{84}$  show opposite trends when one of them is minimized (see  $f_d = 2.3$  and  $f_d = 2.7$ ). Looking at the average performance for these floc fractions, the first, second and third option are  $f_d = 2.7, 2.6$  and  $2.4$ , respectively (see dashed black line in Figure 3.9a). This final result can also be obtained when computing the mean value of  $RMSEfp$  (see Figure 3.9b).

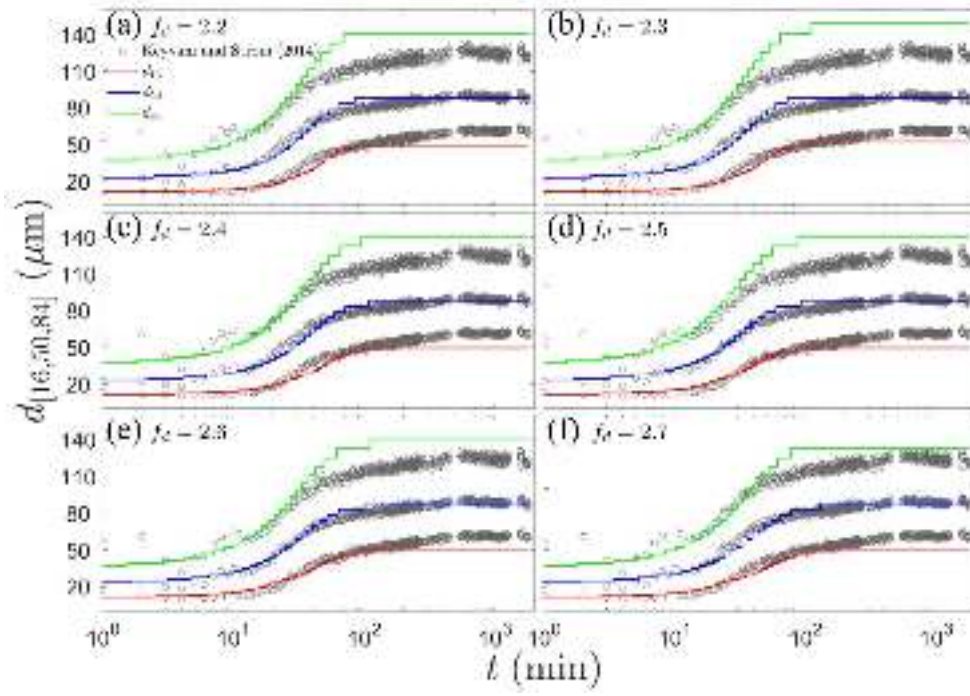


Figure 3.8 Temporal evolution of the tri-floc size statistics  $d_{16}$ ,  $d_{50}$  and  $d_{84}$  for different fractal dimensions minimizing the entire flocculation process error values  $RMSEfp_{d_{50}}$ .

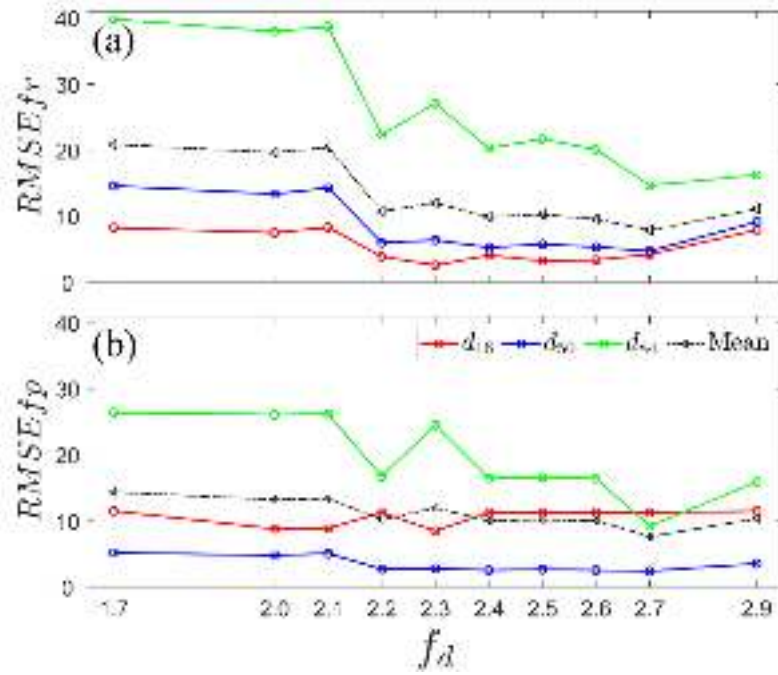


Figure 3.9 Root-Mean-Square-Error for tri-temporal floc size statistics ( $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ) by applying the criterion  $\min(RMSE_{fp_{d_{50}}})$  of minimizing the errors in the measured time series of the median fraction  $d_{50}$ . (a) Root-Mean-Square-Error for the growth stage of flocculation ( $RMSE_{fr}$ ). (b) Root-Mean-Square-Error for the entire temporal evolution ( $RMSE_{fp}$ ).

### 3.2.3 Tri-temporal floc size statistics using $\min(RMSE_{fp_{d_{16}}})$ or $\min(RMSE_{fp_{d_{84}}})$

Through a systematic error analysis of  $d_{50}$  for the initial floc growth and the entire flocculation process presented in the previous sections, optimal model parameters are obtained. However, the predicted fine ( $d_{16}$ ) and coarse ( $d_{84}$ ) floc fractions are adversely affected. That is, better agreement in the fine fraction comes at the expense of worse agreement in the coarse fraction. Now, we evaluate the possibility to narrow the flocculation model parameters and improve the overall agreement by minimizing

the fine or coarse floc sizes statistic errors (i.e.,  $\min(RMSEfp_{d_{16}})$  or  $\min(RMSEfp_{d_{84}})$ ) using the same systematic error analysis.

The criterion of minimizing the fine fraction  $\min(RMSEfp_{d_{16}})$  produces non-satisfactory results for the overall floc size statistics since the coarse fraction  $d_{84}$  stands out for its high error values ( $RMSEfp_{d_{84}} \geq 34.62 \mu m$ ) as illustrated in Figure 3.10. This magnitude is higher than  $RMSEfp_{d_{84}}$  obtained by using the previous criterion  $\min(RMSEfp_{d_{50}})$ . Conversely, applying the criterion  $\min(RMSEfp_{d_{84}})$  shows satisfactory results especially in the  $RMSEfr$  values since the best value is distinguished from the other acceptable errors (see  $f_d = 2.5$  in Figure 3.11a). However, the minimum value of  $RMSEfp$  averaged over the three size statistics is located at  $f_d = 2.9$  (Figure 3.11b). This is a limitation in the flocculation model since  $f_d = 2.9$  is a much higher than expected value for typical flocs. Considering the error analysis criterion for the initial floc growth stage, the optimum fractal dimension is selected to be  $f_d = 2.5$ .

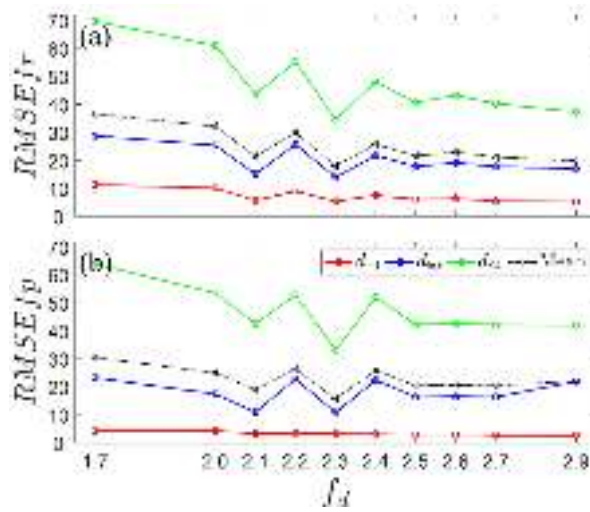


Figure 3.10 Root-Mean-Square-Error for tri-temporal floc size statistics by applying  $\min(RMSEfp_{d_{16}})$ . (a) Root-Mean-Square-Error for the initial floc growth stage. (b) Root-Mean-Square-Error for the entire temporal evolution of  $d_{16}$ ,  $d_{50}$  and  $d_{84}$ .

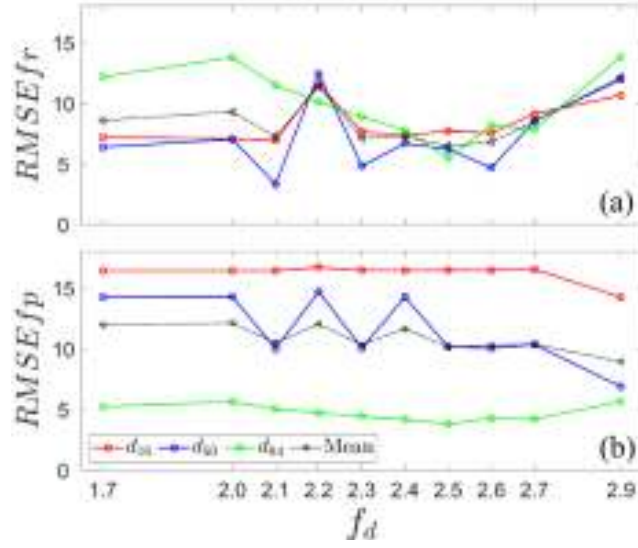


Figure 3.11 Root-Mean-Square-Error for tri-temporal floc size statistics by applying  $\min(RMSE_{fp_{d_{84}}})$ . (a) Root-Mean-Square-Error for the initial floc growth stage. (b) Root-Mean-Square-Error for the entire temporal evolution of  $d_{16}$ ,  $d_{50}$  and  $d_{84}$ .

The tri-temporal floc size statistics for three selected cases are presented in Figure 3.12. We established previously for the equilibrium state that minimizing the median floc size errors leads to over- and under-predicted results for coarse and fine flocs, respectively (see also Figure 3.12a and 3.12b). Hence, the difference between Case 1 with  $f_d = 2.4$  and Case 2 with  $f_d = 2.7$  lies mainly in the degree of agreement to represent the coarse fraction  $d_{84}$  (see  $RMSE_{eq}$  values in Table 3.2) since Case 2 with  $f_d = 2.7$  shows 49.12% better agreement compared to Case 1. This contrast can also be noticed in the distributed mass concentration at the equilibrium state (see blue-dashed line vs red-solid line in Figure 3.13). Comparing with Case 1, Case 2 relocates a small amount of sediment mass in the coarse fraction to the median and fine fractions due to a relatively larger breakup effect signified by smaller  $r = \alpha/\beta$  value in Case 2. Using

a lower fractal dimension of  $f_d = 2.5$  in Case 3 allows for an even lower  $r = 6.7$ , which significantly reduces the sediment mass in the coarse fraction (see smaller  $d_{84}$  in Figure 3.12c) and this is evidently due to a more significant relocation of mass from the coarse fraction to the finer fraction (see a shift of sediment mass distribution to the left represented by the black-dashed line in Figure 3.13).

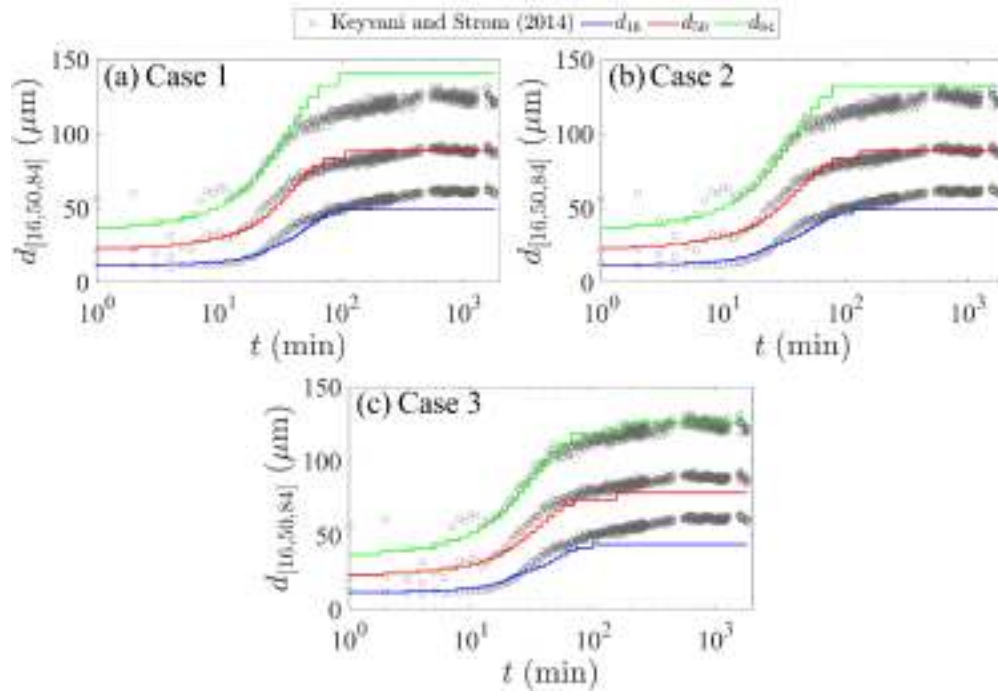


Figure 3.12 Modeled tri-temporal floc size statistics (lines) compared with measured data (symbols) reported by Keyvani and Strom (2014). (a) and (b) are Case 1 and Case 2 results using the criteria  $\min(RMSEfp_{d_{50}})$  and (c) Case 3 results using the criterion  $\min(RMSEfp_{d_{84}})$ .

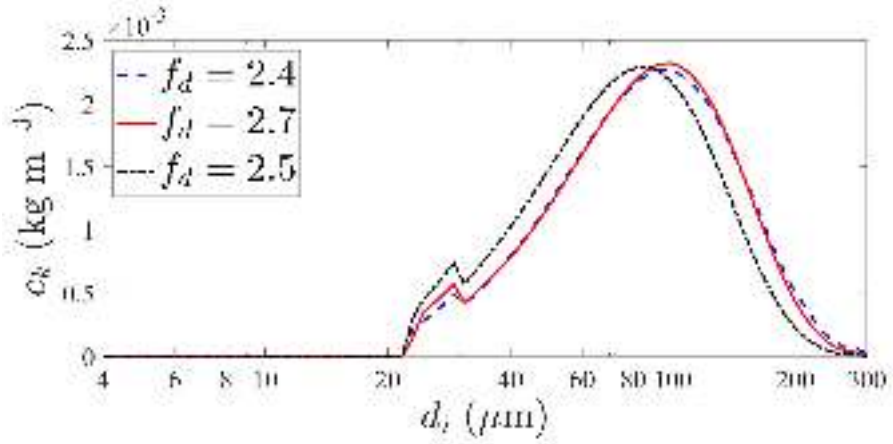


Figure 3.13 Distributed mass concentration at the equilibrium state for Case 1 ( $f_d = 2.4$ ) and Case 2 ( $f_d = 2.7$ ) with the criterion  $\min(RMSEfp_{d_{50}})$ , and Case 3 ( $f_d = 2.5$ ) with the criterion  $\min(RMSEfp_{d_{84}})$ .

Table 3.3. A summary of recommended cases for their model parameters and errors (in  $\mu\text{m}$ )

| Case | $f_d$ | $d_i$ | $\alpha$ | $\beta$ | $r$   | $RMSEfr$ | $RMSEfp$ | mean<br>( $RMSEfr$ ) | mean<br>( $RMSEfp$ ) |
|------|-------|-------|----------|---------|-------|----------|----------|----------------------|----------------------|
| 1    | 2.4   | 16    | 0.25     | 0.032   | 7.813 | 4.08     | 11.27    | 9.88                 | 10.08                |
|      |       | 50    |          |         |       | 5.27     | 2.54     |                      |                      |
|      |       | 84    |          |         |       | 20.30    | 16.43    |                      |                      |
| 2    | 2.7   | 16    | 0.55     | 0.074   | 7.432 | 4.22     | 11.27    | 7.86                 | 7.63                 |
|      |       | 50    |          |         |       | 4.71     | 2.41     |                      |                      |
|      |       | 84    |          |         |       | 14.65    | 9.22     |                      |                      |
| 3    | 2.5   | 16    | 0.35     | 0.052   | 6.731 | 7.71     | 16.45    | 6.46                 | 10.12                |
|      |       | 50    |          |         |       | 6.20     | 10.15    |                      |                      |
|      |       | 84    |          |         |       | 5.47     | 3.77     |                      |                      |

### 3.3 Discussion – Effect of Floc Yield Strength

The results presented in Section 3.2 indicate that by rigorously calibrating the PBE-based size-class flocculation model against measured tri-temporal floc size statistics ( $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ), we can identify several combinations of the model

parameters ( $\alpha$ ,  $\beta$  and  $f_d$ ) that show good agreement with measured data. However, there are still uncertainties in the selection of the best model parameters, particularly in Case 2, which has the best agreement but with a high value of the fractal dimension of 2.7. In this section, we include one other significant physical quantity in the model parameters to improve the overall agreement. To avoid overfitting model results, the choice of the additional physics to be included must first be justified.

Motivated by improving the limited capability of the model to represent the coarse and fine fractions simultaneously, and the optimum ratios of collisional efficiency and fragmentation  $\alpha/\beta$  in Case 1~3 seem to be related to such improvement, we evaluate the effect of considering the fragmentation rate  $\beta$  as a function of floc size. As shown in equation (2.12), the fragmentation rate  $\beta$  is a function of the empirical coefficient  $E$ , fluid viscosity  $\mu$  and floc yield strength  $F_y$ . The justification of treating  $\beta$  as a constant is to assume the floc yield strength is a constant. In the literature, floc yield strength is routinely assumed to be  $F_y = 10^{-10}N$  in flocculation modeling and the model calibrations are carried out either through the coefficient  $E$ , or directly using the parameter  $\beta$  (Maggi et al., 2007; Verney et al., 2011; Winterwerp, 1998). However, in the water quality literature, Jarvis et al. (2005) presented a review of many laboratory measurements of floc yield strength (or yield stress) which indicated that the floc yield strength  $F_y$  is inversely proportional to the floc size (e.g., Bache et al., 1999; Yeung and Pelton, 1996). In other words, the larger the floc size is, the easier the floc can be broken by turbulent shear. This fact is supported by our error analysis presented in Section 3.2. Figure 3.14 presents the best calibrated  $\beta$  values by minimizing the error in the three size fractions ( $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ) plotted as a function of fractal dimension between 2.3 and 2.6. We observe a clear trend in each fractal dimension that the larger the size

fraction when the error is minimized, the larger the value of  $\beta$  (or smaller  $F_y$ ) is required. Hence, we investigate the effect of considering the floc yield strength  $F_y$  inversely proportional to floc size.

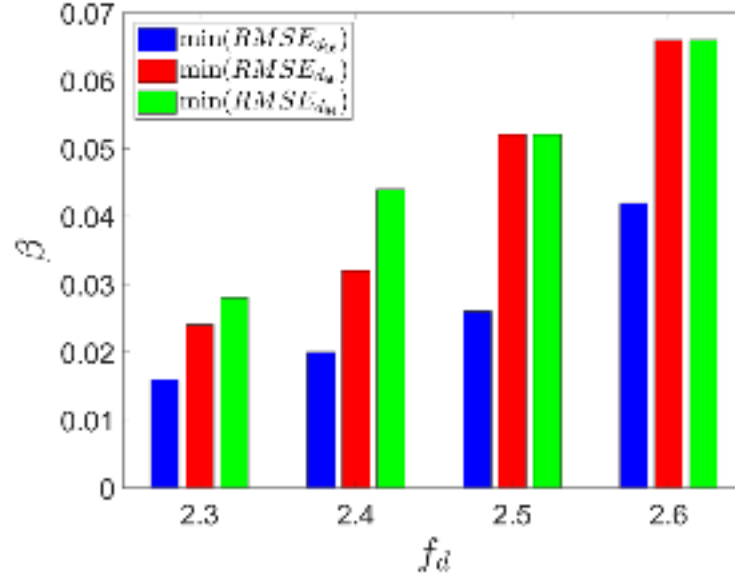


Figure 3.14 Fragmentation rate  $\beta$  variation with respect to size fraction based on the criterion  $\min(RMSE_{d_{[16,50,84]}})$  for fractal dimension  $f_d = 2.3 \sim 2.6$ .

Since measuring the floc yield strength as a function of floc size can be very difficult and most studies of cohesive sediment transport do not report such data, as a first step we propose to model the floc yield strength in terms of microflocs and macroflocs (Manning and Dyer, 2007) and divide the fragmentation rate  $\beta$  into two different values accordingly. To distinguish these two groups, a floc size limit  $d_L$  is defined such that the fragmentation rate of flocs with a size smaller (larger) than  $d_L$  is specified as  $\beta_{\text{micro}}$  ( $\beta_{\text{macro}}$ ). The parameter  $\alpha$  and  $f_d$  remain constant and the same

values found in Section 3.2 for Case 1 and Case 3 (see Table 3.3) are applied. As for  $\beta_{\text{micro}}$  and  $\beta_{\text{macro}}$ , the mean value between these two fragmentation rates is matched with a constant  $\beta$  in each of these two cases, while satisfying the physical behavior of higher tendency for breakup in macroflocs with  $\beta_{\text{macro}} > \beta_{\text{micro}}$ .

