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Temporal Variability in Cohesive Sediment Dynamics in a Partially Mixed Estuary, the York River Estuary, Virginia, USA: A Numerical Study Developed from Observations

A Dissertation
Presented to
The Faculty of the School of Marine Science
The College of William & Mary

In Partial Fulfillment
of the Requirements for the Degree of
Doctor of Philosophy

by
Danielle Rae Nicole Tarpley
May 2020
This dissertation is submitted in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy

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This Ph.D. is dedicated to my father Gilbert A. Tarpley, for always supporting my dreams no matter how far away from home they took me, and always making sure I had everything I needed.
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- Amy Poehler (Harvard Graduation, 2011)

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Author’s Note

Chapter 2 of this dissertation was originally prepared as a manuscript for publication in a peer-reviewed journal. As a result, this chapter was formatted for the *Journal of Marine Science and Engineering*. Additionally, the numbering of the figures, tables, and equations were formatted for publication and differ from Chapters 3 and 4.

The citation for Chapter 2 is:
Abstract

Fine-grained material such as silts and clays are the predominant sediment type in low energy systems such as micro-tidal embayments and estuaries. Due to its cohesive nature, fine sediment typically moves through marine systems as aggregated particles, or flocs, rather than as individual mineral grains. The particle’s components, local hydrodynamics, and concentration influence floc size, density, and fall velocity. These, in turn, impact suspended sediment transport, which complicates predictions of the fate of sediment for water quality, contaminant distribution, and dredging purposes in these systems. This dissertation used a state-of-the-art modeling system and observations to examine the variability in sediment distribution due to cohesive processes along a partially mixed estuary and to determine the role of flocculation on sediment transport for a muddy site within the York River estuary, Virginia. The Coupled Ocean-Atmosphere-Wave-Sediment Transport (COAWST) modeling system was used to simulate the hydrodynamics and suspended sediment transport in a muddy estuarine system. The model accounted for flocculation dynamics with a population balance model, FLOCMOD, changes in the erosion of sediment from the bed due to compaction or bed consolidation, and sediment-induced density gradients.

The sensitivity of the sediment distribution was performed using an idealized two-dimensional (vertical and longitudinal) model that produced key estuarine features such as salinity-driven circulation and an estuarine turbidity maximum (ETM). The reference model included the effects of flocculation, bed consolidation, and sediment-induced density gradients. Results from the reference model were compared to test cases, each of which removed one of these processes. This showed that the effects of flocculation on suspended sediment concentrations (SSC) were most significant in the surface waters and in the ETM; whereas bed consolidation decreased SSC along the full length of the estuary. Another test case demonstrated that calculations of SSC and median floc diameter ($D_{50}$) were sensitive to the number of sediment classes used to represent the floc population.

The capabilities of the idealized two-dimensional estuary were extended and used to examine the contribution of flocculation compared to other sediment transport mechanisms such as advection, diffusion, settling, and erosion. The dominant processes that impacted the sediment mass balance in the idealized estuary were flocculation, vertical diffusion, and erosion. Next, the $D_{50}$ produced by FLOCMOD in the idealized estuary was compared to a theoretical equilibrium floc size ($D_{eq}$) estimated based on the ratio of SSC to the square root of the shear rate ($G$). This analysis also produced an estimate for a timescale for flocculation. In general, $D_{50}$ reached $D_{eq}$ in the bottom boundary of the estuary when the flocculation timescales were on the order of minutes. However, immediately above the sediment bed, $D_{eq}$ was very similar to $D_{50}$ when erosion was minimal or when finer flocs were eroded from the bed. However, the computed $D_{50}$ most often differed widely from $D_{eq}$, indicating that equilibrium theory was not appropriate for much of the idealized estuary.