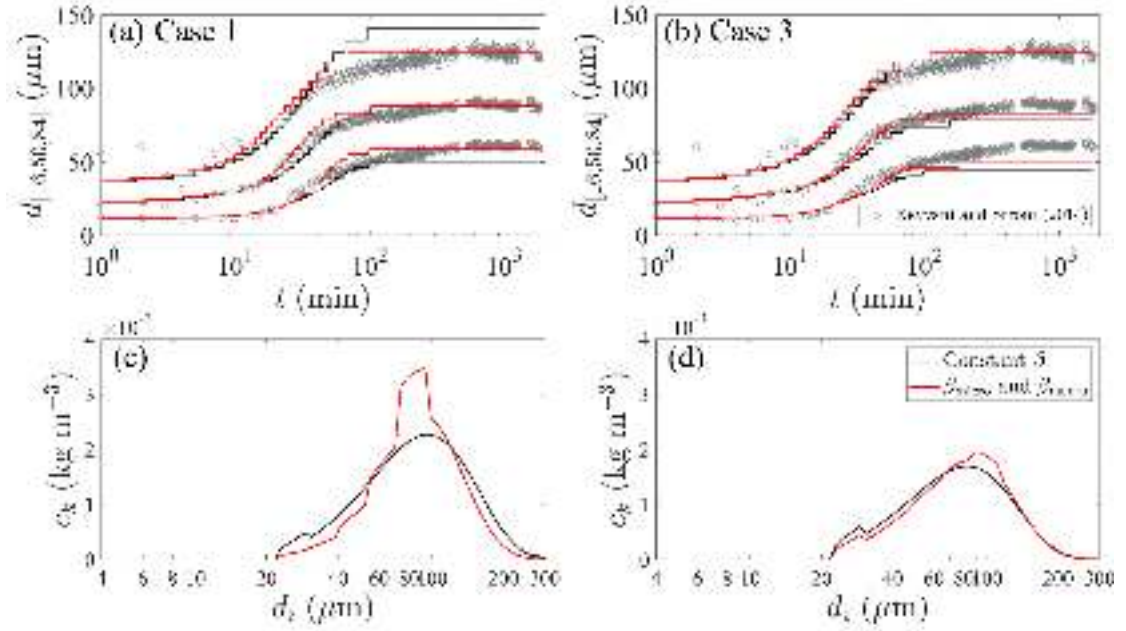


Figure 3.15 Comparison between constant fragmentation rate ( $\beta$ ) and two-value fragmentation rate ( $\beta_{\text{micro}}$  and  $\beta_{\text{macro}}$ ) for Case 1 and Case 3. (Upper panel) Tri-temporal floc size statistics ( $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ) based on the (a) criterion  $\min(RMSE_{d_{50}})$  and (b)  $\min(RMSE_{d_{84}})$ . (Lower panel) mass concentration distribution over the floc size classes using the criterion (c)  $\min(RMSE_{d_{50}})$  and (d)  $\min(RMSE_{d_{84}})$ .

Table 3.4. A summary of the two-value fragmentation rate cases for their model parameters and errors (in  $\mu m$ ).

| Case | $f_d$ | $d_i$ | $\alpha$ | $\beta_{\text{micro}}$ | $\beta_{\text{macro}}$ | $r$   | $d_L$ | $RMSEfr$ | $RMSEfp$ | mean<br>( $RMSEfr$ ) | mean<br>( $RMSEfp$ ) |
|------|-------|-------|----------|------------------------|------------------------|-------|-------|----------|----------|----------------------|----------------------|
| 1a   | 2.4   | 16    | 0.25     | 0.020                  | 0.044                  | 1.953 | 95.0  | 5.81     | 3.38     | 7.18                 | 3.57                 |
|      |       | 50    |          |                        |                        |       |       | 5.85     | 2.67     |                      |                      |
|      |       | 84    |          |                        |                        |       |       | 9.87     | 4.66     |                      |                      |
| 3a   | 2.5   | 16    | 0.35     | 0.045                  | 0.059                  | 1.683 | 110.0 | 4.86     | 11.30    | 4.98                 | 7.05                 |
|      |       | 50    |          |                        |                        |       |       | 2.47     | 5.68     |                      |                      |
|      |       | 84    |          |                        |                        |       |       | 7.60     | 4.16     |                      |                      |

The use of the two-value  $\beta_{\text{micro}}/\beta_{\text{macro}}$  fragmentation rate shows remarkable improvement compared to using a constant  $\beta$  method in Case 1 with  $f_d = 2.4$ . For the coarse fraction  $d_{84}$  under the criterion  $\min(RMSEfp_{d_{50}})$ , the over-predicted errors  $RMSEfp_{d_{84}}$  for the entire time series in Case 1 (Figure 3.15a) are significantly reduced from  $16.43 \mu m$  to  $4.66 \mu m$  (nearly a factor 4 reduction of error, compare Table 3.3 and 3.4). The same improvement can be seen for the fine fraction  $d_{16}$  with an error value  $RMSEfp_{d_{16}}$  reducing from  $11.27 \mu m$  to  $3.38 \mu m$ . Furthermore, these improvements preserve the excellent agreement of  $d_{50}$  because the  $RMSEeq_{d_{50}}$  maintains its low error values (errors slightly increase by 5% from  $2.54 \mu m$  to  $2.67 \mu m$ ). For the initial floc growth stage, using the two-value  $\beta_{\text{micro}}/\beta_{\text{macro}}$  fragmentation rate in Case 1 significantly improves the agreement for the coarse fraction (error associated with  $d_{84}$  decreases from  $20.3 \mu m$  to  $9.87 \mu m$ , about a factor 2 smaller) while only marginally decreasing the agreement for the median (11% increase of error) and fine (42% increase of error) fraction. Evaluating the overall performance through the mean error values, we observe a factor 3 reduction of errors for the entire time series ( $\text{mean}(RMSEfp)$  reduces from  $10.08 \mu m$  to  $3.57 \mu m$ ). The improvement by using the two-value  $\beta_{\text{micro}}/\beta_{\text{macro}}$  fragmentation rate is particularly significant for equilibrium floc sizes.

Relatively minor improvement is observed for Case 3 ( $f_d = 2.5$ ) when the two-value fragmentation rate is applied. This is partly because the agreement in the coarse fraction when using a single value  $\beta$  is already good (see Table 3.3, e.g.,  $RMSEfp$  for  $d_{84}$  is only  $3.77 \mu m$ ). The improvement for median fraction (fine fractions) by using the two-value fragmentation rate for the entire time series can be quantified by an error reduction from  $10.15 \mu m$  to  $5.68 \mu m$  (from  $16.45 \mu m$  to  $11.3 \mu m$ ). As for the initial floc growth stage, the two-value fragmentation rate reduces the errors by a factor of about 1.6 and 2.5 for  $d_{16}$  and  $d_{50}$ , respectively. However, the corresponding error is increased by 39% for the coarse fraction. A numerical experiment has been carried out for Case 2 with a fractal dimension of 2.7. We obtain the similar conclusion that the improvement by using a two-value fragmentation rate in Case 2 is very good but not as effective as in Case 1.

The distributed mass concentration at the equilibrium state is another important characteristic that can be used to compare the two-value fragmentation rate approach with the constant  $\beta$  approach (see Figure 3.15c and 3.15d). When the fractal dimension is  $f_d = 2.4$ , a reduction of the mass concentration is observed for floc classes lower than  $55.25 \mu m$  and higher than  $118 \mu m$  (compare the red line with the black line in Figure 3.15c). As a result of mass conservation, the mass concentration distribution over the floc size classes is squeezed laterally, and the concentration between the floc classes  $55.25 \sim 118 \mu m$  increases. Consequently, the equilibrium floc statistics for coarse  $d_{84}$  (fine  $d_{16}$ ) fraction must decrease (increase). A similar behavior can be seen when the fractal dimension is  $f_d = 2.5$  (in Case 3) but with a different feature. For instance, using a single-value fragmentation rate, the equilibrium floc size for the coarse fraction  $d_{84}$  is already in good agreement with measured data. Interestingly, the use of a two-value

fragmentation rate effectively decreases the mass concentration in the fine fraction and moves the mass toward the median fraction (Figure 3.15d), while the coarse fraction is nearly unchanged. Specifically, the mass concentration increases between  $69.77 \sim 157.9 \mu m$  (see Figure 3.15d) and decreases in finer fraction ( $d_i \leq 69.77 \mu m$ ). There is a very small increase of mass concentration in the coarser fraction ( $d_i \geq 157.9 \mu m$ ).

### 3.4 Conclusions

We present a systematic investigation of the key model parameters for the PBE-based size class flocculation model of Verney et al. (2011) using the experimental data reported by Keyvani and Strom (2014). An analysis on constraining the key model parameters, namely the collisional efficiency, fragmentation rate, and fractal dimension, is first carried out for the median floc size statistics  $d_{50}$ . A criterion based on minimizing the equilibrium state median floc size errors provides multiple options of model parameters with many of them misleading since they fail to match the measured initial floc growth. The agreement can be significantly improved by applying a second criterion sequentially minimizing the error for the initial floc growth stage, or equivalently by minimizing the entire flocculation time series of  $d_{50}$ . Interestingly, utilizing the objective function of simply minimizing the error for the initial floc growth stage ( $\min(RMSEfr_{d_{50}})$ ) shows generally good agreement with the entire measured time series of flocculation, confirming a good predictive ability of the present PBE-based flocculation model. The resulting model parameters are constrained to multiple options of fractal dimension in the range of  $f_d = 2.2 \sim 2.7$  and we conclude that the median floc size  $d_{50}$  alone is insufficient to constrain the flocculation model parameters.

The PBE-based flocculation model can reasonably predict  $d_{16}$  and  $d_{84}$  using solely the calibration results from the median floc sizes  $d_{50}$  in the range of  $f_d = 2.2 \sim 2.7$ . The best two options with minimum errors are selected for  $f_d = 2.4$  and  $f_d = 2.7$  with the latter selected because of its good agreement with measured coarse fraction  $d_{84}$  even though the  $f_d$  value is higher than expected. Evaluating two different criteria based on minimizing the entire temporal floc size statistic errors of  $d_{16}$  and  $d_{84}$  indicates that minimizing the errors in the fine fraction is not viable due to the high errors in the coarse fraction. On the contrary, minimizing the error in the coarse fraction shows good agreement with the measured initial floc growth at  $f_d = 2.5$ .

To improve the model's predictive ability for fine, median, and coarse fractions at typically expected fractal dimension ranges for cohesive sediment, we propose a two-value fragmentation rate approach (floc yield strength is smaller for macroflocs than microflocs) motivated by limited measured data in the water quality literature and the present model analysis for a single fragmentation rate  $\beta$ , which clearly shows a positive correlation between calibrated  $\beta$  and floc size (see Figure 3.14). The results from the two-value fragmentation rate approach demonstrate significant improvement in representing the tri-temporal floc size statistics compared with data from using a constant  $\beta$ , especially for the case of lower fractal dimension at  $f_d = 2.4$ .

Findings reported in this study call for future research on expanding the knowledge of floc yield strength, for instance, through a series of laboratory experiments to directly measure floc yield strength as a function of floc size and other environmental factors. Future studies on other model parameters, such as the collision efficiency  $\alpha$ , fractal dimension  $f_d$ , and the distribution function of fragmented flocs, are

important as they are known to represent the physicochemical properties of flocs, which may change with floc size.

## **Chapter 4**

### **FLOCCULATION AND COHESIVE SEDIMENT TRANSPORT IN THE CURRENT BOTTOM BOUNDARY LAYER**

The main goal of this chapter is to investigate Research Question 3 to advance the understanding and modeling of flocculation effects on cohesive sediment transport processes in the current bottom boundary layer. The specific objectives of this chapter are to (1) develop a modeling framework that incorporate flocculation in cohesive sediment transport modeling in the bottom boundary layer, (2) evaluate how the flocculation process affects the floc size and settling velocity for a range of floc properties and environmental conditions, and (3) investigate how the variability of floc properties controls cohesive sediment distribution in the current bottom boundary layer. The model framework is discussed in detail in Chapter 2. Section 4.1 presents a description of the data processing methods for the DNS data. Section 4.2 and 4.3 provide a local sensitivity analysis for PBE flocculation model and main results from the modeling framework of cohesive sediment transport, respectively. Section 4.4 is dedicated to a discussion on the model applicability and limitation and Section 4.5 provides concluding remarks. In Chapter 5, the extension for the present modeling framework for wave bottom boundary layer application is reported.

#### **4.1 Turbulent-averaged quantity**

Since the cohesive sediment modeling framework requires input of turbulence-averaged profiles (see Step I in Figure 2.1), the streamwise velocity and sediment concentration fields from the DNS data are decomposed into statistically-averaged

mean quantities, denoted by angular brackets  $\langle \cdot \rangle_{12t}$ . The subscript 1 and 2 indicates applying a plane average process in streamwise  $x_1$  and spanwise  $x_2$  directions while the subscript  $t$  corresponds to the time average after the flow reaches a statistical statistically-steady state. Hence, a turbulence-averaged quantity can be calculated by the following expression

$$\langle \psi \rangle_{12t}(x_3) = \frac{1}{\mathcal{T} L_1 L_2} \sum_{t=t_0}^{t=t_0+T} \sum_{x_1=0}^{x_1=L_1} \sum_{x_2=0}^{x_2=L_2} \psi(x_1, x_2, x_3, t) \Delta x_1 \Delta x_2 \Delta t, \quad (4.1)$$

where  $\psi$  is a representative quantity,  $t_0$  is the time instant at which the flow becomes statistically steady and  $\mathcal{T}$  is the duration of time average. The turbulent fluctuation component  $\psi'$  is then obtained by the Reynolds decomposition

$$\psi'(x_1, x_2, x_3, t) = \psi(x_1, x_2, x_3, t) - \langle \psi \rangle_{12t}(x_3). \quad (4.2)$$

Using the fluctuating components of velocity  $u'_i$  and mass concentration  $c'$ , the turbulent diffusivity of sediment  $K_t$ , defined in Equation 2.3 can be calculated from the DNS data as follows

$$K_t = - \frac{\langle u'_3 c' \rangle_{12t}}{\frac{d\langle c \rangle_{12t}}{dx_3}}. \quad (4.3)$$

In this study, the DNS data is used as input to the modeling framework and Equation (4.3) is applied directly to calculate the turbulent diffusivity. Similarly, the eddy viscosity can be calculated from the DNS data as

$$\nu_t = - \frac{\langle u'_1 u'_3 \rangle_{12t}}{\frac{d\langle u_1 \rangle_{12t}}{dx_3}}. \quad (4.4)$$

The main driving force of flocculation is the turbulent shear rate  $S$ , or the turbulent dissipation rate  $\varepsilon$  (see Equation (2.1)), which is determined by the

environmental flow conditions. Here, the turbulent dissipation rate  $\varepsilon$  ( $m^2 s^{-3}$ ) is calculated directly from the DNS data using its original definition as

$$\varepsilon = \nu \left\langle \left( \frac{\partial u'_i}{\partial x_j} \right)^2 \right\rangle_{12t}. \quad (4.5)$$

The turbulent shear rate can be associated with the Kolmogorov length scale as  $\eta = \sqrt{\nu/S}$ , which means that the higher the turbulent shear  $S$ , the smaller the Kolmogorov length scale. Indeed, it is difficult to estimate the turbulent dissipation rate directly from measured data because it requires the calculation of spatial gradients of turbulent velocity fluctuations with a very high-resolution. A key reason for using DNS for the present study of flocculation and cohesive sediment transport is that it provides high resolution temporal and spatial data, allowing us to accurately calculate the turbulent dissipation rate.

## 4.2 Local analysis of flocculation model

For a given set of cohesive particle parameters (i.e., collision efficiency  $\alpha$ , fragmentarion rate  $\beta$  and fractal dimension  $f_d$ ) and driving factors from the environmental flows (i.e., turbulent share rate  $S$  and the turbulence-averaged sediment concentration  $C$ ), 246 simulations are performed (see Table 4.1). Following Penaloza-Giraldo et al. (2023), all simulations are discretized with  $N_f = 75$  floc size classes distributed logarithmically for a better representation of the coarse floc fractions. The smallest floc size class in the modeled distribution corresponds to the primary particle diameter  $d_p = 4 \mu m$  and the maximum floc size is selected to be  $\max(d_f) = 2500 \mu m$ . The floc size distribution is initialized by specifying the entire sediment mass at floc size class  $d_f = 20 \mu m$ . As stated by Verney et al. (2011) and verified by Penaloza-Giraldo et al. (2023), the equilibrium floc size distribution is insensitive to the initial

floc size distribution. Finally, the simulation time in each case is sufficiently long to ensure that all floc size classes reach the equilibrium state.

Table 4.1. A summary of all cases simulated for local sensitivity analysis.

| Local Sensitivity Analysis                   | Scenario                              | $\alpha$ | $\beta \text{ (s}^{1/2} \text{ m}^{-1})$ | $r = \frac{\alpha}{\beta}$ | $S \text{ (s}^{-1})$ | $C \text{ (kg m}^{-3})$ | $f_d$ |
|----------------------------------------------|---------------------------------------|----------|------------------------------------------|----------------------------|----------------------|-------------------------|-------|
| Cohesive Sediment Parameters (CSP)           | CSP1                                  | 0.05     | 0.02                                     | 2.5                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.2      | 0.02                                     | 10.0                       | 50                   | 0.05                    | 2.0   |
|                                              | CSP2                                  | 0.1      | 0.04                                     | 2.5                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.01                                     | 10.0                       | 50                   | 0.05                    | 2.0   |
|                                              | CSP3                                  | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.2   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.4   |
|                                              | Aquatic Environmental Variables (AEV) | 0.1      | 0.02                                     | 5.0                        | 10                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 100                  | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.01                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.05                    | 2.0   |
|                                              |                                       | 0.1      | 0.02                                     | 5.0                        | 50                   | 0.1                     | 2.0   |
| $W_a$ affected by ratio $r$ at different AEV | WCSP1                                 | 0.2      | 0.08                                     | 2.5                        | 10~50                | [0.01, 0.05, 0.1]       | 2.0   |
|                                              | WCSP2                                 | 0.2      | 0.02                                     | 10.0                       | 10~50                | [0.01, 0.05, 0.1]       | 2.0   |
| $W_a$ affected by $f_d$ at different AEV     | WFD1                                  | 0.05     | 0.02                                     | 2.5                        | 10                   | [0.01, 0.05, 0.1]       | 2.0   |
|                                              |                                       | 0.05     | 0.02                                     | 2.5                        | 10                   | [0.01, 0.05, 0.1]       | 2.2   |
|                                              |                                       | 0.05     | 0.02                                     | 2.5                        | 10                   | [0.01, 0.05, 0.1]       | 2.4   |
|                                              | WFD2                                  | 0.05     | 0.02                                     | 2.5                        | 40                   | [0.01, 0.05, 0.1]       | 2.0   |
|                                              |                                       | 0.05     | 0.02                                     | 2.5                        | 40                   | [0.01, 0.05, 0.1]       | 2.2   |
|                                              |                                       | 0.05     | 0.02                                     | 2.5                        | 40                   | [0.01, 0.05, 0.1]       | 2.4   |
| $t_e$ with the same $r$ at different AEV     | ETF1                                  | 0.2      | 0.08                                     | 2.5                        | 10~50                | [0.01, 0.05, 0.1]       | 2.0   |
|                                              | ETF2                                  | 0.05     | 0.02                                     | 2.5                        | 10~50                | [0.01, 0.05, 0.1]       | 2.0   |

The collisional efficiency  $\alpha$  quantifies the floc cohesion/stickiness in the aggregation process. A large value of  $\alpha$  encourages floc growth. This direct proportionality can be noted when comparing the mass concentration distribution  $c_f$  at the equilibrium state for three different collisional efficiency values (see Scenario CSP1 in Table 4.1 and results in Figure 4.1a). The lowest collisional efficiency value (i.e.,  $\alpha = 0.05$ ) provides a mass concentration distribution  $c_f$  in the range between

$\min(d_f) = 20.9 \mu m$  and  $\max(d_f) = 200.6 \mu m$  (see the blue solid line in Figure 4.1a) with a weighted average floc size of  $d_a = 52.5 \mu m$  (blue dashed line). By doubling the collisional efficiency value from  $\alpha = 0.05$  to  $\alpha = 0.1$ , the mass concentration distribution  $c_f$  expands toward larger size classes with  $\min(d_f) = 22.79 \mu m$  and  $\max(d_f) = 368.8 \mu m$ , respectively (compare red and blue solid lines in Figure 4.1a). The weighted average floc size increases by a factor of 1.8 to  $d_a = 94.5 \mu m$  (compare blue and red dashed lines). Doubling the collisional efficiency again from  $\alpha = 0.1$  to  $\alpha = 0.2$  leads  $c_f$  to continue to expand and to shift to larger floc size classes since the  $\min(d_f)$ ,  $\max(d_f)$  and  $d_a$  increase to  $24.86 \mu m$ ,  $739.6 \mu m$  and  $184 \mu m$ , respectively.

Conversely, higher values of the fragmentation rate  $\beta$  represent weaker floc yield strengths and encourage floc breakup (see Equations (2.11) and (2.12)) and produce smaller flocs (see blue line in Figure 4.1b). However, decreasing  $\beta$  can cause a relatively larger aggregation effect since these two processes are inversely related in the balance equation (2.5). In fact, the three mass concentration  $c_f$  distributions associated with the three (decreasing) fragmentation rates  $\beta$  (Figure 4.1b) in Scenario CSP2 are identical to those in Scenario CSP1 shown in Figure 4.1a for the three (increasing) collisional efficiency  $\alpha$  values because each identical pair has the same ratio between  $\alpha$  and  $\beta$  (compare  $r = \alpha/\beta$  in Table 4.1). This confirms that the ratio  $r$  quantifies the participation balance between aggregation and the breakup process and controls the equilibrium floc size distributions (Verney et al., 2011).

We further investigate the effect of fractal dimension, which is associated with the parameterization of the floc structure in the breakup terms (i.e.,  $G_{bS}$  and  $L_{bS}$ , see Equations (2.9), (2.10)) via the rate function  $B$  (see Equation (2.11)). A larger fractal dimension produces slightly larger flocs and narrower size distributions (see Figure

4.1c). Overall, the distributed mass concentration  $c_f$  over the floc size class  $d_f$  is not sensitive to the fractal dimension  $f_d$ . However, fractal dimension determines the floc structure and the resulting floc density and settling velocity via Equations (2.13) and (2.16). A local sensitivity analysis for the weighted average settling velocity  $w_a$  will be reported later in this section.

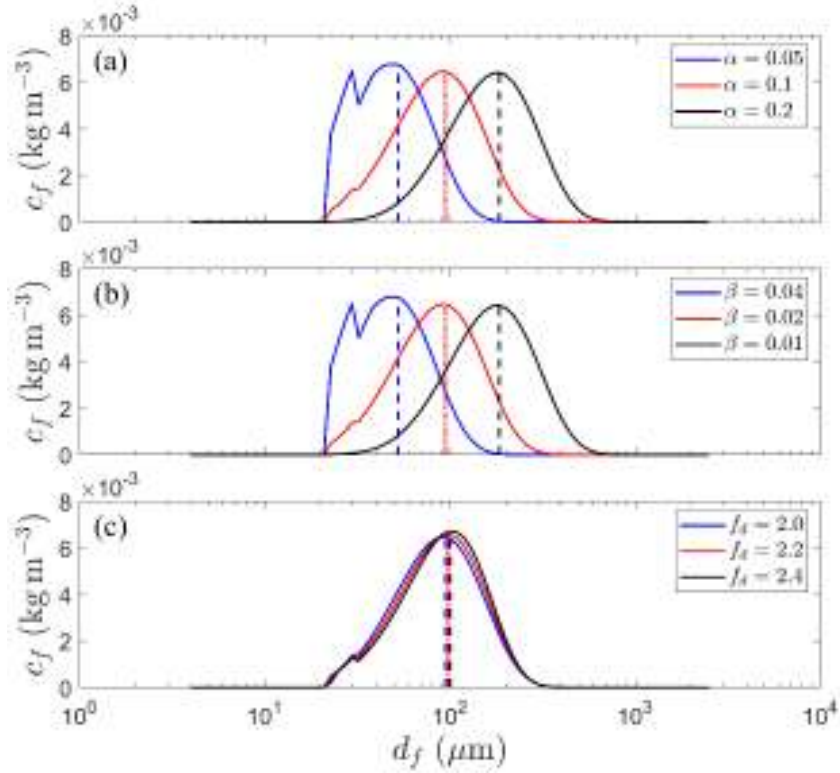


Figure 4.1. Distributed mass sediment concentration  $c_f$  over the floc size classes  $d_f$  at the equilibrium state by varying (a) collisional efficiency  $\alpha$ , (b) fragmentation rate  $\beta$ , and (c) fractal dimension  $f_d$ . These simulations correspond to  $S = 50 \text{ s}^{-1}$  and  $C = 0.05 \text{ kg m}^{-3}$ .

The turbulent shear rate  $S$  is the main driving factor to induce both aggregation and fragmentation (breakup). However, it is noted that the fragmentation term depends on the turbulent shear rate  $S$  with a higher power of 1.5 compared to that of the aggregation term (compare Equations (2.11) and (2.8)). For instance, a low value of the turbulent shear rate (i.e.,  $S = 10 \text{ s}^{-1}$ ) produces a wide mass concentration distribution  $c_f$  with floc size ranges from  $\min(d_f) = 24.86 \text{ }\mu\text{m}$  to  $\max(d_f) = 806.8 \text{ }\mu\text{m}$ , and a weighted average floc size  $d_a$  of  $206.3 \text{ }\mu\text{m}$  (see the blue lines Figure 4.2a). On the other hand, using a high turbulent shear rate of  $S = 150 \text{ s}^{-1}$  generates a floc size range from  $\min(d_f) = 22.79 \text{ }\mu\text{m}$  to  $\max(d_f) = 183.9 \text{ }\mu\text{m}$  with a weight-averaged floc size  $d_a$  of  $58.46 \text{ }\mu\text{m}$  (see the black lines in Figure 4.2a). Therefore, it can be concluded that a higher turbulent shear rate enhances the influence of fragmentation and produces smaller floc sizes at the equilibrium state and vice versa.

Regarding the local sediment concentration  $C$ , the trend is opposite since it promotes the aggregation process (Winterwerp, 1998). The lowest concentration (i.e.,  $C = 0.01 \text{ kg m}^{-3}$ ) shows the  $c_f$  distribution shifting to lower floc sizes with floc size classes ranging between  $\min(d_f) = 22.79 \text{ }\mu\text{m}$  and  $\max(d_f) = 64.73 \text{ }\mu\text{m}$  and a weighted average floc size of  $d_a = 29.25 \text{ }\mu\text{m}$  (see blue lines in Figure 4.2b). Increasing the sediment mass concentration  $C$  to  $0.05 \text{ kg m}^{-3}$  favors the emergence of larger flocs, where the minimum floc size class endures (i.e.,  $\min(d_f) = 22.79 \text{ }\mu\text{m}$ ) but the maximum  $d_f$  and weighted average floc size are increased to  $\max(d_f) = 183.9 \text{ }\mu\text{m}$  and  $d_a = 52.5 \text{ }\mu\text{m}$ , respectively (compare blue with red solid lines in Figure 4.2b). This direct proportionality remains for the maximum concentration  $C = 0.1 \text{ kg m}^{-3}$  investigated with  $\min(d_f) = 22.79 \text{ }\mu\text{m}$ ,  $\max(d_f) = 368.8 \text{ }\mu\text{m}$  and  $d_a = 94.63 \text{ }\mu\text{m}$  (see black lines in Figure 4.2b).

Importantly, the sensitivity analysis also reveals a trend related to the types of floc size distribution. A bimodal floc size distribution is obtained for the three physical conditions investigated here. The first one is related to cohesive sediment properties of low  $r$  values either when the stickiness properties are low (see  $\alpha = 0.05$  in Figure 4.1a), or the floc yield strengths are weak (see  $\beta = 0.04$  Figure 4.1b). The second condition is for an energetic environment where high turbulent shear can break large flocs (see black line in Figure 4.2a). The last circumstance is associated with the limited availability of cohesive sediment at low sediment concentration (see the red and blue lines in Figure 4.2b).

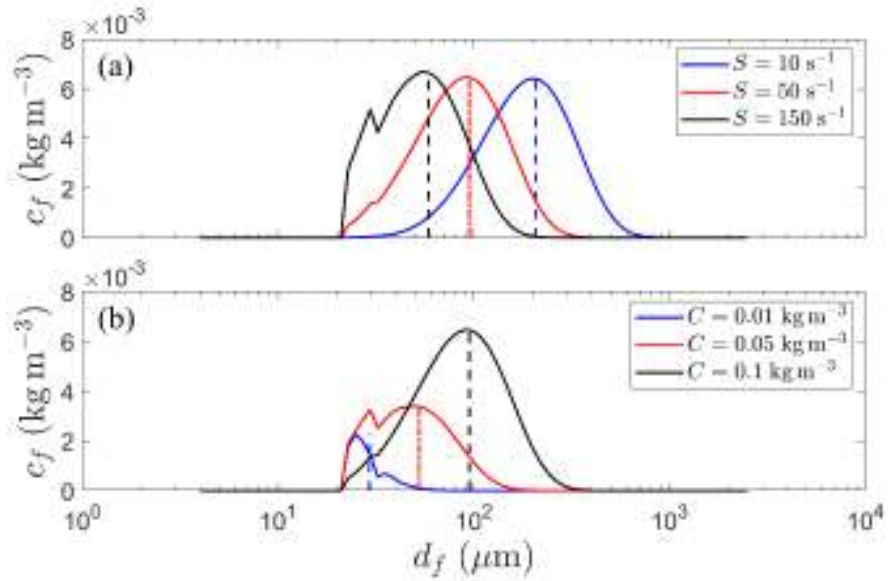


Figure 4.2 Distributed mass sediment concentration  $c_f$  over the floc size classes  $d_f$  at equilibrium by varying (a) the turbulent shear rate  $S$ , and (b) the sediment concentration  $C$ . The floc properties correspond to  $r = 5$  and  $f_d = 2.0$

The previous analysis revealed that the ratio  $r = \alpha/\beta$  controls the distributed mass concentration  $c_f$  at equilibrium since varying  $\alpha$  or  $\beta$  separately show irrelevance if their ratio  $r$  remains the same. The same conclusion is obtained for the weighted average floc size class  $d_a$ , floc density  $\rho_a$ , and settling velocity  $W_a$  since they are all derived from  $c_f$ . To have a better understanding of the flocculation effect on the weighted average settling velocity  $W_a$ , additional simulations are carried out with detailed variation of  $S$  from  $10 \text{ s}^{-1}$  to  $50 \text{ s}^{-1}$ , maintaining the same sediment concentration values (i.e.,  $C_1 = 0.01 \text{ kg m}^{-3}$ ,  $C_2 = 0.05 \text{ kg m}^{-3}$  and  $C_3 = 0.1 \text{ kg m}^{-3}$ ). The group data are classified into two categories for this analysis, the low cohesion scenario WCSP1 with  $r = 2.5$  (see solid lines in Figure 4.3) and high cohesion WCSP2 with a  $r = 10$  (see dashed lines in Figure 4.3). The results show that high cohesion properties (higher stickiness or floc yield strength) and sediment concentration produce larger flocs, and consequently a larger floc settling velocity  $W_a$ . The settling velocity decreases with increasing turbulent shear  $S$ . However, its rate of decrease is smaller for flocs of lower sediment concentration  $C$  and lower  $r$ . At sediment concentrations around  $0.01 \text{ kg m}^{-3}$ , the settling velocity is nearly constant around  $0.1 \sim 0.2 \text{ mm/s}$  regardless of  $r$  and  $S$  (see the solid and dashed blue lines in Figure 4.3). For high  $S$ , the dependence of the settling velocity on  $S$  is negligible because the floc size is mainly controlled by breakup, and it is limited by the Kolmogorov length scale. Larger sediment concentrations and higher stickiness (larger  $r$ ) act together to increase the floc settling velocity and its variability with  $S$ .

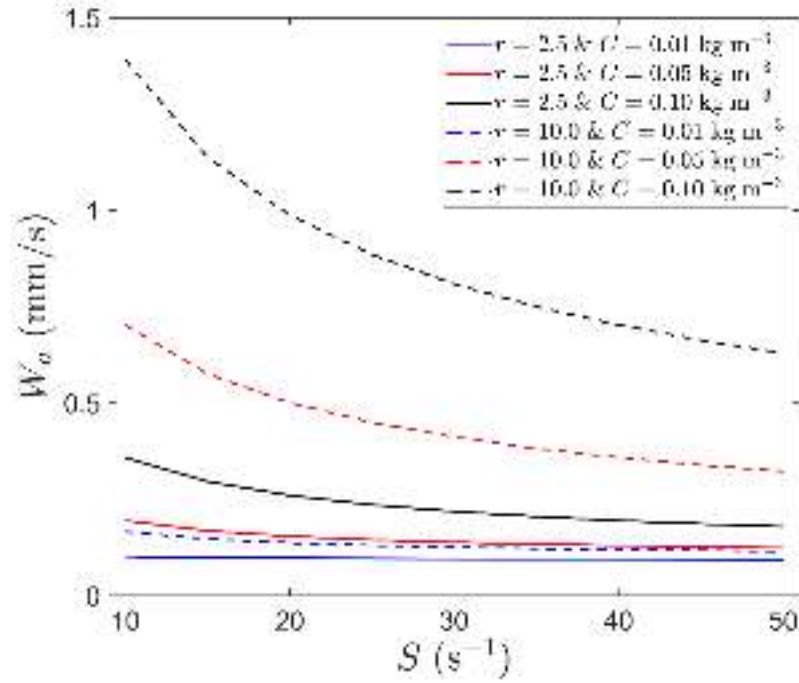


Figure 4.3 Weighted average settling velocity  $W_a$  in the equilibrium state considering the variation of turbulent shear rate  $S$  and sediment concentration  $C$ . The floc fractal dimension corresponds to  $f_d = 2.0$  and results from  $r = 2.5$  and  $10.0$  are shown.

The fractal dimension affects the modeling of the weighted average settling velocity  $W_a$  in two ways. Firstly, the fractal dimension plays a role in floc fragmentation (see Equation (2.11)), but its effect on the calculated floc size distribution is minor (see Figure 4.1c). Secondly and more importantly, the fractal dimension directly controls the floc density (Equation (2.13)) and hence the floc settling velocity (Equations (2.16)). To explore the effect of the fractal dimension on the weighted average settling velocity  $W_a$ , we compare the results of three different values of the fractal dimension (i.e.,  $f_d = 2.0$ ,  $f_d = 2.2$  and  $f_d = 2.4$  in Figure 4.4) at  $r = 2.5$ . Increasing the fractal dimension clearly increases the weighted average settling velocity  $W_a$ . At a low turbulent shear

rate of  $S = 10 \text{ s}^{-1}$  and a high sediment concentration of  $C = 0.10 \text{ kg m}^{-3}$  (black-solid line in Figure 4.4), increasing the fractal dimension from 2.0 to 2.4 causes a factor 4 increase of the settling velocity, while at a higher shear rate of  $S = 40 \text{ s}^{-1}$  at a low sediment concentration of  $C = 0.01 \text{ kg m}^{-3}$ , only a factor 2 increase of the settling velocity is observed (blue-dashed line). For higher cohesion at  $r = 10$ , similar trends are observed, but a factor 7 increase in the settling velocity is observed when the fractal dimension increases from 2.0 to 2.4 at a relatively the low turbulent shear rate of  $S = 10 \text{ s}^{-1}$  and a rather high sediment concentration of  $C = 0.10 \text{ kg m}^{-3}$  (not shown for brevity). We must, therefore, acknowledge that the uncertainty in the fractal dimension can cause large uncertainties in the settling velocity, especially in the condition of low turbulent shear rate, high sediment concentration, and sediments with high cohesion and high yield strength.

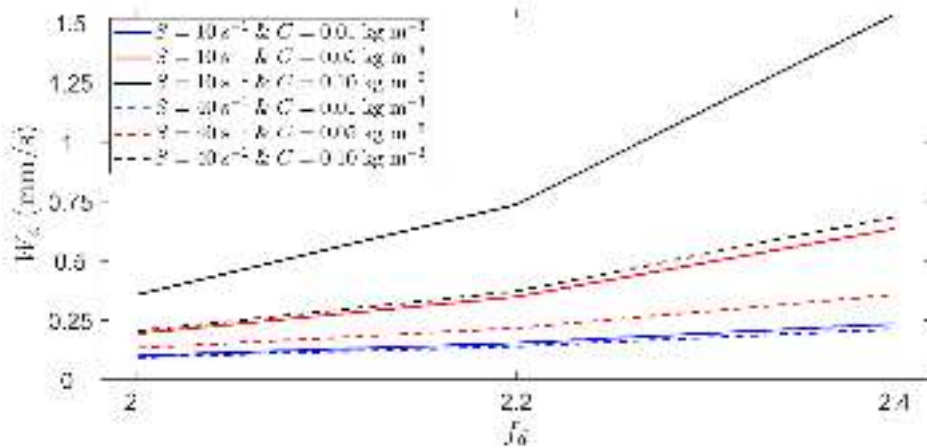


Figure 4.4 Weighted average settling velocity  $W_a$  in the equilibrium state as a function of the fractal dimension  $f_d$  with a ratio  $r = 2.5$  and three different local statistically averaged sediment concentrations  $C$ . The turbulent share rate  $G$  corresponds to (a)  $S = 10 \text{ s}^{-1}$ , (b)  $S = 25 \text{ s}^{-1}$ , and (c)  $S = 40 \text{ s}^{-1}$ .

Up to this point, the local analysis reveals that the ratio parameter  $r = \alpha/\beta$  controls the resulting floc size distribution in the equilibrium state, regardless of varying  $\alpha$  or  $\beta$  as long as their ratio  $r$  remains constant. However, the temporal evolution of the floc size distribution does depend on the magnitudes of  $\alpha$  and  $\beta$  even when their ratio  $r$  is kept constant. This can be characterized by the time required to reach the equilibrium state for a distributed concentration  $c_f$  over the floc size distribution  $d_f$ , which is called equilibrium flocculation time  $t_e$ . In the simulation results,  $t_e$  is calculated at the instant when  $c_f$  over  $d_f$  becomes time independent. A sensitivity analysis for  $t_e$  is carried out using the established turbulent shear rate (from  $10 \text{ s}^{-1}$  to  $50 \text{ s}^{-1}$ ) and sediment concentration ( $C_1 = 0.01 \text{ kg m}^{-3}$ ,  $C_2 = 0.05 \text{ kg m}^{-3}$  and  $C_3 = 0.1 \text{ kg m}^{-3}$ ) values at  $f_d = 2.0$  and  $r = 2.5$ . To demonstrate the individual influence of  $\alpha$  and  $\beta$  with a constant  $r = 2.5$ , the data are classified in two scenarios ETF1 and ETF2 (see Table 4.1), where the first corresponds to high values of  $\alpha$  and  $\beta$  (see black contour lines in Figure 4.5), and the second to low values (see dashed red contour lines in Figure 4.5). Higher magnitudes of  $\alpha$  and  $\beta$  decrease the equilibrium flocculation time. This suggests that stronger cohesion properties reach an equilibrium floc distribution faster. Regarding the aquatic environment variables, higher  $S$  and  $C$  contribute to shorter equilibrium flocculation time.

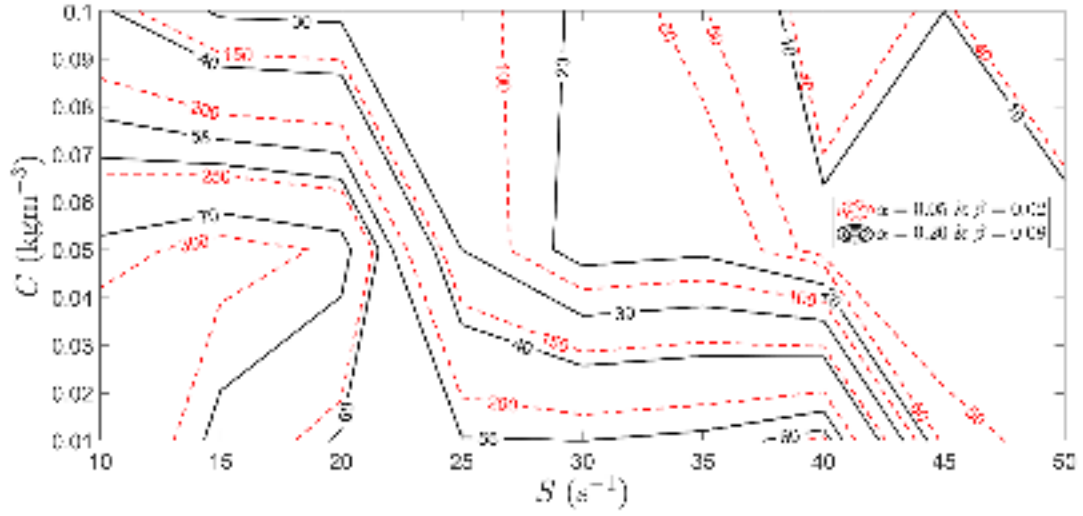


Figure 4.5 Contours of the equilibrium flocculation time in minutes as a function of the turbulent shear rate  $S$  and the sediment concentration  $C$  for  $\alpha = 0.05, \beta = 0.02$  (red-dashed lines) and by increasing both parameters by four times to  $\alpha = 0.2, \beta = 0.08$  (black lines). Notice that both cases have the same  $r = \alpha/\beta = 2.5$ .

### 4.3 Transport analysis using the modeling framework

The transport analysis using the proposed modeling framework (see Section 2.1) investigates how flocculation dynamics control the settling velocity of cohesive sediment and the resulting sediment distribution in a current bottom boundary layer. We use the DNS model of Yue et al. (2020) and carry out two simulations at Reynolds number  $Re_\tau = u_\tau L_3 / \nu = 180$  defined based on the friction velocity specified to be  $u_\tau = 0.009 \text{ m/s}$ , channel depth  $L_3 = 0.02 \text{ m}$  and water viscosity of  $\nu = 10^{-6} \text{ m}^2/\text{s}$ . The first simulation is for clear fluid without sediment, whereas the second simulation incorporates the suspended sediment by specifying a critical bottom shear stress  $\tau_c = 1 \times 10^{-1} \text{ Pa}$  and a constant settling velocity of  $0.5 \text{ mm/s}$ . Figures 4.6a and 4.6b show the turbulence-averaged velocity profiles  $\langle u_1 \rangle_{12t}$  and turbulent shear rate  $S$  from the clear fluid simulation, the sediment-laden simulation and another clear fluid DNS data

at the same Reynolds number reported by Vreman et al. (2014). The comparison between clear fluid cases shows an averaged error of 0.17%. A very small discrepancy in the  $S$  profile near the top boundary with the data of Vreman et al. (2014) can be explained by the different top boundary conditions., Vreman et al. (2014) imposed a no-slip boundary condition while the present study imposes a free-slip boundary. Moreover, the nearly identical results for the simulations with and without sediment confirm that the sediment concentration produced in this dataset is sufficiently dilute and turbulence is not affected by the presence of sediment. By identifying the sediment concentration at  $x_3 = 0.4 \text{ cm}$  ( $x_3^+ = 36$ ) to be  $0.039 \text{ kg m}^{-3}$  from the DNS data, we generate the analytical solution for suspended fine sediment using the well-known Rouse profile (Rouse 1941). The agreement between the simulation data and the Rouse profile (see Figure 4.6c) again proves that these simulation data satisfy the dilute assumption used in the modeling framework.