To facilitate the direct application of the flocculation model to the York River estuary, a one-dimensional (vertical) model was designed using observations of hydrodynamics and floc properties from the Claybank site for the vertical water column structure. The sensitivity of SSC and floc distribution to the parameterization of FLOCMOD was assessed using a model representing a spring-neap tidal cycle. The SSC was more sensitive to parameterization in the bottom boundary layer, $D_{50}$ was less sensitive than SSC, and the grain size distribution width (spread) was more sensitive to the fractal dimension. Model results were then compared to observations to choose parameters to represent the floc population in the York River estuary. Parameterization was challenging, but the preferred representation for the York floc population had a low relative error for SSC and acceptable error for the distribution mode and spread. For the spring-neap tidal cycle in general, vertical diffusion, settling, and erosion accounted for more sediment mass transport than flocculation, but flocculation played an important role in the vertical distribution of sediment via changes in floc size.
Temporal Variability in Cohesive Sediment Dynamics in a Partially Mixed Estuary, the York River Estuary, Virginia, USA: A Numerical Study Developed from Observations
Chapter 1: Introduction

1 Motivation and Background

1.1 Motivation

Poor water quality in estuarine and coastal environments causes damage to nursery habitats and the reduction of living resources that can negatively affect the economy of coastal communities (Dennison et al. 1993; Kemp et al. 2005). Degradation in water quality can be a direct result of elevated suspended sediment concentrations (SSC) partially due to changes in land use (Thrush et al. 2004). In the Chesapeake Bay, specifically, efforts to reduce sediment loads have focused on restoring natural lands by replanting buffers, creating improved development plans that preserve lands and open space, reducing loads from urban areas by promoting infiltration, modifying storm water management techniques, and reducing the dependence on septic systems (National Research Council 2011). The Chesapeake Bay Program (CBP) uses a monitoring program combined with a suite of numerical models to assess the effectiveness of different management techniques and evaluate the current status of the Bay (CBP 2012). These models need to include the prediction of SSC and depositional fluxes in order to fully assess conditions in the system.

A considerable portion of the suspended sediment in the Chesapeake Bay is composed of fine-grained material, i.e. silts and clays, which are cohesive in nature. Predicting SSC and deposition of cohesive sediment in an estuary is challenging due to the complexity of hydrodynamics, suspended sediment properties, and bed
characteristics. In suspension, silts and clays undergo flocculation, i.e., the aggregation of smaller particles, which causes sediment properties such as size, shape, and density, and the resulting settling velocity to range over several orders of magnitude (Droppo 2001; Droppo 2004). Upon deposition, the flocculated particles retain water at first, but over time the deposits de-water and gel (Dankers and Winterwerp 2007). Given enough time, the bed consolidates and becomes more difficult to erode (Grabowski et al. 2011). Therefore, to properly estimate erosional, depositional, and suspended fluxes of fine-grained material, the contribution of processes such as flocculation and consolidation should be considered. Several field, laboratory, and numerical studies have provided the framework to describe these cohesive processes mathematically (Burban et al. 1989; Fennessy et al. 1994; Dyer and Manning 1999; Winterwerp 2001; Winterwerp 2006; Dickhudt et al. 2009). Recent efforts also include the incorporation of these cohesive processes into numerical community models (Winterwerp et al. 2006; Sanford 2008; Gong and Shen 2009).

The York River estuary, Virginia, a tributary of the Chesapeake Bay, has a sediment bed that is predominantly fine-grained. It exhibits many classic estuarine characteristics, and is subject to water quality issues including elevated suspended sediment loads and declines in submerged aquatic vegetation and oyster beds (Moore 2009; Reay 2009; zu Ermgassen et al. 2013). Additionally, the maintenance of shipping channels is required for military ships to access the Coast Guard and Naval bases in the York River estuary. As a smaller, and more accessible system than the entire Chesapeake Bay, the York is an
ideal location to examine the influence of cohesive processes on sediment dynamics that are also important to the Bay as a whole.

1.2 Estuarine Sediment Distributions

Sediment moving through an estuary can be affected by a variety of processes before being buried or exiting the estuary. A portion of the fluvial suspended sediment moving down-estuary is trapped near the head of the salt intrusion creating an estuarine turbidity maximum (ETM; Schubel 1968; Burchard and Baumert 1998; Sanford et al. 2001; Dickhudt et al. 2009). Many factors contribute to sediment trapping in the ETM, including residual gravitational circulation, asymmetrical responses in tidal velocity, tidal resuspension, the formation of fast settling aggregates, salinity, temperature, and sediment-induced density gradients that create a stratified water column, and the formation of an easily erodible pool of sediment (Burchard and Baumert 1998; Sanford et al. 2001; Winterwerp 2011; van Maren et al. 2015).