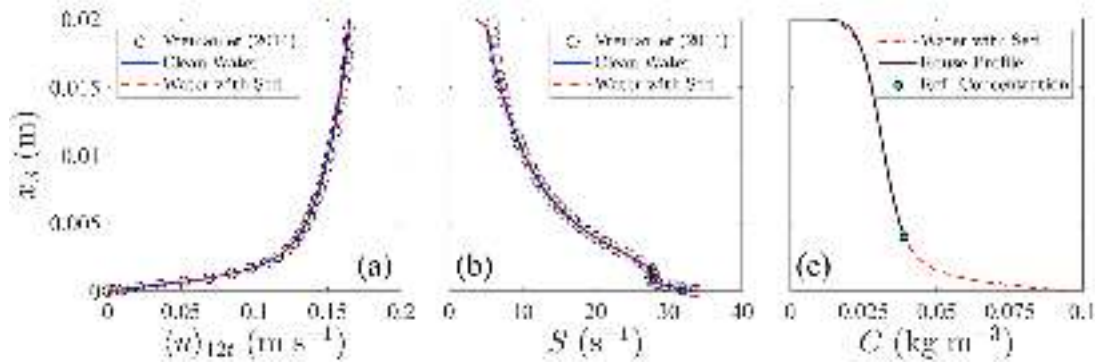


Figure 4.6. Turbulence-averaged profiles for (a) streamwise velocity, (b) turbulent shear rate and (c) sediment concentration.

The turbulent shear rate  $S$  and the turbulence-averaged sediment concentration  $C$  profiles from the DNS results are provided as input to the modeling framework (i.e., Step I in Figure 2.1). The PBE flocculation model (Verney et al., 2011) is applied at every vertical location  $x_3$ , identical to the DNS grid locations, to obtain the corresponding equilibrium floc size distribution  $c_f$  (Step II in Figure 2.1). Identical to the local analysis presented in Section 4.2, the PBE flocculation model is discretized into 75 floc size classes from 4  $\mu\text{m}$  to 2500  $\mu\text{m}$  with a size class interval distributed logarithmically. Three different ratios between the collisional efficiency and fragmentation rate ( $r = \alpha/\beta = [2.5, 5.0, 10.0]$ ) are evaluated to examine the number of iterations required to reach the converged solutions, which uses the Root-Mean-Square error  $E_W$  between the previous and the present settling velocity profiles is less than a tolerance  $\epsilon_W = 1 \times 10^{-6} \text{ m s}^{-1}$  as a threshold (see the dashed-black line in Figure 4.7). The analysis reveals that the number of iterations and the Root-Mean-Square error are proportional to the ratio  $r$ . When a floc is of lower cohesion or low yield stress at  $r = 2.5$  (easier to break), four iterations are sufficient to reach the converged solution with a very small error of  $O(10^{-8}) \text{ m s}^{-1}$  (see the blue line in Figure 4.7). By doubling the influence of cohesion at  $r = 5.0$ , the same number of iterations is needed (see the green line in Figure 4.7) but the error increases by an order of magnitude  $O(10^{-7}) \text{ m s}^{-1}$ . When the floc is of high cohesion or more difficult to break (i.e.,  $r = 10$ ), the number of iterations increases to six as the convergence error  $E_W = 9.7 \times 10^{-7} \text{ m s}^{-1}$  is just below the tolerance criterion  $\epsilon_W$  (see the red line in Figure 4.7).

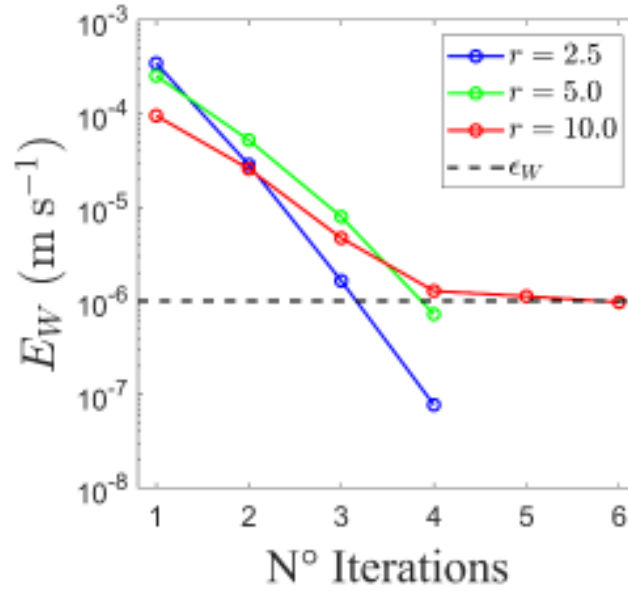


Figure 4.7. Convergence analysis shown as the Root-Mean-Square error of the settling velocity profiles ( $E_W$ ) plotted against the number of iterations for three different  $r$  values.

A sample of how the iterations of the weighted average floc property profiles reach a converged solution (Iteration between Step II and IV in Figure 2.1) is presented for  $r = 5$  in Figure 4.8. Although the first iteration achieves a solution with 5% error from the converged concentration profile  $C$  (compare the magenta line with the blue dashed line in Figure 4.8b), the weighted average floc size, floc density and settling velocity profiles show much more significant errors (compare the magenta line with the blue dashed line in Figure 4.8c, 4.8d and 4.8e). Better agreement is achieved in the second iteration (see the green lines in Figure 4.8c, 4.8d and 4.8e). However, notable errors can still be seen near the bottom. This visual disagreement disappears in the 3rd iteration with  $E_W = 7.9 \times 10^{-6} \text{ m s}^{-1}$ , which is still significantly above the prescribed tolerance (see the green line in Figure 4.7). The error  $E_W$  decreases by one order of

magnitude to  $E_w = 7.2 \times 10^{-7} \text{ m s}^{-1}$  in the 4th iteration, which is lower than the tolerance criterion  $\epsilon_w = 10^{-6} \text{ m s}^{-1}$ , and converged solutions are obtained. It is interesting to point out that even though the prescribed initial uniform settling velocity of  $0.5 \text{ mm/s}$  is about a factor two larger than the final solution, the convergence in the present modeling framework is still very fast.

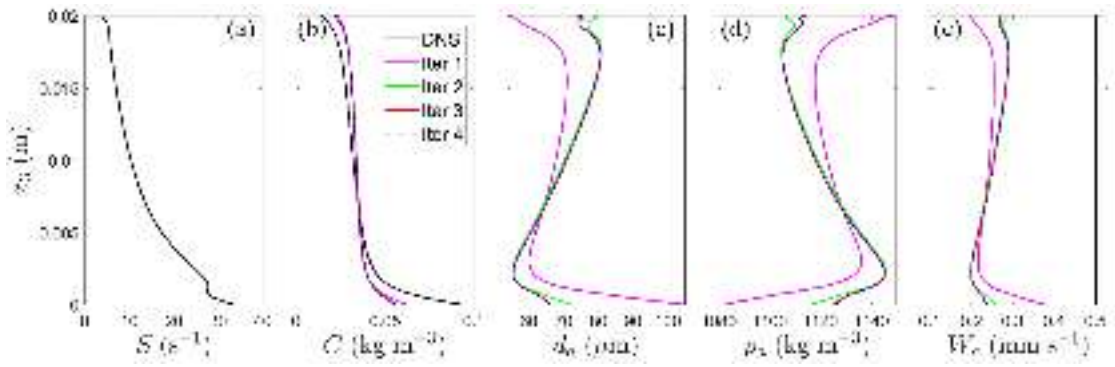


Figure 4.8. Convergence of weighted average profiles at different iteration stages for  $r = 5.0$ . (a) the prescribed turbulent shear rate  $S$  from DNS, (b) turbulence-averaged sediment concentration  $C$ , (c) floc diameter  $d_a$ , (d) floc density  $\rho_a$  and (e) settling velocity  $W_a$ . The black lines in (b) and (e) represent the initial concentration profile and constant settling velocity of  $0.5 \text{ mm s}^{-1}$ .

The converged weighted average concentration profiles for the three different  $r$  ratios ( $r = \alpha/\beta = [2.5, 5.0, 10.0]$ ) are presented in Figure 4.9b. Depending on the aggregation and breakup influences on floc size and, hence, settling velocity, the sediment mass is redistributed in the water column due to vertical transport. For instance, a reasonably well-mixed profile is generated when the breakup process is relatively more important at a low  $r = 2.5$  value (low cohesion or low floc yield strength). Decreasing the breakup influence (or increasing the aggregation effects) by

doubling  $r$  to 5.0 or further doubling it to 10, more sediment is relocated near the bottom and the negative concentration gradient becomes sharper (compare the blue with the green and red lines in Figure 4.10b). According to the vertical mass balance shown in Equation (2.4), a large negative sediment concentration gradient must be due to larger settling velocity. Indeed, the weighted average floc size  $d_a$  and settling velocity  $W_a$  exhibit a positive correlation with respect to the  $r$  value (Figures 4.9c and 4.9e). The other weighted average floc property to be noted is the density  $\rho_a$ . As the floc stickiness or yield strength decreases (i.e.,  $r = [10.0 \rightarrow 2.5]$ ), the weighted average floc density  $\rho_a$  increases in the water column (Figure 4.9d). This agrees with the interpretation that finer flocs, generated by the dominance of the breakup process via turbulent shear, are of larger density, which is a direct outcome of the fractal concept shown in Equation (2.13). For this reason, variability of  $\rho_a$  around the corresponding depth-averaged value is inverted in proportion compared to  $d_a$  and  $W_a$ . Nevertheless, the direct proportionality between floc size  $d_a$  and settling velocity  $W_a$  can be seen from Equation (2.16) with  $f_d = 2.0$ .

In summary, the relative importance of aggregation and breakup effects in flocculation dynamics, parameterized by  $\alpha$  and  $\beta$  to represent floc cohesion and yield strength, directly controls the magnitude of floc size and settling velocity in the current bottom boundary layer and hence the vertical distribution of cohesive sediment. Flocs with larger cohesion (easier to stick together) and larger yield strength (more difficult to break) produce larger floc sizes and settling velocity and hence more sediments are trapped near the bed.

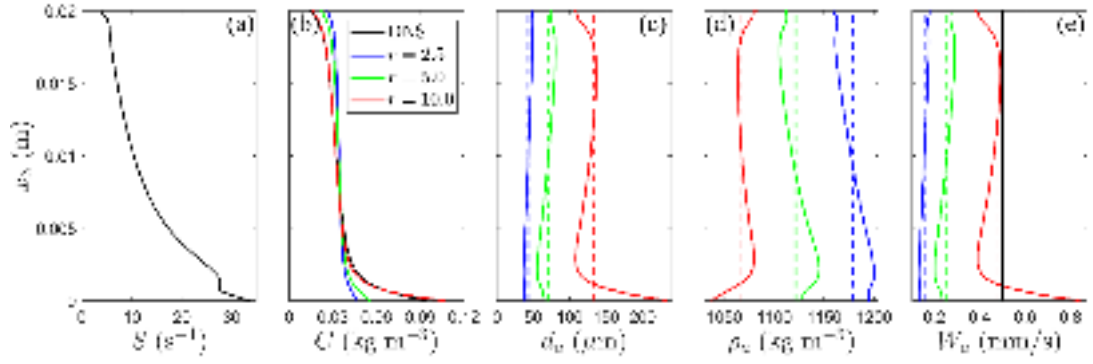


Figure 4.9. Floc stickiness or floc yield strength effects via the parameter ratio  $r$  on weighted average floc property profiles at the fractal dimension  $f_d = 2.0$ . (a) Turbulent shear rate, (b) statistically averaged sediment concentration  $C$ , (c) floc diameter, (d) floc density and (e) settling velocity. The dashed lines correspond to the depth-averaged values.

Typical bottom boundary layer profiles show that both turbulent shear rate and sediment concentration are largest near the bed and decay away from the bed (see Figure 4.9a and 4.9b). Interestingly, according to the local analysis presented in Section 4.2, large floc size and settling velocity exist when the turbulent shear rate is small or/and sediment concentration is large. As the turbulent shear rate dictates the floc breakup process while the sediment concentration encourages floc growth, the vertical structure of the floc size and settling velocity profiles in a bottom boundary layer depend on the intensities of these two quantities at a given vertical location via a competition of floc growth and breakup terms in the PBE equations. More insight into the aggregation or breakup influence on the vertical structure of the cohesive sediment can be obtained by comparing the vertical profiles with their depth-averaged values. For low stickiness or low yield strength, flocs (i.e.,  $r = 2.5$  and  $r = 5.0$ ),  $d_a$  and  $W_a$  are smaller than their depth averaged value in the lower water column (see the blue and green lines in Figure 4.9c) where both the turbulent shear rate and the sediment concentration are large. Since

the smaller floc size near the bed can only be explained by the higher turbulent shear rate causing breakup, the observed vertical variations of  $d_a$  and  $W_a$  are dictated by the turbulent shear rate, not by the sediment concentration. This is consistent with the idea that at low stickiness or low yield strength flocs are easier to break by turbulent shear while the aggregation effect quantified by sediment concentration is relatively minor. On the contrary, increasing the floc stickiness or the yield strength with ratio  $r = 10.0$  causes an increase of  $d_a$  and  $W_a$  to exceed their depth averaged values within the bottom 5.34% of the water column (see the red solid line surpassing the dashed line near the bed in Figure 4.9c). This is explained by the high mass concentration near the bed that encourages floc growth via aggregation, also consistent with the idea that flocs with high stickiness or yield strength encourage floc growth. Notice that once the sediment concentration becomes lower away from the bed,  $d_a$  and  $W_a$  drop below the depth-averaged value suggesting the increasing dominance of turbulent shear as sediment concentration decreases.

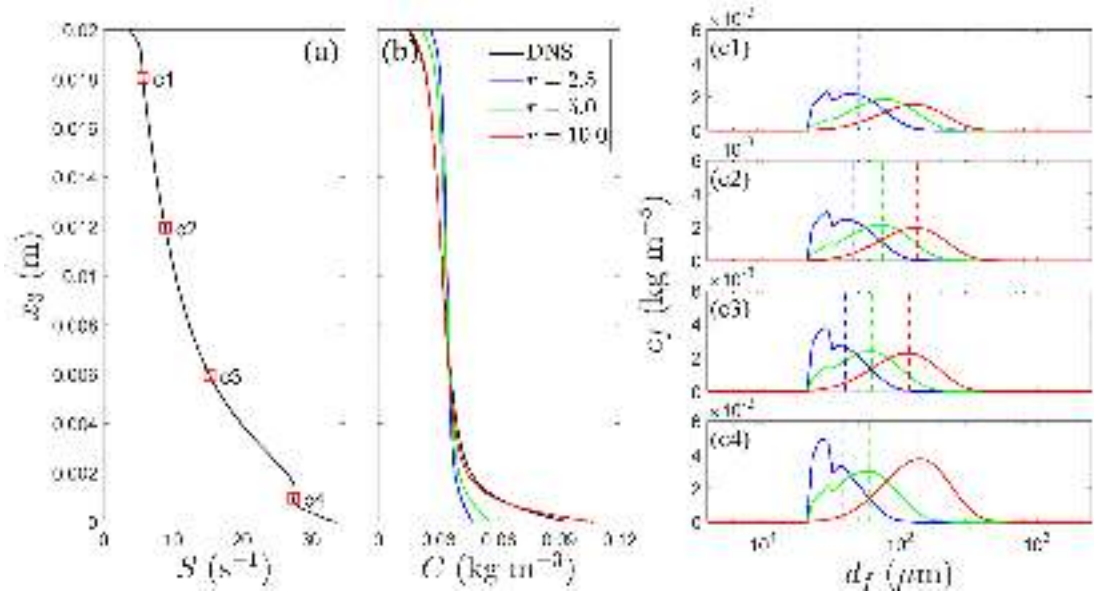


Figure 4.10. (a) Turbulent shear rate profile, (b) mass concentration profile, (c) mass concentration distributions over floc size classes at four different locations (c1)  $x_3 = 0.018\ m$ , (c2)  $x_3 = 0.012\ m$ , (c3)  $x_3 = 0.006\ m$ , and (c4)  $x_3 = 0.001\ m$ . The dashed lines correspond to  $d_a$ .

The floc size distributions shown in Figure 4.10 reveal important results regarding the formation of a bimodal floc size distribution in the current boundary layer. The local analysis presented in Section 4.2 concluded that bimodal distributions exist in three circumstances: low  $r$  value, high turbulent shear, and very low sediment concentration. Floc size distributions shown in Figure 4.10 confirmed that at the lowest  $r$  value ( $r = 2.5$ , see blue lines), bimodal distributions are obtained at all four locations throughout the boundary layer. For the highest  $r$  value ( $r = 10.0$ , see red lines), the bimodal distribution disappears for the entire water column. For moderate  $r$  value investigated here ( $r = 5.0$ , see green lines), a bimodal distribution can be observed in the lower water column (see (c3) and (c4) in Figure 4.10) where turbulent shear is strong.

An important characteristic obtained from the weighted average settling velocity is its variability in the water column due to the flocculation process. Implementing a variable settling velocity in space and time can be computationally intensive in cohesive sediment transport models. As a result, many models opt for using a constant settling velocity instead. Following this idea, the depth-averaged settling velocity  $\overline{W_a}$  is implemented directly in the mass balance equation (Equation (2.2)) to evaluate the ability to recover the sediment concentration profile  $C$  obtained using variable settling velocity. The results show reliable predictions of concentration profiles with low mean-square-errors of 3% and 5% (see Figure 4.11a and 4.11b) when the flocs are of low stickiness or low yield strength (i.e.,  $r = 2.5$  and  $r = 5.0$ , respectively). This means that a variability of the settling velocity below 20% in the whole water column can be a good indicator of using  $\overline{W_a}$  in the present modeling framework (see the blue and red lines in Figure 4.12). In contrast, a less accurate estimate with a mean-square-error of 11.6% can be observed for high stickiness or high yield strength (i.e.,  $r = 10.0$ ). The intense aggregation effect near the sediment bed ( $x_3 < 0.001\text{ m}$ ) induces settling velocity variability significantly above 20% (see the red line in Figure 4.12), causing over-predictions of the sediment concentration  $C$  (see Figure 4.11c). In general, adopting  $\overline{W_a}$  in the mass balance equation is viable when the breakup processes are relatively important to induce well-mixed concentration profiles.

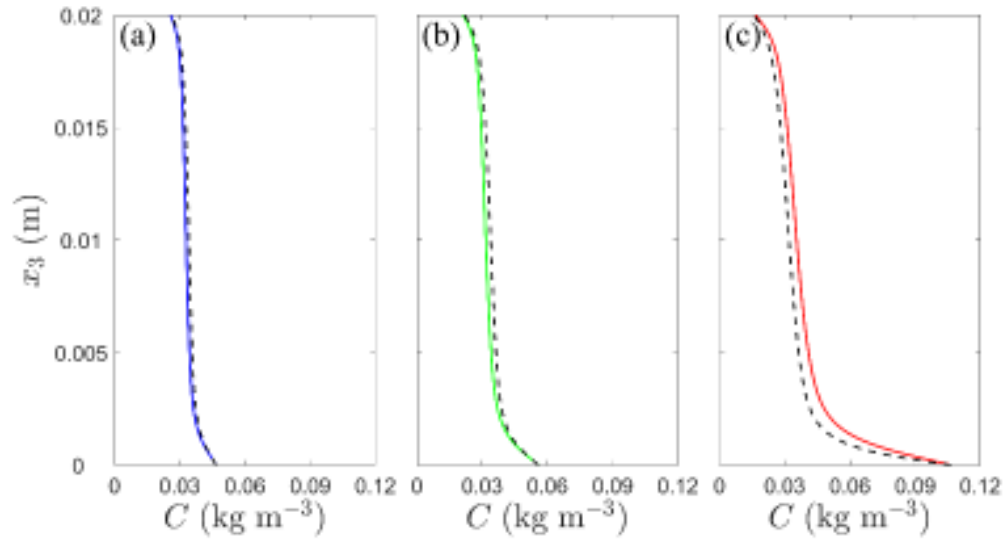


Figure 4.11 Predicted sediment mass concentration profiles using depth-averaged settling velocity (solid line) versus those calculated from the modeling framework (dashed line)  $r = 2.5$  (a),  $r = 5.0$  (b) and  $r = 10.0$  (c).

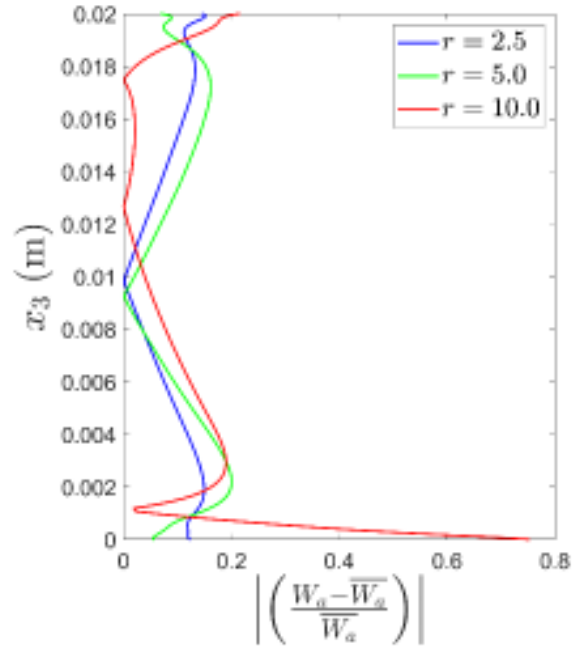


Figure 4.12 Variability of the settling velocity relative to the depth-averaged mean in the water column for the three different  $r$  ratios.

Until now, the weighted average floc property profiles have been determined with a constant fractal dimension of  $f_d = 2.0$ . For a better understanding of its role, the weighted average floc property profiles are calculated for two additional values of  $f_d = 2.2$  and  $f_d = 2.4$  with the cohesion properties set to be  $r = 2.5$  (low cohesion). As far as sediment concentration and settling velocity profiles are concerned, increasing the fractal dimension apparently is similar to increasing the  $r$  value (compare Figure 4.9b and Figure 4.13b). However, the reasons behind the observed features are different. Since the local sensitivity analysis (Section 4.2) indicates a small effect of  $f_d$  on the floc sizes (Figure 4.1c), increasing  $f_d$  only slightly increases the depth averaged settling velocity (dashed lines in Figure 4.13c). A main effect of increasing  $f_d$  is to significantly increase the weighted average floc density  $\rho_a$  (Figure 4.13d) and this is the reason that the settling velocity  $W_a$  also increases accordingly. We notice that in the present transport analysis, the vertical variation of the floc size is seemingly more sensitive to the fractal dimension than in the local analysis. However, we need to remember that the floc size variabilities observed here are mainly due to large vertical variability in turbulent shear rate and sediment concentration.

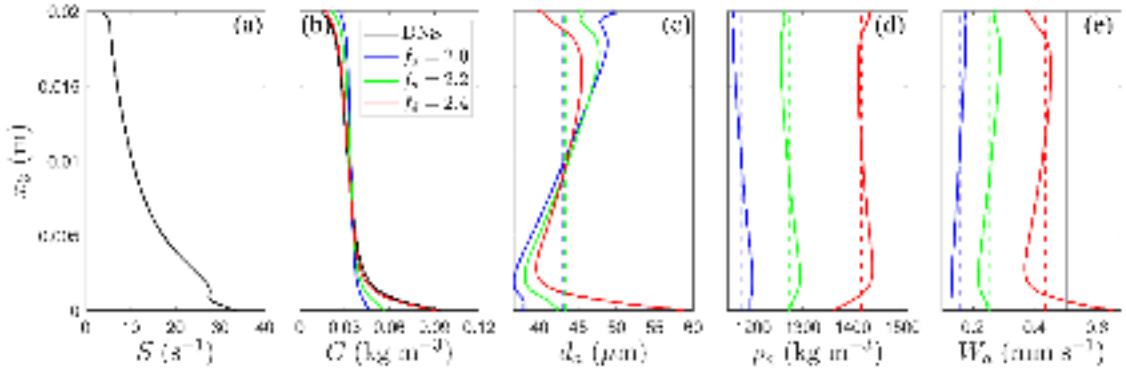


Figure 4.13 Effect of fractal dimension on the weighted average floc properties profiles at  $r = 2.5$ . (a) Turbulent shear rate, (b) sediment concentration  $C$ , (c) floc diameter, (d) floc density and (e) settling velocity. The dashed lines correspond to the depth-averaged values.

#### 4.4 Discussion

The results presented in Section 4.3 indicate that the present modeling framework can quantify the equilibrium flocculation effects on dilute cohesive sediment transport in the bottom boundary layer. This section discusses two important subjects to generalize the use of this modeling framework and to evaluate its limitations.

##### 4.4.1 Closure turbulent Schmidt number

The results presented here are driven by the DNS data in which the turbulent kinetic energy cascade is fully resolved and the turbulent diffusivity  $K_t$  is directly estimated from the calculated sediment turbulent flux and turbulence-averaged concentration gradient (See Equation (4.3)). This procedure can be difficult to apply if the data comes from a Reynolds-Averaged Navier-Stokes (RANS) model or from measurements where the turbulent sediment flux is not available. Usually, these types of models calculate eddy viscosity  $\nu_t$ , and an assumed value of the turbulent Schmidt number  $Sc_t$  is further used to calculate turbulent diffusivity  $K_t$ . Using the DNS data,

both turbulent diffusivity  $K_t$  and eddy viscosity  $\nu_t$  are computed via Equation (4.3) and (4.4) and compared in Figure 4.14a. The results show that it is a good approximation to use the eddy viscosity  $\nu_t$  and  $Sc_t = 1$  to represent the turbulent diffusivity  $K_t$  in most of the water column, where the turbulence is fully developed (see Figure 4.14b at  $x_3^+ = 19.8 \sim 153$ ). The deviations near the bottom correspond to transitional turbulence effects in the viscous sub-layer and buffer layer. The deviation near the top is simply due to the applied free-slip boundary condition. It is important to point out that near the bed with  $x_3^+ < 19.8$ ,  $Sc_t$  increases rapidly toward the bed.

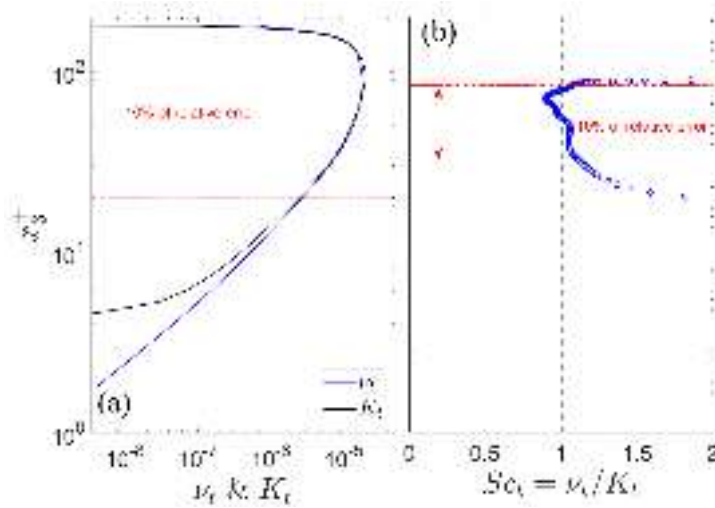


Figure 4.14 (a) Profiles of sediment turbulent diffusivity, eddy viscosity and (b) the corresponding turbulent Schmidt number (circles). The vertical dashed line represents  $Sc_t = 1$  and dotted horizontal lines represent locations of 10% relative error.

Although the previous analysis of  $\nu_t$  and  $K_t$  shows considerable differences near the bottom where the flow is not fully turbulent, the implementation of the approximation that turbulent diffusivity  $K_t$  equals to  $\nu_t$ , or namely  $Sc_t = 1$ , into the

modeling of sediment transport in the vertical water column appears to be appropriate for cohesive sediments of lower  $r$  value. The modeled weighted average settling velocity profiles are used to compare the difference between using  $K_t$  directly (i.e., results from Figure 4.9e) and using  $v_t$  by assuming  $Sc_t = 1$  (see Figure 4.15). For  $r = 2.5$ , assuming  $Sc_t = 1$  can well represent the settling velocity profile in 93% of the water column with a relative error lower than 2%. The maximum relative error corresponds to 3%, which occurs near the top boundary, while near the bed the error is less than 1%. Doubling the ratio to  $r = 5.0$ , assuming  $Sc_t = 1$  reproduces 81% of the settling velocity profile within 2% relative error. The highest relative errors near the bed are just above 2%. For  $r = 10.0$ , assuming  $Sc_t = 1$  reproduces 69% of the settling velocity profile and higher relative errors exceeding 2% are found within  $x_3^+ < 8.1$  near the bed.

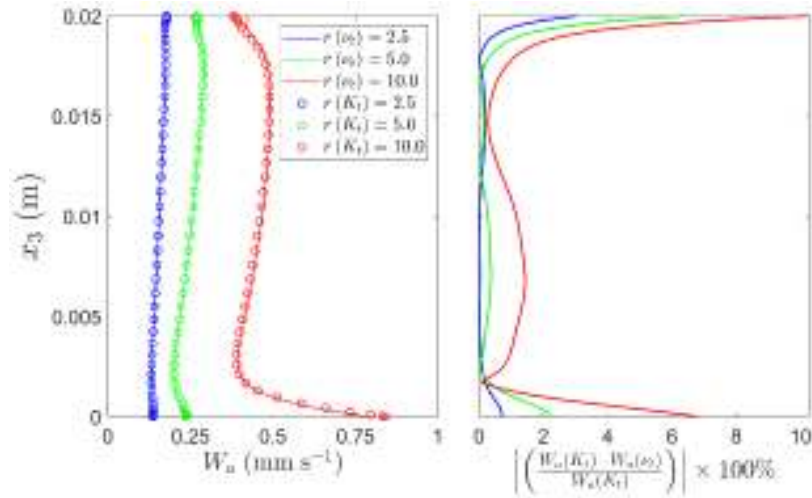


Figure 4.15 (a) Settling velocity profiles calculated by directly using turbulent diffusivity  $K_t$  (circles) or by using eddy viscosity  $v_t$  and assuming  $Sc_t = 1$  (lines) for three different  $r$ . Panel (b) shows their absolute errors.

#### 4.4.2 Equilibrium flocculation time

The present modeling framework requires a turbulent shear rate  $S$  and turbulence-averaged sediment concentration  $C$  profiles as input data to calculate floc properties in the equilibrium state (Step II in Figure 2.1). According to the local analysis (see Figure 4.5), the equilibrium flocculation time is short when sediment concentration, turbulent shear rate and the magnitude of  $\alpha$  and  $\beta$  values are large. In the boundary layer,  $S$  and  $C$  profiles vary in the water column and, hence, the equilibrium flocculation time  $t_e$  must vary accordingly. Figure 4.16 shows the equilibrium flocculation time profiles for three cases with  $r = 2.5, 5.0$  and  $10$  at  $\alpha = 0.1$  and  $f_d = 2.0$ . The  $t_e$  profile is inversely proportional to the increase of the turbulent shear rate  $S$  and the sediment concentration  $C$  toward the sediment bed, consistent with the local analysis (see section 4.2). Regarding the cohesive properties, the equilibrium flocculation time is longer for flocs with high stickiness or yield strength (i.e., large  $r$  values). However, close to the bed, flocs with the largest  $r$  value of  $10$  show a very short  $t_e$  due to high sediment concentration. This shows that a dominance of environmental parameters over cohesive sediment properties is expected near the bottom of the boundary layer.

Moreover, the importance of analyzing  $t_e$  as a function of the water columns is to test our equilibrium assumption. For the cases considered here, the equilibrium flocculation time is generally shorter than 2 hours within  $0.005$  m from the bed, which is about 25% of the water column where both sediment concentration and turbulent shear rate are high, and the most intensive flocculation and variability of the settling velocity occurs (see Figure 4.16). From the local analysis shown in Figure 4.5, if the  $\alpha$  and  $\beta$  values were increased by 4 times, the present equilibrium floc time profile would be shorter by 4 times, and the limitation of the equilibrium assumption can be further relaxed. As an example, Penaloza-Giraldo et al. (2023) carried out a comprehensive

model calibration of the flocculation experiment of Keyvani and Strom (2014) using mixed Kaolinite-Bentonite clay and obtained  $\alpha = 0.25$  and  $\beta = 0.032$ , indicating that the equilibrium flocculation time shown in Figure 4.16 may decrease by about 2.5 times.

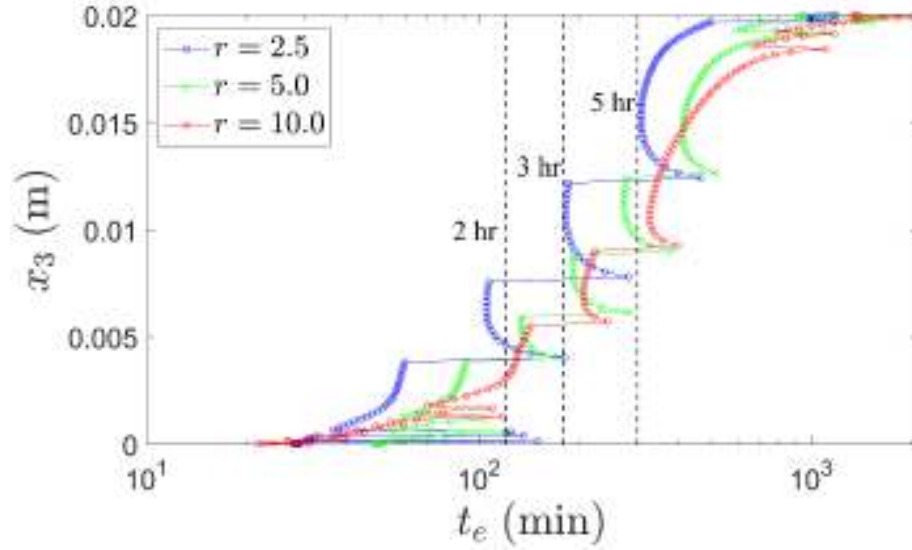


Figure 4.16. Equilibrium flocculation time profiles for three different  $r$  values with  $f_d = 2.0$  and  $\alpha = 0.1$ .

#### 4.5 Conclusions

A cohesive sediment transport modeling framework for a statistically-steady, fully developed current bottom boundary layer is presented, incorporating settling velocity as a variable influenced by flocculation under equilibrium and dilute conditions. The flocculation model is based on solving the PBE for the size distribution of the number concentration of flocs using the open-source model of Verney et al. (2011). Accurate initial input profiles of turbulent shear rate  $S$  and turbulence-averaged sediment concentration  $C$  are generated using DNS data for a statistically steady fully-

developed current bottom boundary layer using the pseudo-spectral model developed by Yue et al. (2020). With the settling velocity treated as a variable due to flocculation, the vertical distribution of the sediment concentration is updated using a turbulence averaged mass balance equation. Although DNS data is used in this study, input profiles from other Reynolds averaged models or measured data can be used as input to the model framework.

The results demonstrate that including the flocculation changes the concentration profile due to variation in the floc size distribution and the resulting settling velocity. A reasonably well-mixed concentration profile is obtained for flocs of lower cohesion or yield strength (smaller  $r$  value), i.e., flocs are easier to break. This condition changes as the aggregation influence increases due to higher floc cohesion or yield strength, relocating more sediment near the bed. The vertical variability of  $W_a$  from its depth-averaged mean value is generally small for flocs of lower  $r$  value. For the highest value  $r = 10$  investigated in this study, a very large settling velocity is obtained near the bed due to high sediment concentration. Using a depth-averaged settling velocity can generally reproduce the sediment concentration profile in the current bottom boundary layer with errors smaller than about 10% when  $r$  is smaller than 10.

Findings reported in this study are based on flocs in the equilibrium state. This study calls for future research on expanding the knowledge and develop a more efficient model framework of flocculation and cohesive sediment transport in non-equilibrium conditions. Laboratory experiments characterizing the floc sediment concentration and settling velocity under inhomogeneous turbulent flow are needed to further validate the present model framework.

## Chapter 5

### FLOCCULATION AND COHESIVE SEDIMENT TRANSPORT IN THE WAVE BOTTOM BOUNDARY LAYER

In this Chapter, the proposed modeling framework (Chapter 2) is used to quantify the flocculation effects on cohesive sediment transport in the wave bottom boundary layer to address Research Question 3. However, an additional assumption is required for the wave bottom boundary layer problem. We investigate the problem driven by a periodic oscillatory motion and the variables now depend on wave phase. Therefore, a double-averaging procedure, namely, turbulence-average and wave-period averaging process must be applied (Nielsen 1992) to the advection-diffusion-settling equation for sediment concentration. Since we formulate the bottom boundary layer process in a tunnel without an actual surface, the present study models wave bottom boundary layers similar to those in oscillating tunnel (U-tube) and the surface wave induced vertical velocity and horizontal velocity and the corresponding surface wave induced boundary layer streaming are neglected. The turbulence-averaged mass balance equation for oscillatory boundary layer can be written as

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_3} \left[ K_s \frac{dC}{dx_3} + W_a C - \langle u'_3 c' \rangle \right] = 0 \quad (5.1)$$

To study wave-period-averaged process, we apply wave-period-average operation over equation (5.1), represented by an overbar " $\overline{\quad}$ ". Since the first term in equation (5.1) become zero after wave-period-average, we can integrate the resulting equation and with further simplification, we obtain:

$$K_s \frac{d\bar{C}}{dx_3} + \bar{W}_a \bar{C} - \overline{\langle u'_3 c' \rangle} = 0 \quad (5.2)$$

By using equation (5.2) for wave-period-averaged mass balance, we ignore the intra-wave correlation between settling velocity variation and sediment concentration variation. This approximation is justified for dilute condition in which the flocculation time-scale is much longer than typical wave period (Winterwerp 2002). The third term represents the wave period averaged turbulent sediment flux. Here we further assume that it can be calculated as:

$$-\overline{\langle u'_3 c' \rangle} = \bar{K}_t \frac{\partial \bar{C}}{\partial x_3}. \quad (5.3)$$

When applying this approximation, we ignore the intra-wave correlations of turbulent diffusivity and sediment concentrations. This approximation can be justified for small settling velocity, or in terms of nondimensional parameters, a small Rouse number defined as the ratio of settling velocity to friction velocity, in which the intra-wave variation of sediment concentration is expected to be small. With these additional assumptions, we can integrate the wave-period-averaged mass balance equation to obtain wave-period-averaged sediment concentration as:

$$\frac{d\bar{C}}{dx_3} = - \frac{\bar{W}_a \bar{C}}{\bar{K}_t + K_s}. \quad (5.4)$$

The above equation is mathematically identical to equation (2.4) for current bottom boundary layer. In other words, the model framework applied for wave (oscillatory) bottom boundary layer is mathematically identical to that in Chapter 4 for current bottom boundary layer, except that we need to keep in mind that the physical quantities are defined as wave-period-averaged quantities with additional

approximation discussed here. To simplify the notation, we will further drop the overbar for the remaining of this chapter.

To address Research Question 3, the scientific objectives are to (1) evaluate how the flocculation process redistributes sediment concentration in the wave bottom boundary layer, (2) investigate how lutocline formations are affected by the cohesive floc properties, and (3) examine the feasibility of implementing a depth-average settling velocity to model cohesive sediment transport in the wave bottom boundary. For these purposes, six baseline cases of DNS are carried out for different constant settling velocity  $w_s$  and critical shear stress of erosion  $\tau_c$  (see section 5.1). The decomposition methodology for analyzing DNS data is presented in section 5.2 with the intention to define the initial wave-period-averaged and turbulence-averaged (double-averaged) shear rate  $S$  and sediment concentration  $C$  profiles to be used by the flocculation model. Simulation results for fine sediment dynamics in the wave boundary layer for constant settling velocity without considering flocculation are presented in Section 5.3. Section 5.4 further investigates how flocculation affect the settling velocity and cohesive sediment distribution in the wave bottom boundary layer by considering three different cohesion properties ( $r = 2.5$ ,  $r = 5.0$  and  $r = 10.0$ ). Section 5.5 provides a summary of this investigation.

## **5.1 Direct numerical simulation baseline cases**

Before incorporating the flocculation process using the modeling framework, six DNS cases, each with a constant settling velocity, are carried out to generate the initial double-averaged shear rate  $S$  and sediment concentration  $C$  profiles (see Table 5.1) and to understand the baseline fine sediment dynamics in the wave bottom boundary layer without considering altered settling velocities by flocculation. The Stoke

Reynolds number of  $Re_\Delta = 800$  is specified for all cases based on its Stokes boundary layer thickness of  $\Delta = \sqrt{2\nu/\Omega_w} = 0.0018 \text{ m}$  as a length scale with a oscillatory (wave) period  $T_w = 2\pi/\Omega_w = 10 \text{ s}$ , and an orbital velocity amplitude of  $U_w = 0.4484 \text{ m/s}$  associated to a prescribed free-stream velocity time series. To re-suspend sediment, three critical bottom shear stress of erosion  $\tau_c$  are used (i.e.,  $\tau_c = [0.8, 0.9, 1.0] \text{ Pa}$ ) with a constant empirical erosion rate of  $m_e = 3 \times 10^{-7} \text{ m/s}$ . Since the magnitude of settling velocity also controls the depositional flux and hence it is a sensitive parameter determining the amount of sediment in the wave boundary layer. Simulations are carried out for two different constant settling velocity  $w_s$ . The first set corresponds to  $0.5 \text{ mm/s}$  (cases C1, C2, and C3 in Table 5.1), following the previous study (Yue et al., 2020). To significantly increase the sediments in the wave boundary layer, the second set of simulation specifies  $w_s = 0.25 \text{ mm/s}$  (cases C4, C5, and C6 in Table 5.1).

The computation domain for all the cases corresponds to  $[L_1 \times L_2 \times L_3] = [60\Delta \times 60\Delta \times 60\Delta] = [0.1070 \times 0.1070 \times 0.1070] \text{ m}$ , where the coordinate origin is located at the bottom-left-front corner, as shown in Figure 2.2. The number of the grid points for the discretization is  $[n_1 \times n_2 \times n_3] = [288 \times 192 \times 161]$ , respectively. The domain size is evaluated to be sufficiently large to contain the largest turbulent eddies and grid resolution is identical to previous DNS simulation studies at an even higher Stokes Reynolds number of 1000 reported by Yue et al. (2020).