Sediments may be episodically removed from the ETM through pulses in river discharge or strong wind events that promote down-estuary transport (Kniskern and Kuehl 2003; North et al. 2004). Outside of the ETM, sediment is redistributed and eventually buried or transported out of the estuary.

Some estuaries, including the York and Hudson River estuaries, exhibit a secondary turbidity maximum (STM) that is downstream of the ETM (Lin and Kuo 2001; Ralston et al. 2012). A numerical study in the York suggested that bed resuspension, turbulent reduction due to stratification, convergence of residual flow, and tidal asymmetry interact to form the STM (Lin and Kuo 2001). In the Hudson River estuary, a steep
change in the bathymetry produces a salinity front, which traps sediment to form an STM and a local pool of erodible sediment (Ralston et al. 2012). Similarly, bathymetry, along with salinity stratification, may play a role in forming the STM in the York River estuary (Lin and Kuo 2001). Additionally, resuspended bottom sediment, tidal asymmetries in velocity, and weak convergence of residual flow has been shown to impact the STM location in the York (Lin and Kuo 2003). Uncertainties in these results lie in the simplified representation of sediment characteristics. Despite this, it is clear STMs influence sediment distributions for some estuaries, including the York River estuary.

Estuarine models that couple hydrodynamics with sediment transport processes can be used to examine the distribution of sediment. These models resolve hydrodynamics by solving initial boundary value problems using the continuity and conservation of mass equations with various initial and boundary conditions (Dornhelm and Woolhiser 1968; Walters and Cheng 1979; Shchepetkin and McWilliams 2005). Over the years, model capabilities have expanded to better represent complex systems. Modern hydrodynamic models can have higher-resolution and complex grids, use higher order approximation methods, have more complex boundary conditions, assimilate data, and can be coupled with other process models, such as cohesive sediment transport models (Le Provost et al. 1998; Shchepetkin and McWilliams 2005; Warner et al. 2005; Fennel et al. 2006; Warner et al. 2008; Warner et al. 2010).

1.3 Cohesive sediment processes

Clay particles have charged surfaces that naturally repel one another, but ions from saline water or biological compounds counter this to promote attraction between clays
which, in turn, encourages the aggregation of particles and formation of flocculated particles (flocs). Flocs in freshwater form due to biological secretions and typically have diameters that range from several microns to <200 μm, but aggregation is more frequent in salinities >0.6-2.6 (Krone 1978; Droppo and Ongley 1994; de Boer et al. 2000; McAnally and Mehta 2001; Guo and He 2011). The probability of aggregation increases with organic content, SSC (<100 mg L⁻¹), turbulence, and differential settling (McAnally and Mehta 2002; Winterwerp 2002; Cross et al. 2013; Soulsby et al. 2013). Moderate turbulent shear stresses increase collisions that allows flocs to form, but at high levels of turbulence the shear can tear flocs apart (Fugate and Friedrichs 2003; Verney et al. 2011; Wang et al. 2013; Mehta 2014). The smallest constituents of flocs, known as “primary particles”, are typically ~1 to 5 μm in diameter (Fettweis et al. 2012). As flocs grow, the diameters and settling velocities increase causing faster deposition. Primary particles can be packaged in tightly compacted microflocs (10s of μm in diameter), or loosely bound macroflocs (~100 to 1000 μm in diameter) that are often a conglomerate of primary particles and microflocs (Lee et al. 2011; van Leussen 2011; Manning and Schoellhamer 2013). Organic material incorporated into the floc and the floc porosity also affect the size, shape, density, and settling rate of flocs (Dyer and Manning 1999; Manning and Schoellhamer 2013). Thus, in cohesive environments such as a muddy micro-tidal estuary, temporal and spatial variation in SSC, turbulence, and organic material impact floc settling velocities, resulting in changes in sediment suspension and deposition rates.
The vertical distribution of suspended sediment is largely governed by the balance between turbulent shear and settling, which is parameterized by the Rouse number. Generally, suspended particles with slow settling velocities are more uniformly distributed vertically, whereas fast settling particles are concentrated near the bed. As described above, settling velocities for cohesive sediment varies with turbulence and SSC. Increases in turbulence cause an increase in SSC, to a degree, via erosion from the bed. In the absence of stratification, vertical mixing is enhanced with higher turbulence levels, distributing sediment vertically, and enhancing the potential for longitudinal transport. However, elevated SSC (a few hundred mg L\(^{-1}\) or greater) can alter the turbulent structure by forming a density gradient that limits mixing and inhibits the upward flux of sediment (Winterwerp 2001; Winterwerp 2006). The relative impact of turbulent damping compared to turbulent production can be parameterized with the non-dimensional gradient Richardson number (Trowbridge and Kineke 1994; Friedrichs et al. 2000). Stratified conditions reduce the drag of the fluid on near-bed sediment, and sediment remains closer to the bed, often forming a lutocline (Friedrichs et al. 2000; Dyer et al. 2004). Lutoclines are known to form in ETMs, but little is known about the occurrence and the associated hydrodynamic conditions, stability, and effects of lutoclines in other locations in an estuary (Dyer et al. 2004; Wang 2010; Wu et al. 2012).