Table 5.1. DNS wave cases

| Cases ID  | $NT_w$ | $[M_1 \sim M_2]$ | $\tau_c$ (Pa) | $w_s$ (mm/s) |
|-----------|--------|------------------|---------------|--------------|
| <b>C1</b> | 50     | [30, 50]         | 1.0           | 0.5          |
| <b>C2</b> | 50     | [30, 50]         | 0.9           | 0.5          |
| <b>C3</b> | 50     | [30, 50]         | 0.8           | 0.5          |
| <b>C4</b> | 100    | [80, 100]        | 1.0           | 0.25         |
| <b>C5</b> | 100    | [80, 100]        | 0.9           | 0.25         |
| <b>C6</b> | 100    | [80, 100]        | 0.8           | 0.25         |

## 5.2 Turbulent averaging procedure

As established in Chapter 2, the proposed modeling framework relies on two critical assumptions: the dilute condition and the equilibrium state. To satisfy the second assumption under wave motions, we consider a wave-period-averaged formulation since the time scale of a wave (i.e., seconds) is much smaller than the flocculation time scale (i.e., minutes). Therefore, wave-period-averaged and turbulence-averaged turbulent shear  $S$  and sediment concentration  $C$  profiles are needed to drive the model framework (step I in Figure 2.1). Before computing any wave-averaged quantity, the quasi-steady state needs to be identified via calculating the volume averaged quantities, which is written as follows

$$\langle \psi \rangle_{123}(t) = \frac{1}{L_1 L_2 L_3} \sum_{x_3=0}^{x_3=L_3} \sum_{x_1=0}^{x_1=L_1} \sum_{x_2=0}^{x_2=L_2} \psi(x_1, x_2, x_3, t) \Delta x_1 \Delta x_2 \Delta x_3, \quad (5.5)$$

where  $\psi$  is an arbitrary variable and the angular brakes  $\langle \cdot \rangle$  represents the averaging process in  $x_1$ ,  $x_2$  and  $x_3$ -directions following the subscript notation (i.e., 1, 2 and 3).

Subsequently, the plane- and wave-phase averaging process is applied to calculate turbulence-averaged quantities for the number of wave periods  $M = M_2 - M_1$  in the time range  $[M_1 T_w, M_2 T_w]$  after the quasi-steady is reached. This is computed by

$$\langle \psi \rangle_{12p}(x_3, t) = \frac{1}{M L_1 L_2} \sum_{M_1}^{M_2} \sum_{x_1=0}^{x_1=L_1} \sum_{x_2=0}^{x_2=L_2} \psi(x_1, x_2, x_3, t) \Delta x_1 \Delta x_2, \quad (5.6)$$

Finally, the wave-period-averaged quantities are calculated as follows

$$\langle \psi \rangle_{12pw}(x_3) = \frac{1}{(M_1 - M_2) T_w} \sum_{t=M_1 T_w}^{t=M_2 T_w} \langle \psi \rangle_{12p}(x_3, t) \Delta t, \quad (5.7)$$

### 5.3 DNS oscillatory flow simulations

The volume-averaged (Equation 5.5) concentration  $\langle c \rangle_{123}$  field is used to identify the temporal development to quasi-equilibrium steady state for the six DNS cases. In general, this state is reached after 30 waves for lower sediment loads when the constant settling velocity  $w_s = 0.5 \text{ mm/s}$  is specified (see Figure 5.1). The volume-averaged concentration is also controlled by the critical shear stress of erosion, and it is larger when critical shear stress of erosion is lower. In contrast, more waves are required for cases with lower settling velocity  $w_s = 0.25 \text{ mm/s}$  due to increased sediment load in the water column and a quasi-equilibrium state is obtained after 80 waves (see Figure 5.2).

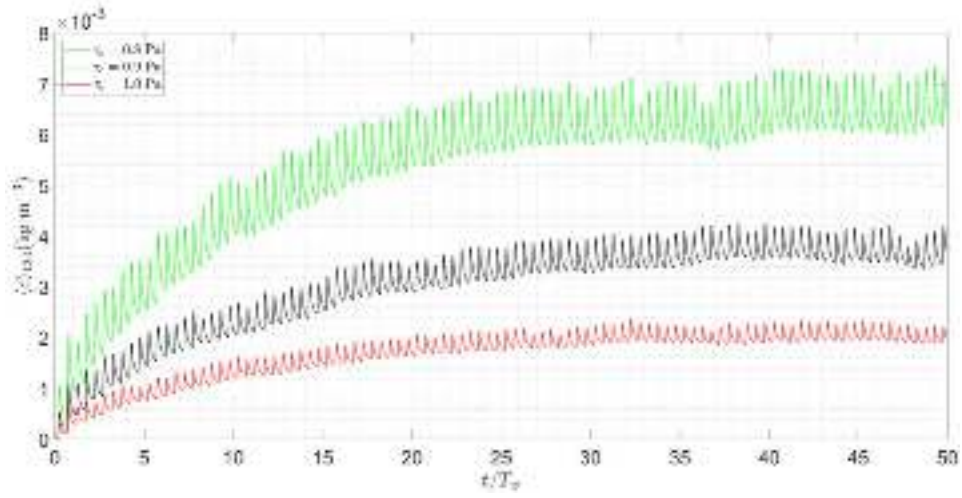


Figure 5.1. Domain-averaged concentration time series for different critical shear stress with a constant settling velocity of  $w_s = 0.5 \text{ mm/s}$ .

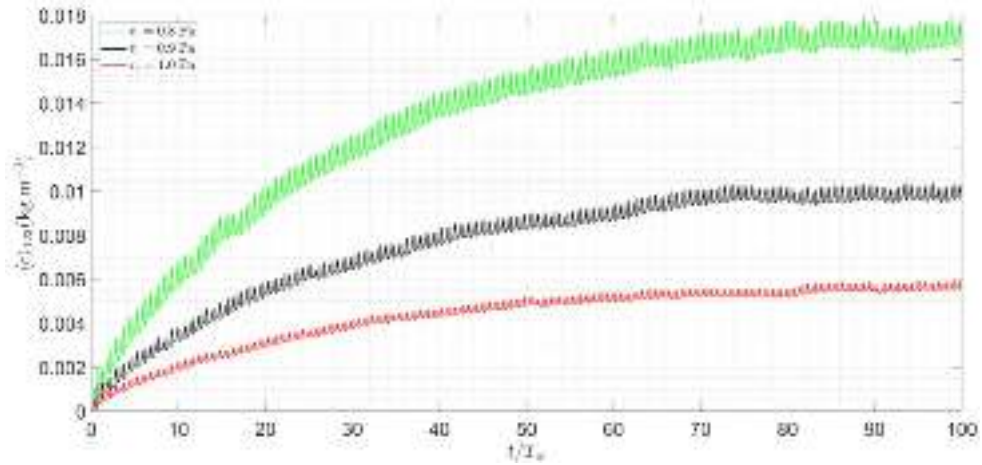


Figure 5.2. Domain-averaged concentration time series for different critical shear stress with a constant settling velocity of  $w_s = 0.25 \text{ mm/s}$ .

Once the quasi-steady state has been identified, the next step is to apply the turbulence-averaging operation (Equation 5.7), using 20 waves in the ranges of [30 ~ 50] and [80 ~ 100] for the higher (Figure 5.1) and lower settling velocity (Figure 5.2)

cases, respectively. Successively, the wave-period-average operation (Equation 5.8) is implemented to compute the turbulence- and wave-period averaged shear rate  $S$  and sediment concentration  $C$  profiles for flocculation calculation.

Analyses are also applied to an additional DNS case in a clear water condition by turning off the resuspension of sediment to evaluate the variability due to wave-period averaging and dilute assumption adopted in this study. The present oscillatory bottom boundary layer at  $Re_\Delta = 800$  is categorized as in the lower range of intermittently turbulence regime and the wave boundary layer is of transitionally turbulent features (Ozdemir et al., 2014). Unlike the fully turbulent condition, the existence of a unique statistically-averaged turbulence shear rate profile in transitionally turbulent flow is hardly observed unless a very large number of wave periods are simulated and used for averaging. This is due to the intermittent turbulence burst events not necessarily repeating every wave cycle. To assess this variability on the calculated wave-period-averaged turbulent statistics, two wave-period averaged shear rate profiles (i.e.,  $S_{w1}$  and  $S_{w2}$ ) are obtained due to the two different wave ensembles (i.e.,  $t/T_w = [30\sim50]$  and  $t/T_w = [80\sim100]$ ). We compare  $S_{w1}$  and  $S_{w2}$  to evaluate their difference (see Figure 5.3a). The results show high similarities with relative errors below 5% in the lower  $\frac{3}{4}$  of the wave bottom boundary layer ( $x_3 \leq 0.08$ ). As we will present later, the lower  $\frac{3}{4}$  of the wave bottom boundary layer is where most sediments are distributed, and flocculation process is likely to be important. In contrast, larger discrepancies (error exceeds 15%) are found near the top of the wave bottom boundary layer, due to using different averaging ranges reflecting intermittency. However, turbulence shear rates in the top  $\frac{1}{4}$  of the boundary layer are lower than  $0.3 \text{ s}^{-1}$ . We conclude that the difference

in turbulent statistics due to averaging ranges is of minor importance for sediment transport and flocculation investigation to be presented next.

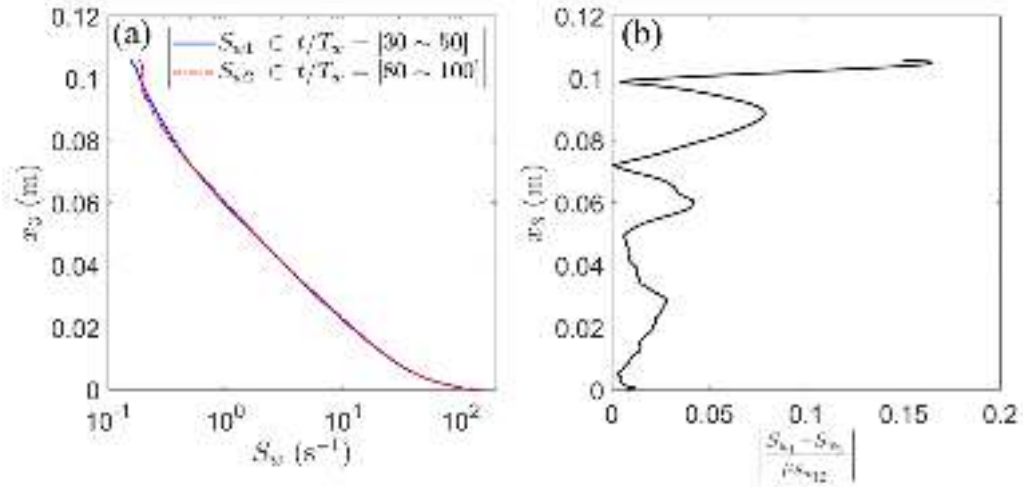


Figure 5.3. (a) Comparison of turbulent shear rate profiles calculated using two different simulation ranges for clear fluid condition and their relative errors (b). The symbol  $\mu_{S_{w12}}$  represents the local mean values between  $S_{w1}$  and  $S_{w2}$ .

The resulting wave-period-averaged sediment concentration  $C$  profiles, considering a critical bottom shear stress of erosion  $\tau_c = 0.8 Pa$ , are compared for higher and lower settling velocity (i.e., C3 and C6 in Table 5.1). As expected, decreasing the settling velocity increases the amount of sediment in the water column in C6 (see Figure 5.4) and generate a lutocline, which can be identified by the local peak in (negative) concentration gradient away from the bottom at  $x_3 = 0.07 m$ . In this study, we use the local peak of (negative) sediment concentration gradient to identify the existence and location of lutocline (see red-dashed lines in Figure 5.4). On the other hand, sediment concentration associated with higher settling velocity case in C3 is two

to three times lower than that of C3 and there is nearly no peak of sediment concentration gradient exists in the water column, and we consider no lutocline is formed (see black curve in Figure 5.4b). The existence of a lutocline attenuates turbulence via sediment-induced stable density stratification (Ozdemir et al., 2010a). Strictly speaking, it violates the dilute assumption required by the modeling framework. A comparison of wave-period-averaged shear rates (Figure 5.4c) provides a more quantitative picture. The shear rate profiles of C3 and C6 are nearly identical below  $x_3 = 0.06 \text{ m}$ . However, for  $x_3 > 0.06 \text{ m}$ , shear rate profile of C6 (red curve in Figure 5.4c) is notably smaller than that of C3 (black curve). Comparing the shear rate profile with clear water conditions (without sediment), we observe that the relative error for C3 is smaller than 5% below  $x_3 = 0.08 \text{ m}$  and it increase to about 15% near the top of the wave bottom boundary layer. This behavior is similar to the variability in clear fluid condition via using different averaging interval and therefore, we can conclude that turbulence is intact due to sediment in C3, and this case satisfies the dilute assumption required by the flocculation model framework.

On the contrary, for case C6 the relative error is within 5% in the lower water column  $x_3 < 0.05 \text{ m}$  but the error increase rapidly to 20% at the location of lutocline. This comparison suggests that the lutocline formation under sufficient concentration in C6 causes attenuation of turbulence in the upper portion of the wave bottom boundary layer. However, it is also important to point out that according to the DNS data presented here, the turbulence shear rate  $S$  is smaller than  $1 \text{ s}^{-1}$  when  $x_3 > 0.06 \text{ m}$ , making turbulent induced flocculation hardly feasible. Moreover, the lutocline formation is initiated at the top of the more turbulent region above  $x_3 = 0.05 \text{ m}$  where the turbulent shear rate is about  $S = 2 \text{ s}^{-1}$  and below it, turbulence is intact by sediment. Hence, even

for this highest sediment load case, it is still interesting to evaluate how flocculation may affect the onset of lutocline formation.

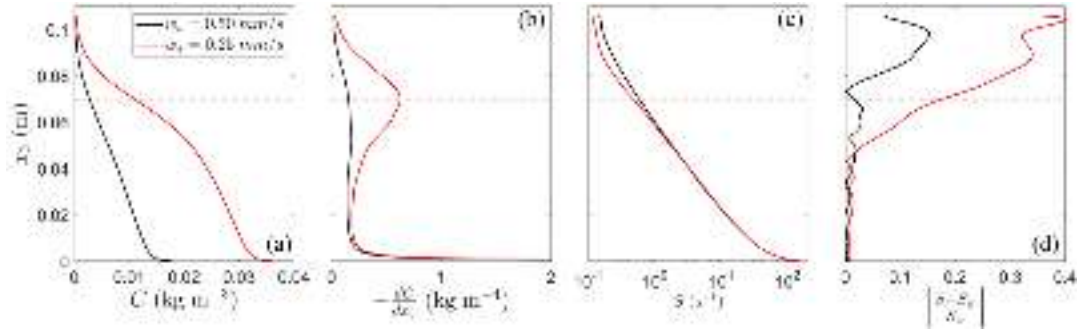


Figure 5.4. Comparisons of wave-period-averaged profile of sediment concentration  $C$  (a), sediment concentration gradient (b), turbulent shear rate  $S$  (c) and absolute relative error of  $S$  using clear water simulation results as a reference (d) for case C3 and C6 using a critical shear stress of erosion  $\tau_c = 0.8$  Pa. The red-dashed line shows the lutocline location.

The next four baseline DNS cases are generated by increasing the critical shear rate of erosion to  $\tau_c = 0.9$  Pa (i.e., C2 and C5 in Table 5.1) and  $\tau_c = 1.0$  Pa (i.e., C1 and C4 in Table 5.1) for the two constant settling velocity, respectively. As expected, the wave-period-averaged sediment concentration  $C$  profiles decrease compared to the previous cases C3 and C6 (compare Figure 5.5a and b with 5.4a). In addition, the negative correlation between sediment concentration magnitude and settling velocities  $w_s$  persist (see Figure 5.5a and 5.5b). We can confirm that there is no lutocline formulation in case C1 and C2 using a higher constant settling velocity of 0.5 mm/s. For cases with a lower settling velocity of  $w_s = 0.25$  mm/s (i.e., C4 and C5), the lutocline formation remains with a lower value in the peak concentration gradient at slightly higher location of  $x_3 = 0.077$  m and  $x_3 = 0.0806$  m, respectively compared to the case

C6 (see Figure 5.5c and d compared with Figure 5.4b). This indicates that a decrease in suspended sediment results in a weaker lutocline formation and smaller attenuation of turbulence due to sediment.

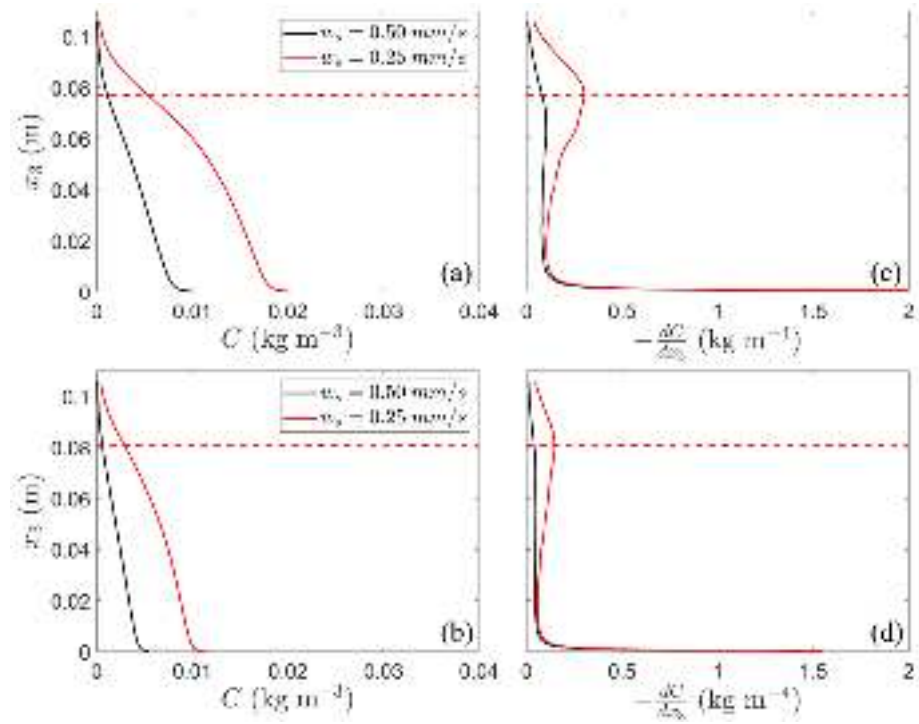


Figure 5.5. Comparisons of wave-period-averaged profile of sediment concentration  $C$  using a critical shear stress of erosion  $\tau_c = 0.9 \text{ Pa}$  (case C2 and C5) shown in (a) and  $\tau_c = 1.0 \text{ Pa}$  (Case C1 and C4) shown in (b) with their sediment concentration gradient shown in (c) and (d).

#### 5.4 Flocculation effects

With the initial wave-period-averaged shear rate  $S$  and sediment concentration  $C$  profiles established previously for the six cases (See Table 5.1), the modeling framework is applied to evaluate the flocculation effects on the sediment concentration and weighted average settling velocity  $W_a$  profiles in the wave bottom boundary layer.

The same three cohesion properties defined in the current boundary layer case (Chapter 4) are also selected here (i.e.,  $r = [2.5, 5.0, 10.0]$ ) with a fractal dimension  $f_d = 2.0$ , and the convergency tolerance criterion for  $W_a$  is specified to  $\epsilon_w = 3 \times 10^{-6} \text{ m/s}$ .

#### 5.4.1 Flocculation effects for large settling velocity cases

The flocculation effects are first evaluated for large (constant) settling velocity cases C1, C2, C3 (see Table 5.1). For the critical shear stress of erosion specified in the range of  $\tau_c = 0.8 \sim 1.0 \text{ Pa}$  in this study, these three cases are characterized by low sediment load (maximum concentration near the bed never exceeds  $0.02 \text{ kg m}^{-3}$ ) without the formation of lutoclines. The results shown in Figure 5.6 reveal several important findings. Regardless of the variation of the cohesion floc properties, represented by the parameter  $r$  (stickiness or yield strength), including flocculation produces a more well-mixed sediment concentration profile in the wave bottom boundary layer (compare color lines in Figure 5.6). This is mainly because the flocculation model indicates rather small floc sizes in the range of  $22 \sim 66 \mu\text{m}$  (see Figure 5.7a, b and c) in such low sediment concentration and high turbulent shear rate condition. As a result, the settling velocities are in the range of 0.1 to 0.25 mm/s, which is significantly smaller than the constant settling velocity of 0.5 mm/s specified in the DNS (see Figure 5.7d, e and f). Moreover, the effect of using different  $r$  values produce nearly identical floc size and settling velocity profiles, especially for the cases C1 and C2 of higher critical shear stress of  $\tau_c = 0.9 \text{ Pa}$  and  $\tau_c = 1.0 \text{ Pa}$  when the peak sediment concentration near the bed is less than  $0.01 \text{ kg m}^{-3}$ . This suggests that the turbulent shear rate  $S$  is the main driver to induce flocculation and redistribute the sediment concentration in the water column, resulting in a more homogeneous, well-

mixed profile. The magnitude of the initial sediment concentration profile needs to be larger to activate the influence of the floc cohesion properties quantified by  $r$ .

Lastly, the C3 with a lower  $\tau_c = 0.8 \text{ Pa}$  show a higher sediment concentration with the near-bed value peaked just below  $0.018 \text{ kg m}^{-3}$  and in this case, we observe a slightly larger dependency with respect to cohesive floc properties  $r$ . For flocs of higher stickiness or yield strength ( $r = 10$ , see green line in Figure 5.6c), the resulting concentration profile shows larger concentration gradient compared to those of lower  $r$  values. This feature can be understood by examining the floc size and settling velocity shown in Figure 5.7c, f. Flocs with high magnitude of  $r = 10$  cause larger floc sizes and the resulting settling velocity is more than a factor two larger than those of lower  $r$  values. The peak settling velocity of about  $0.25 \text{ mm/s}$  occurs at  $x_3 = 0.055 \text{ m}$  where we also observe a stronger negative sediment concentration gradient. In the present wave bottom boundary layer, turbulent shear rate is large which prevents floc growth, especially close to the bed (see Figure 5.4c where  $S$  exceed  $10 \text{ s}^{-1}$  in the lower 20% of the wave bottom boundary layer). However, away from the bed when  $S$  drops to about  $2 \text{ s}^{-1}$  in the middle of the wave bottom boundary layer, more cohesive flocs work in conjunction with higher sediment concentration in case C3 encourage floc size growth and produce higher settling velocity flocs that further increase the negative concentration gradient observed around  $x_3 = 0.055 \text{ m}$ . Results demonstrated in case C3 show an interesting interplay among settling velocity variability controlled by flocculation and sediment concentration in the wave bottom boundary layer. These important dynamics can be more pronounced in cases with higher sediment load to be discussed in the next subsection.

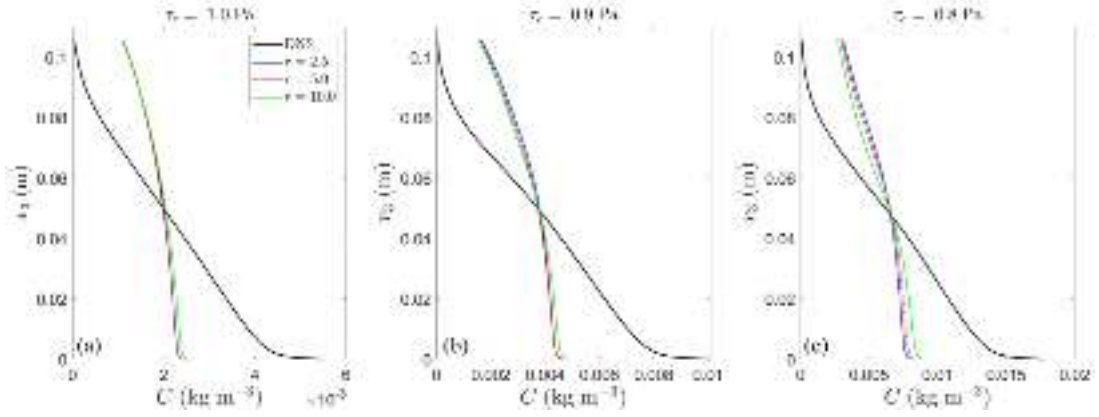


Figure 5.6 Concentration profiles for (a) case C1 ( $\tau_c = 1.0$  Pa), (b) case C2 ( $\tau_c = 0.9$  Pa) and (c) case C3 ( $\tau_c = 0.8$  Pa) for three different cohesive floc properties (ratio  $r = \alpha/\beta$ ). The initial concentration profile (black lines) is established from DNS with a constant settling velocity  $w_s = 0.5$  mm/s.

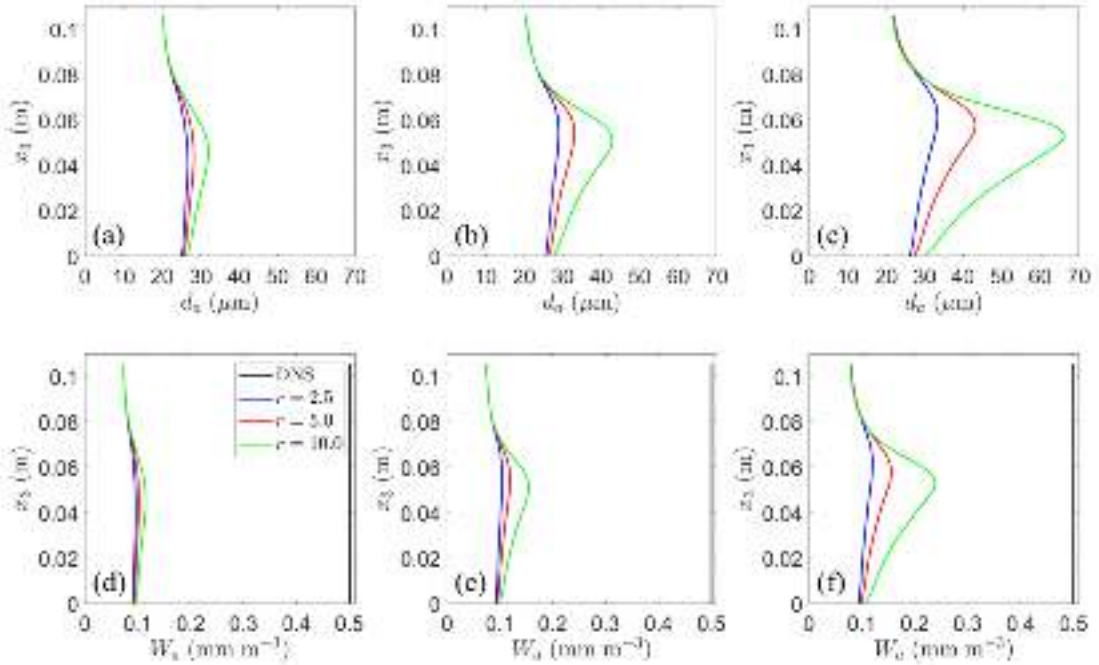


Figure 5.7. Weight averaged floc size for case C1 ( $\tau_c = 1.0$  Pa) (a), C2 ( $\tau_c = 0.9$  Pa) (b), and C3 ( $\tau_c = 0.8$  Pa) (c) with the corresponding weighted average settling velocity profiles shown in (d), (e) and (f) at different  $r$ . The vertical black line indicates the constant settling velocity of 0.5 mm/s used by the DNS.

The variability of  $W_a$  is another essential characteristic to evaluate since low values are an indicator of using a depth-averaged settling velocity  $\overline{W_a}$  in cohesive sediment transport modeling. Generally, flocs with low cohesion properties (i.e.,  $r = 2.5$ ) show lower vertical variability in  $W_a$ , while high cohesion properties (i.e.,  $r = 10.0$ ) show larger variability as illustrated Figure 5.8 (compare blue lines with green lines). However, the initial sediment concentration profile plays a significant role in the magnitude of variabilities since concentration values significantly activate cohesion floc properties as shown in Figure 5.6. For instance, when a quarter of the water column possesses an initial sediment concentration magnitude higher than  $0.01 \text{ kg m}^{-3}$  (see Figure 5.6c), the settling velocity variability reaches maximum values about 77.5%, 41% and 21% for  $r = 10.0$ ,  $r = 5.0$  and  $r = 2.5$ , respectively (see Figure 5.8c). These maximum variabilities decrease to 44%, 24%, and 14%, correspondingly when the initial concentration profile decrease by increasing the critical shear rate of erosion to  $\tau_c = 0.9 \text{ Pa}$ . The continuous decrease in the availability of sediments in the water column via the critical shear rate of erosion (i.e.,  $\tau_c = 1.0 \text{ Pa}$ ) generate low variabilities in  $W_a$  (i.e.,  $> 22\%$ ). These results suggest that the implementation of the depth-averaged settling velocity approach is viable for either low cohesion properties or low sediment concentration in the water column.

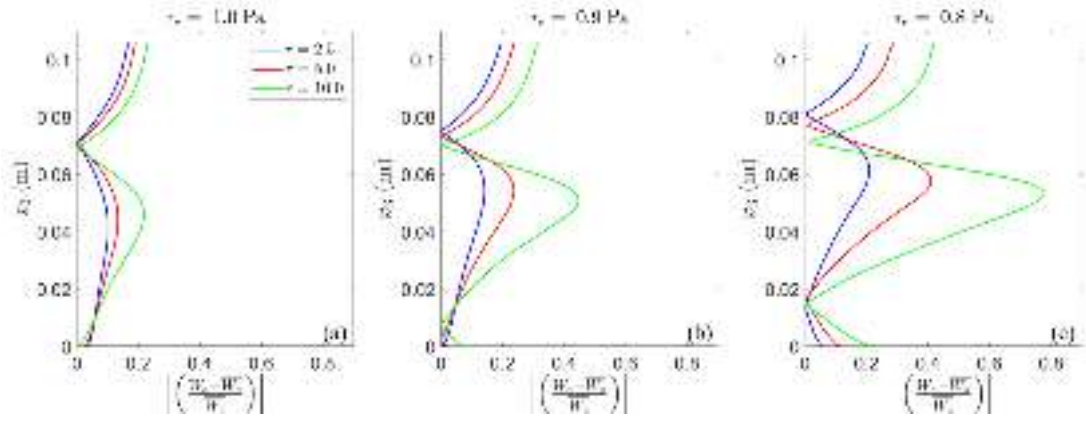


Figure 5.8. Vertical variability of the weighted average settling velocity profiles for case (a) C3, (b) C2 and (c) C1 for three different cohesive sediment properties represented by  $r = 2.5, 5.0, 10.0$ .

#### 5.4.2 Flocculation effects for small settling velocity cases

The flocculation effects are evaluated for initial sediment concentration profile obtained via a prescribed constant settling velocity  $w_s = 0.25 \text{ mm/s}$  from the DNS (i.e., cases C4, C5 and C6 in Table 5.1). When sediment concentration is low due to high critical shear stress  $\tau_c = 1.0 \text{ Pa}$  (see the case C4 in Table 5.1), including flocculation produces a more well-mixed sediment concentration profile (see Figure 5.9a), consistent with those discussed in Section 5.4.1. This is because the calculated mean floc size by including flocculation is in the range of  $20\sim70\mu\text{m}$  (Figure 5.9c) and the resulting settling velocity is between  $0.1\sim0.25 \text{ mm/s}$  (Figure 5.9d), lower than the prescribed constant settling velocity of  $0.25 \text{ mm/s}$  in the DNS. Also, the direct proportionality between the bottom sediment concentration and floc cohesive properties (larger  $r$  value) remains. Since total sediment mass in the domain is conserved in the present modeling framework, a larger near bed sediment concentration indicates that overall sediments are distributed lower in the wave bottom boundary layer. Importantly, a weak lutocline formation is obtained with high stickiness/yield strength flocs, i.e.,  $r =$

10.0 (see the green line in Figure 5.9b). According to the location of peak (negative) sediment concentration gradient, the lutocline is located at  $x_3 = 0.058 \text{ m}$ , which is just slightly above the location  $x_3 = 0.055 \text{ m}$  where peak floc size and settling velocity are predicted (see Figure 5.9c and d).

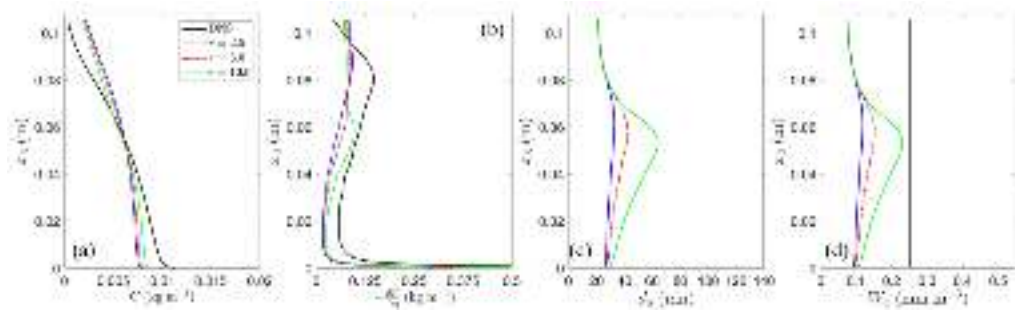


Figure 5.9. Profiles of sediment concentration (a), vertical gradient of sediment concentration (b), weighted average floc size (c) and settling velocity (d) for C4 for three different cohesive sediment properties represented by  $r = 2.5, 5.0, 10.0$ . The prescribed constant settling velocity of  $0.25 \text{ mm/s}$  in DNS is also indicated by the black line in (d).

The flocculation effects vary when the sediment load increases with a critical shear stress of erosion reduces to  $\tau_c = 0.9 \text{ Pa}$  (see case C5 in Table 5.1). Including flocculation effect still produces more well-mixed sediment concentration profiles for low to medium cohesion flocs at  $r = 2.5$  and  $r = 5.0$  (see blue and red lines in Figure 5.10a) as compared to the DNS results (black line) due to the lower settling velocities than the prescribed value of  $0.25 \text{ mm/s}$  in DNS (Figure 5.10d). However, the vertical variabilities of floc size and settling velocity become sufficiently large to cause weak lutocline formations with the lutocline located higher in the domain at  $x_3 = 0.078 \text{ m}$  for flocs of low cohesion ( $r = 2.5$ ), while for medium cohesion flocs ( $r = 5.0$ ), the

lutocline is located lower at  $x_3 = 0.064 \text{ m}$ . For the results with the highest cohesion floc property (i.e.,  $r = 10.0$ ), lutocline is clearly formed at  $x_3 = 0.06 \text{ m}$ . This is not only due to the vertical variability of floc settling velocity but also the fact that the predict floc settling velocity by the flocculation model is larger than the prescribed constant value of  $0.25 \text{ mm/s}$  in DNS.

In essence, the lutocline tends to disappear in lower sediment load condition (see Figure 5.9) due to the rupture of larger flocs and generation of small flocs driven by the breakup effect. Conversely, increasing the floc cohesion and sediment concentration encourages aggregation that produces larger floc size and settling velocity and leading to the formation of sharper lutocline located closer to the bed. This point can be further strengthened if we further increase sediment load in C6.

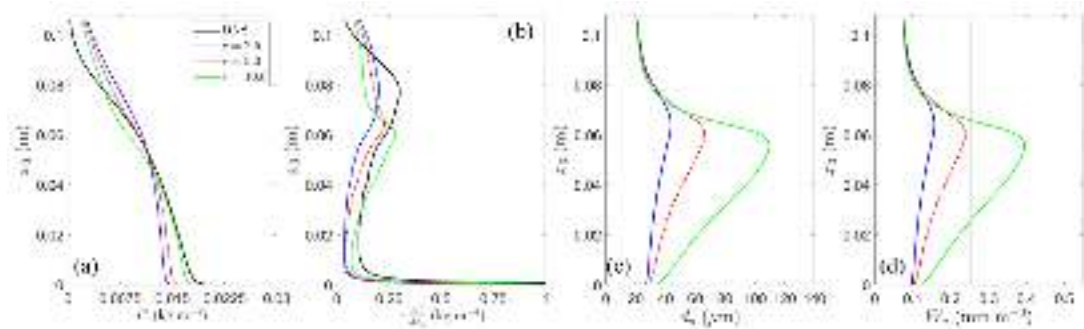


Figure 5.10. Profiles of sediment concentration (a), vertical gradient of sediment concentration (b), weighted average floc size (c) and settling velocity (d) for C5 for three different cohesive sediment properties represented by  $r = 2.5, 5.0, 10.0$ . The prescribed constant settling velocity of  $0.25 \text{ mm/s}$  in DNS is also indicated by the black line in (d).

In the case of high sediment load by further reducing the critical shear stress of erosion to  $\tau_c = 0.8 \text{ Pa}$  (case C6), both high and low cohesive properties cause an increase in sediment concentration near the bed compared to the value of  $0.036 \text{ kg m}^{-3}$  from the DNS results (see Figure 5.11a). In the DNS result using a constant settling velocity of  $0.25 \text{ mm/s}$ , the maximum (negative) concentration gradient away from the bed, defined here as the lutocline location, occurs at  $x_3 = 0.07 \text{ m}$  with a value of  $0.626 \text{ kg m}^{-4}$  (see the black line in Figure 5.11b). The lutocline location and intensity undergoes different alterations according to cohesion floc properties. In the instances of lowest cohesion properties investigated (i.e.,  $r = 2.5$ ), the maximum concentration gradient away from the bed is slightly reduced to  $0.56 \text{ kg m}^{-4}$  (10.54% smaller than the DNS result) but the lutocline is located closer to the sediment bed at  $x_3 = 0.057 \text{ m}$  (see the blue line in Figure 5.11b). For  $r = 5.0$ , the peak concentration gradient away from the bed becomes  $0.67 \text{ kg m}^{-4}$ , which is 7.03% larger than the DNS result and the lutocline descends further close to the bed at  $x_3 = 0.042 \text{ m}$ . According to Ozdemir et al. (2011), the significance of lutocline in the wave bottom boundary layer is that it separates a turbulent region of sediment transport below the lutocline from the quasi-laminar region above the it. Since turbulence must become zero near the bed (e.g., viscous sublayer), the thickness of the turbulent layer that maintains the suspension of sediment is essentially limited by the lutocline. Results presented here show that when sediment concentration becomes sufficiently large and when flocs are more cohesive (or high yield strength), flocculation may affect settling velocity variation and reduce the height of lutocline in the wave bottom boundary layer.

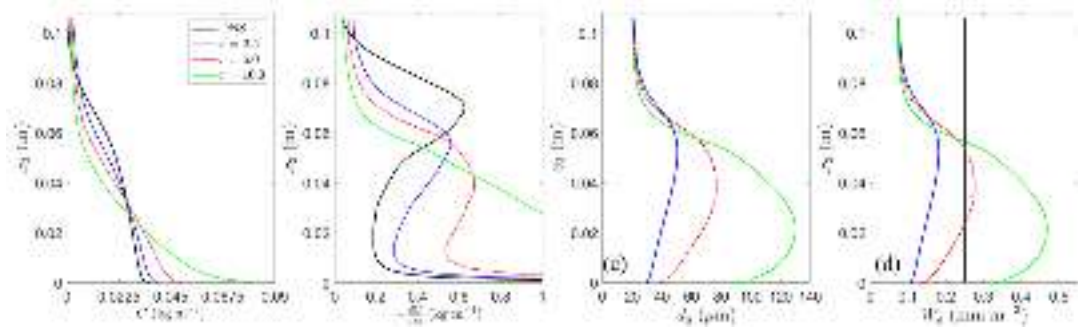


Figure 5.11. Profiles of sediment concentration (a), vertical gradient of sediment concentration (b), weighted average floc size (c) and settling velocity (d) for C6 for three different cohesive sediment properties represented by  $r = 2.5, 5.0, 10.0$ . The prescribed constant settling velocity of 0.25 mm/s in DNS is also indicated by the black line in (d).

Notably, when the floc stickiness or yield strength is high (i.e.,  $r = 10.0$ ), the concentration at the bottom experiences a substantial 132.22% increase from the DNS results (i.e., from  $0.036 \text{ kg m}^{-3}$  to  $0.0836 \text{ kg m}^{-3}$ ), consistent with the formation of large flocs greater than  $100 \mu\text{m}$  (green line in Figure 5.11c) and the resulting large settling velocity nearly doubles that used in the DNS (Figure 5.11d). More importantly, the lutocline no longer exists in the water column while the peak concentration gradient only occurs at the bed. Essentially, we observe a trend that flocs with higher cohesion/yield strength can further lower the lutocline and eventually for the high value of  $r = 10.0$  the lutocline disappears. Due to high settling velocity, the entire sediment concentration profile shows a concave upward shape, consistent with those of sand with a high Rouse number.

The present model framework is limited by the dilute assumption and cannot predict the attenuation of turbulence due to sediment-induced density stratification. However, following the previous DNS study of Ozdemir et al. (2011) investigating the

lutocline location using different constant settling velocities, we can reasonably expect that any mechanism that can effectively lower the lutocline, in this case it is the flocculation effect changing the settling velocity, may eventually cause the disappearance of lutocline, laminarize the wave bottom boundary layer and hence reduce sediment carrying capacity.

In summary, flocculation of cohesive sediments of higher cohesion and yield strength in higher sediment load can cause the lowering of lutocline, and eventually its disappearance due to formation of large flocs near the bed. This implies that the flocculation process may also directly control the turbulence state and transport mode of fine sediment in the wave bottom boundary layer via modifying settling velocity. Further study using a fully coupled model is needed to confirm this finding.

The potential use of a depth-averaged settling velocity  $\overline{W}_a$  for cohesive sediment transport modeling in wave bottom boundary layer is evaluated for C4, C5 and C6. As expected, the positive correlation between cohesion floc properties (magnitude of  $r$ ) and the variability of  $\overline{W}_a$  persists (compare colors lines in Figure 5.12). The degree of this variability depends on how the initial sediment concentration profile interacts with the cohesion floc properties (i.e., the parameter  $r$ ). In the lowest concentration in case C4 using high  $\tau_c = 1.0 Pa$ , the maximum variabilities reach 75.79%, 66.39% and 21.16% for  $r = 10.0$ ,  $r = 5.0$ , and  $r = 2.5$ , respectively (see Figure 5.12a). Increasing the initial sediment concentration profile via using  $\tau_c = 0.9 Pa$ , the variabilities increase to 110.7%, 78.5%, and 42.88%, consistent with the trend found in Figure 5.8. Nevertheless, this trend is interrupted in the highest initial concentration profile scenario (i.e., case C6 using  $\tau_c = 0.8 Pa$ ) for  $r = 10.0$  and  $r = 5.0$  since their maximum variabilities decrease to 75.65%, 66.39% (see the red and green lines in Figure 5.12c).