Erodibility of the sediment bed can be defined as the amount of sediment that can be removed from the bed under a given applied shear stress (Sanford 2008). Sediment deposited to the bed begins to dewater, compress and consolidate since the structure of the flocs is no longer supported by surrounding fluid (Dankers and Winterwerp 2007).
The weight of the flocs causes the structure to compact and begin to form a space-filling bed structure. Initially after deposition, the deposit can easily be re-suspended, but as compaction progresses, the bed becomes less erodible (Mehta et al. 1988; Dankers and Winterwerp 2007). The sediment bed is susceptible to suspension and deposition cycles as flow energy fluctuates, and biological activity further adds to the variability in sediment erodibility. It can therefore take weeks to months after deposition to form a consolidated bed (Mehta et al. 1988).

Bed erodibility controls the supply of sediment from the bed, and is not negligible when examining cohesive sediment transport (Son and Hsu 2011; Fall et al. 2014). Physical, chemical and biological characteristics vary the response of the bed to applied stress (Grabowski et al. 2011). Sediment deposited near slack tide undergoes partial consolidation, but remains fairly easy to erode when tidal currents increase (Dyer 1989; Scully and Friedrichs 2003). Over the spring-neap tidal cycle, the amount of erodible sediment varies as stronger currents and mixing during spring tides increase erosion, and there is less time for consolidation between successive peak tidal flow (Allen et al. 1980; Sanford and Maa 2001; Scully and Friedrichs 2007). Rapid deposition and frequent suspension form pools of highly erodible sediment in frontal trapping regions such as a STM (Dickhut et al. 2009). Other factors that can impact bed erodibility include the average particle or aggregate size, percent clay content, bulk dry density, water content, salinity, temperature, clay mineralogy, pore water chemistry, organic content, biofilms, subaquatic plants, sediment disturbance by bioturbation, and repackaging of sediment grains into fecal pellets (Parchure and Mehta 1985; Mehta et al. 1988; Teal et al. 2008;
The relative contributions of these vary between environments and seasonally, with higher biological activity in the spring/summer seasons.

Several approaches, covering a range of complexity, have been applied to model cohesive sediment dynamics. Flocculated particles have been represented using a constant settling velocity (often ~1 mm s\(^{-1}\)), by increasing settling velocity in >1 g kg\(^{-1}\) water, using multiple sediment classes with different settling velocities, and by tracking shifts in size distribution, median size, or a median equilibrium size (Lick and Lick 1988; Winterwerp 1998; Hill and McCave 2001; Winterwerp 2002; Winterwerp et al. 2006; Maerz et al. 2011; Verney et al. 2011; Ralston et al. 2012; Fall et al. 2014). Population balance equations can be used to track shifts in the size distribution using a set of floc size classes. As an example, the flocculation model, FLOCMOD (Maerz et al. 2011; Verney et al. 2011), uses population balance equations and has been integrated into a community model, the Coupled Atmosphere-Wave-Sediment Transport (COAWST) modeling system (Sherwood et al. 2018). Observations from laboratory experiments when compared to model results showed FLOCMOD has the ability to be parameterized to represent different floc populations (Verney et al. 2011; Sherwood et al. 2018).