This decrease occurs due to the resulting concentration profile exhibiting features of concave upward profile (see the dashed red and green lines in Figure 5.11a). Exclusively, for relatively low flocc stickiness or yield strength (i.e.,  $r = 2.5$ ), the trend continues as the variability increases to 46.96%.

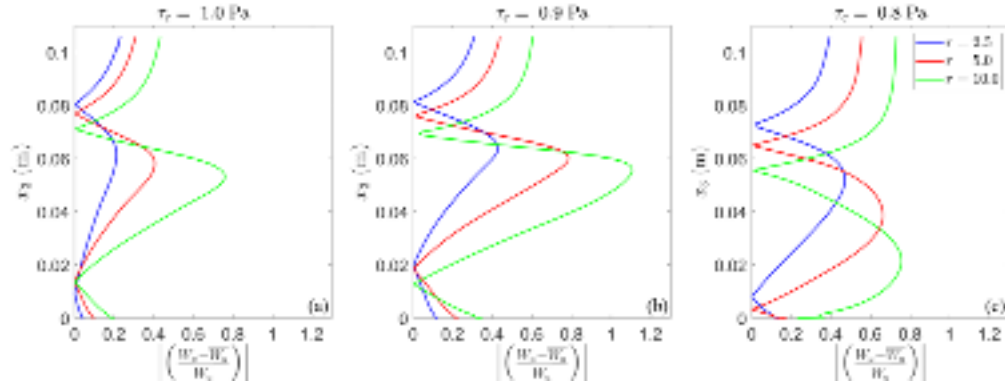


Figure 5.12. Vertical variability of the weighted average settling velocity profiles for case (a) C4, (b) C5 and (c) C6 for three different cohesive sediment properties represented by  $r = 2.5, 5.0, 10.0$ .

The variability analysis in  $W_a$  suggests that implementing the depth-averaged settling velocity approach in the wave bottom boundary layer may be not successful as the vertical variability is significantly larger than that in the current bottom boundary layer discussed in Chapter 4. To verify this argument, the depth-averaged settling velocity is implemented directly in the mass balance formulation (Equation 5.4). The resulting sediment concentration profiles (C profiles) are compared with the profiles obtained when the settling velocity is treated as a variable (i.e.,  $W_a$ ). The results confirm that recovering a constant settling velocity is hardly applicable in the wave bottom boundary layer. Notably, for the lowest sediment suspended with  $\tau_c = 1.0 \text{ Pa}$  (i.e., case

C4), the sediment concentration profile reconstructed with  $\overline{W_a}$  exhibit high discrepancies compared to the profile obtained with  $W_a$  in all three cohesive floc properties (see Figure 5.13a, b, and c). The substantial difference persists as the sediment concentration availability increases with  $\tau_c = 0.9 Pa$  for all the cohesive properties cases (see Figure 5.13d, e, and f). These significant discrepancies reaffirm that the use of a constant  $\overline{W_a}$  can hardly predict sediment concentration profiles, even under dilute conditions. In contrast, lower differences are observed when the sediment concentration load increases with  $\tau_c = 1.0 Pa$ . This means that the concentration profile, whether transitioning to a concave-up shape or fully developed concave-up shape, can be reproduced via a constant  $\overline{W_a}$  with acceptable results (see Figure 5.13g, h and i) because this feature is dominated by the large magnitude of settling velocity, not just the variability.

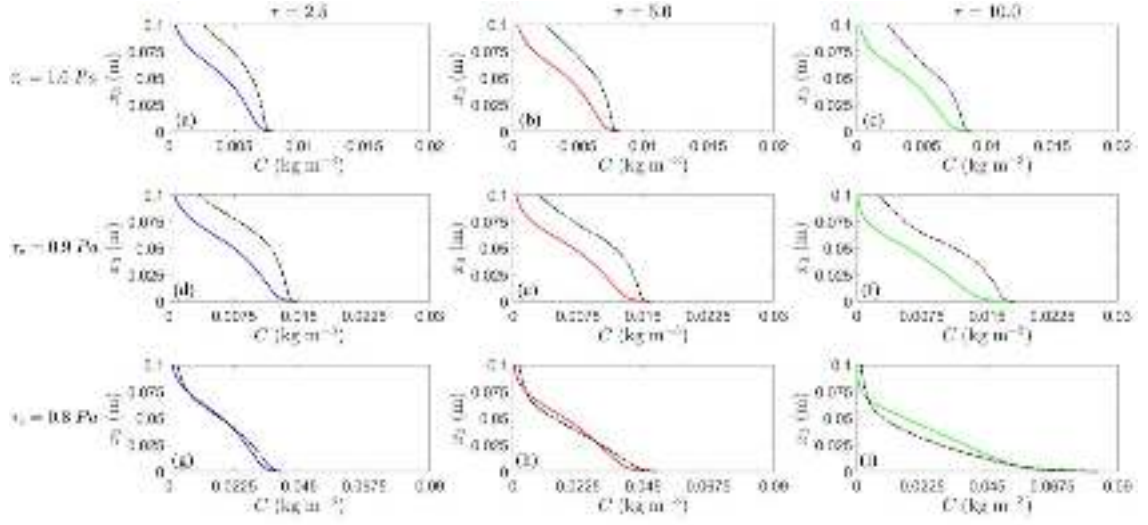


Figure 5.13. Predicted sediment mass concentration profiles using depth-averaged settling velocity (solid line) versus those calculated from the modeling framework (black-dashed line). The first row corresponds to the case C4 with  $r$  values of (a)  $r = 2.5$ , (b)  $r = 5.0$  and (c)  $r = 10.0$ . The second row are associated to the case C5 with  $r$  values of (d)  $r = 2.5$ , (e)  $r = 5.0$  and (f)  $r = 10.0$ . The third row relates with the case C6 with  $r$  values of (g)  $r = 2.5$ , (h)  $r = 5.0$  and (i)  $r = 10.0$ .

## 5.5 Conclusions

The cohesive sediment transport modeling framework is applied to wave bottom boundary layer with a variable settling velocity induced by flocculation in wave-period-average equilibrium and dilute conditions. Here, six initial sediment concentration profiles and turbulent shear rate profiles are generated via Direct Numerical Simulation (DNS), which are computed using two constant settling velocities ( $w_s = 0.50 \text{ mm/s}$  and  $w_s = 0.25 \text{ mm/s}$ ) under three critical shear stress of erosion ( $\tau_c = 0.8 \text{ Pa}$ ,  $\tau_c = 0.9 \text{ Pa}$ , and  $\tau_c = 1.0 \text{ Pa}$ ) at Stokes Reynolds number of 800. When analyzing cases with a constant settling velocity of  $w_s = 0.50 \text{ mm/s}$ , sediment loads are generally lower and the turbulence shear rate  $S$  is the dominant factor that drives flocculation. The

flocculation process produces relatively small flocs and settling velocities in the range of 0.1 to 0.25 mm/s. As results, more well-mixed concentration profiles are obtained by including the flocculation effect. The effect of larger cohesion or floc yield strength is of minor importance. However, a subtle effect of increased near-bed sediment concentration for more cohesive floc is observed because floc settling velocity is slightly larger for floc of higher  $r$  value.

The DNS cases associated with a constant settling velocity of  $w_s = 0.25 \text{ mm/s}$  are of higher sediment load and show the formation of lutocline with different sharpness and vertical position. When sediment concentration is sufficiently large and/or when flocs are of higher cohesion/yield strength, flocculation encourages the formation of lutocline by sharpening the (negative) concentration gradient and lower its position. In a case of highest sediment concentration (Case C6) with largest floc cohesion ( $r = 10.0$ ) investigated, including flocculation produce large floc size exceeding  $120 \mu\text{m}$  near the bed and the corresponding settling velocity nearly doubles the initially prescribed value in DNS. As a result, lutocline disappears and a concave upward concentration profile is obtained. Although the present model does not include the dynamic coupling between sediment concentration profile attenuating turbulence, the concave upward profile obtained here is of similar shape of laminarized wave bottom boundary layer reported by previous DNS study (Ozdemir et al. 2011) using a large constant settling velocity. Essentially, the present study reveals that flocculation in higher sediment concentration condition or for more cohesive flocs tend produce larger floc settling velocity with high vertical variabilities that encourages the formation of sharper lutocline located closer to the bottom. These features indicate that future studies

of cohesive sediment transport in the wave bottom boundary layer should explicitly include the effect of flocculation.

The weighted average settling velocity and its variability are examined to evaluate the feasibility of incorporating a depth-averaged settling velocity in the modeling framework. The application of the depth-averaged settling velocity approach is viable when the initial sediment concentration profile is on the order of  $10^{-3} \text{ kg m}^{-3}$ , and the cohesive floc properties are of low or moderate cohesion/yield strength ( $r \leq 5.0$ ). On the other hand, when the initial sediment concentration is of higher concentration that includes a lutocline formation, the depth-averaged settling velocity should be used with caution.

## **Chapter 6**

### **CONCLUDING REMARKS**

#### **6.1 Summary of Findings**

In this dissertation, a novel modeling framework is developed to include the flocculation effects on cohesive sediment transport in the bottom boundary layer under equilibrium and dilute condition. The open-source population balance equation flocculation model of Verney et al (2011) is adopted to distribute the suspended sediment concentration into different floc size classes at a given location in the bottom boundary layer driven by profiles of turbulent shear rate  $S$  and sediment concentration  $C$ . Using the newly updated floc size distribution and fractal theory, floc settling velocity can be calculated and sediment concentration profile can then be updated via a mass balance. Due to the dilute assumption, turbulent shear rate profile is unchanged. As the main scientific objective of this study is to advance our understanding of how flocculation influences cohesive sediment transport through variable settling velocity in the bottom boundary layers, turbulent shear rate and initial sediment concentration profiles are generated using Direct Numerical Simulation (DNS), ensuring accurate representation of turbulence in both current- and wave-bottom boundary layers (Yue et al., 2020). The subsequent subsections provide a summary of the significant findings.

##### **6.1.1 Population balance equation flocculation model**

To address Research Question 1 and 2 proposed in Chapter 4.1, my research effort embarked to understand the population balance equation flocculation model

FLOCMOD (Verney et al., 2011). A comprehensive study of their several key model parameters is carried out, using laboratory measurements of temporal floc size statistics reported by Keyvani and Strom (2014) under a constant turbulent shear rate  $S$ . The measured time series of the median floc size statistic  $d_{50}$  is divided into three stages (equilibrium state, floc growth stage and the entire time series) to constrain sensitive model parameters in the calibration process. Through comprehensive numerical experiments, the three parameters are identified as (1) floc collisional efficiency  $\alpha$ , representing the cohesion/stickiness of flocs, (2) fragmentation rate  $\beta$ , which is inversely proportional floc yield strength, and (3) fractal dimension  $f_d$ . Results suggest that the temporal evolution of median floc size statistic  $d_{50}$  is not sufficient to constrain these three model parameters. Subsequently, time series of two more floc size statistics,  $d_{16}$  and  $d_{84}$  are included in the evaluation to successfully fulfill the model calibration. Through the rigorous model parameter calibration, we are able to gain more insight into the parameterization of fragmentation rate. Informed by previous laboratory investigation of floc yield strength, a two-value fragmentation rate approach is proposed to highlight the importance of floc yield strength in better predicting the measured temporal evolution of three floc size statistics  $d_{16}$ ,  $d_{50}$  and  $d_{84}$ . This part of the study was published in Penaloza-Giraldo et al. (2023). The main findings can be summarized as follows:

- The median floc size  $d_{50}$  alone is insufficient to constrain the flocculation parameters.
- Adding the floc size statistics  $d_{16}$  and  $d_{84}$  contributes to constrain the flocculation parameters with improved predictions.

- The proposed two-value fragmentation rate approach significantly improves the tri-temporal floc size statistics compared with results obtained by using a constant  $\beta$ .

### **6.1.2 Flocculation effects on cohesive sediment transport in the current bottom boundary layer**

To address Research Question 3, a novel modeling framework is developed to explore the impact of flocculation dynamics on cohesive sediment transport within the current bottom boundary layer. This modeling framework incorporates a settling velocity as a variable, influenced by flocculation under equilibrium and dilute conditions. The Population Balance Equation is implemented and solved by the open-source FLOCMOD developed by Verney et al., (2011), which generates floc size distributions based on the aquatic environmental variables and cohesive floc properties. The floc size statistics are further used to calculate settling velocity. To obtain accurate aquatic environmental variables in current bottom boundary layer at the input (initial condition) to the model (i.e., turbulent shear rate  $S$  and turbulence-averaged sediment concentration  $C$ ), DNS data is produced for a statistically steady fully-developed current with an constant settling velocity (Yue et al., 2020). Given the treatment of settling velocity as a variable, the sediment concentration profile is updated using a turbulence-averaged mass balance equation. A manuscript reporting the findings has been submitted for publication (Penaloza-Giraldo et al. 2024). The main contribution can be summarized as follows:

- A modeling framework coupling flocculation dynamics with cohesive sediment transport in the current bottom boundary layer is developed.

- A series of numerical experiments using the flocculation model for typical range of turbulent shear rate, sediment concentration, and floc cohesive properties reveal the existence of bi-modal floc size distribution.
- Flocs with low cohesion or yield strength induce smaller settling velocity and low settling velocity variability, which result in more well-mixed vertical profiles.
- Depth-averaged settling velocity is a good approximation to calculate sediment distribution in the current boundary layer except for flocs with high cohesion or yield strength.

### **6.1.3 Flocculation effects on vertical structure of sediment concentration in the wave bottom boundary layer**

To address Research Question 4, the modeling framework for cohesive sediment transport is expanded to model the wave bottom boundary layer, incorporating a variable settling velocity induced by flocculation under wave-period-averaged, equilibrium, and dilute conditions. In this context, Direct Numerical Simulation (DNS) is employed to generate six initial sediment concentration profiles and turbulent shear rate profiles. These profiles are computed using two constant settling velocities ( $w_s = 0.50 \text{ mm/s}$  and  $w_s = 0.25 \text{ mm/s}$ ) under three critical shear stress of erosion ( $\tau_c = 0.8 \text{ Pa}$ ,  $\tau_c = 0.9 \text{ Pa}$ , and  $\tau_c = 1.0 \text{ Pa}$ ) at Stokes Reynolds number of 800. The main findings can be summarized as follows:

- With low sediment availability in the wave bottom boundary layer, the dominant mechanism of flocculation is the turbulence shear rate ( $S$ ). Consequently, including flocculation effect produces more well-mixed

concentration profiles due to the generation of small flocs, insensitive to cohesive floc properties.

- With high sediment availability in the wave bottom boundary layer, the cohesive floc properties become crucial and a dominant factor controlling the formation and sharpness of lutoclines. Larger sediment concentration and cohesion encourage the formation of sharper lutocline located closer to the bed.
- When flocs exhibit high cohesion properties (i.e.,  $r = 10$ ) with high sediment availability, the lutocline essentially disappears and it is likely to trigger laminarized wave bottom boundary layer.
- The implementation of depth-averaged settling velocity in the modeling framework may introduce large errors for cohesive sediment transport in the wave bottom boundary layer.

## **6.2 Future work**

In this section, new research directions are proposed based on the findings and limitations identified in this dissertation.

### **6.2.1 Flocculation experiments**

In Chapter 3, the Population Balance Equation (PBE) flocculation model was examined via an extensive calibration process using experimental data on tri-temporal floc size statistics (i.e., floc size fractions of  $d_{16}$ ,  $d_{50}$  and  $d_{84}$ ) from Keyvani and Strom (2014). This work includes a time series of three floc size statistics, and it is one of the most comprehensive datasets. However, it is extremely useful to obtain time series of

full floc size distributions in a given flocculation experiment to fully constrain PBE flocculation models.

Despite limited information, our analysis revealed that the PBE flocculation model lacks consideration of floc yield strength variation in the breakup process (Jorge A Penaloza-Giraldo et al., 2023). Motivated by a laboratory floc yield strength review (Jarvis et al., 2005), a two-value fragmentation rate approach was proposed to improve the model's predictive ability for fine  $d_{16}$ , median  $d_{50}$  and coarse fractions  $d_{84}$ . Evidently, this is our first attempt to address the complex behavior of floc breakup and uncertainties persist in our method since the tri-temporal floc size statistics were successfully predicted by two different sets of parameters, which provided two distinct distributed mass concentration over the floc size classes (see Figure 3.15c and 3.15d). We believe that a more comprehensive understanding of the role of floc yield strength can be gained by observing a complete temporal evolution of distributed mass concentration over floc size classes in a controlled homogenous turbulence flocculation experiment. In addition, with a diverse configuration (i.e., varying turbulent shear rate, concentration, and type of cohesive sediment), a more generalized formulation can be developed for the floc yield strength in the breakup process.

In seeking to advance our understanding of cohesive sediment transport, flocculation experiments that measure temporal evolutions of the physical floc properties over the floc size distributions are needed. While significant efforts have been made to comprehend settling velocities, floc densities and floc structure for pure clays (Ye et al., 2020), as well as their interactions with crucial biotic and abiotic factor such as oil (Daly et al., 2016; Ye et al., 2020), organic matter (Ye et al., 2023), salt concentrations (Krahl et al., 2022), microalgae (Zhu et al., 2022) among others (Ho et

al., 2022), these studies have primarily been conducted under homogeneous turbulence conditions. This means that these experimental data can hardly be used to validate the proposed modeling framework or any other coupled flocculation and cohesive sediment transport model (Liu et al., 2019; Sherwood et al., 2018). Therefore, we consider that controlled flocculation experiments in current and oscillatory channel flow will provide fundamental insights into the physical floc properties over the floc size distributions and concentration profile structures.

### **6.2.2 Fully coupled modeling framework**

The presented modeling framework relies on two fundamental assumptions. The first assumption requires the floc equilibrium conditions. This implies that the PBE flocculation model distributes cohesive sediment concentration until the aggregation and breakup processes reach a balance. Consequently, the floc growth stage (used to estimate flocculation rate) is disregarded in the model framework. Additionally, it is necessary for the carrier flow to be in a fully-developed, statistically steady or quasi-steady state for current or wave cases, respectively. The second assumption relates to dilute sediment flow, indicating that concentration magnitudes are sufficiently low to cause significant damping in the turbulence dissipation rate. From the flocculation modeling perspective, the dilute assumption is probably needed since we assume binary collision and the model parameters are calibrated with laboratory experiments that has a mass concentration around  $0.05 \text{ kg/m}^3$ . For all the cases investigated for current boundary layer in Chapter 4 and most cases in Chapter 5, the dilute assumption is met. However, in for the highest concentration case reported in Chapter 5, results reveal that flocculation with strong stickiness or yield strength (i.e., greater values of  $r$ ) generates a concave upward concentration profile, resembling the shape of the laminarized wave

bottom boundary layer reported by Ozdemir et al. (2011). Due to the dilute assumption, we can only speculate that for high cohesion sediments with sufficient concentration, flocculation may drive laminarization. This emphasizes the necessity for future studies to broaden understanding and develop a more advanced fully coupled model framework for flocculation and cohesive sediment transport in the wave bottom boundary layer.

The present study shows that the minimum number of floc classes is about 75, which is required to better represent the coarse fraction (Jorge A Penaloza-Giraldo et al., 2023) when compare with laboratory data of Keyvani and Strom (2014). Full coupling between PBE flocculation model and cohesive sediment transport equations has been proposed previously for Reynolds-averaged formulations (Sherwood et al., 2018) and Large Eddy Simulations approach (Liu et al., 2019) using a floc size number (15 and 28, respectively) that is significantly below the recommended value obtained in the present study. We consider that a feasible alternative to overcome the computation limitation and construct a modeling framework to simulate more realistic field conditions is to develop a Machine Learning-based surrogate flocculation model. By implementing a Physics-Informed Neuronal Network (PINN) as a surrogate model for the PBE flocculation model, mathematical operations will speed up significantly (Cai et al., 2021; Donnelly et al., 2024; Nazemzadeh et al., 2021). Therefore, quantifying physical floc properties such as settling velocity, and transferring them to solving the cohesive sediment transport governing equations will be computationally efficient. Following the Direct Numerical Simulation approach (Ozdemir et al., 2011; Yue et al., 2020) more fundamental knowledge about the role of flocculation can be provided for turbulence modulation, lutocline formation, laminarization, instability flow, and wave-supported gravity flow in the bottom boundary layer.

An additional advantage of developing the PINN flocculation model is its versatility with Reynolds-Averaged formulation for regional scales modeling of cohesive sediment transport in estuaries and continental shelves. With a fast and efficient flocculation model, investigating the role of flocculation in complex environmental scenarios becomes feasible. For instance, flocculation impacts cycles of erosion and deposition by altering the settling velocities of flocs. Within this cycle, rates of organic matter can be modified, leading to remineralization that may contribute to a decrease in oxygen levels in water columns (Hicks et al., 2017). Up to now, aggregation and breakup process have been neglected (Moriarty et al., 2018). Another future application of PINN flocculation model is to investigate event-timescales scenario, such hurricanes, in a given coastal system. These events generate a massive load of sediment and have the potential to mobilize dissolved and particulate contaminants within the estuary (Harris et al., 2020). However, understanding the contribution of each mechanism in such complex environment through measurements proves challenging. Notably, a more efficient computational tool that integrate flocculation process into a cohesive sediment transport systems is needed.

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