The effects of sediment-induced density gradients and the consolidation of the sediment bed have also been added into numerical models in a variety of ways. Sediment-induced density gradients or stratification have been addressed with adjustments to the turbulence closure model, the equation of state, and the applied bed stress due to elevated SSC (Winterwerp 2001; Neumeier et al. 2008; Warner et al. 2008;
Gong and Shen 2009; Son and Hsu 2011; Bi and Toorman 2015). The impacts of sediment-induced stratification are better represented using higher vertical resolution (Chen et al. 2013). Stages of consolidation have been represented by varying the erosion rate with changes in bed density, depth into the bed, or bed age, and by increasing the critical shear stress for erosion with depth or age (Hayter and Mehta 1986; Cancino and Neves 1999; Liu et al. 2002; Fettweis and Van Den Eynde 2003; Neumeier et al. 2008; Sanford 2008; Fall et al. 2014; Bi and Toorman 2015). Within COAWST, Sherwood et al. (2018) added the bed consolidation model of Sanford (2008), but relatively few applications of this model have been published to date. The choice of the representation of consolidation depends on the modeling application and available observational data. Complex representations typically contain several parameters with a range of applicable values, in which field or laboratory measurements can be used to optimize or constrain (Burban et al. 1989; Winterwerp et al. 2006; Verney et al. 2011; Winterwerp 2011; Fall et al. 2014; Grasso et al. 2015). Simplistic representations may reduce computational costs and require fewer model parameters. Regardless of the model used, in situ measurements are helpful for reducing uncertainties (Fall et al. 2014; Grasso et al. 2015).

1.4 The York River estuary

The York River is a partially mixed, microtidal (<1 m tidal range) estuary that spans ~50 km, with its head at the confluence of the Mattaponi and Pamunkey rivers, to its mouth at the Chesapeake Bay. The salinity within the York ranges from ~6-25 g kg\(^{-1}\); salinity stratification is highest in the lower reaches of the river and is greater during
neap tides compared spring tides (Friedrichs et al. 2000; Friedrichs 2009). Along the muddy main channel, water depths increase from ~6 m to ~20 m from West Point to Gloucester Point. A muddy secondary channel runs along the middle reaches on the southeast side of the river, is ~5 m in depth, and is separated from the main channel by an inactive oyster reef (Dellapenna et al. 2003; Friedrichs 2009). The channels are bordered by sandier shoals ~2 m in depth. Sediment is trapped at the head of the salt intrusion forming an ETM around West Point, and seasonally at the STM located at a transition between the well-mixed upper estuary and partially mixed lower estuary in the Claybank region about ~30 km from the mouth (Lin and Kuo 2001; Friedrichs 2009).

Several field studies focused near Claybank as part of the Multi-Disciplinary Benthic Exchange Dynamics (MUDBED) since 2006 show SSC, the estimated bulk sediment settling velocity, and bed erodibility vary temporally and spatially in the river (Friedrichs et al. 2008; Fall et al. 2014). Near-bed SSC are greatest directly following peak tidal flow, and may result in sediment-induced stratification that dampens turbulence (Friedrichs et al. 2000; Cartwright et al. 2013; Fall et al. 2014). Measured bulk settling velocities indicate faster settling particles such as resilient fecal pellets can contribute to the near-bed suspension near peak tidal flow, whereas flocs dominate further from the bed and during weaker tidal stresses (Cartwright et al. 2011; Fall et al. 2014). The size of these flocs may be controlled by the size of the turbulent eddies in the lower and mid-water column (Fugate and Friedrichs 2003). The bed erodibility is impacted by the composition of deposited sediment, such as whether the bed sediment is composed of flocs or is repackaged into resilient pellets by biota. Physical mixing processes are dominant in the
mid-to upper York River estuary, where erodibility is affected by presence of a mobile bed due to tidal fluctuations in bed stress, the associated resuspension and deposition and/or the presence of the ETM/STM (Schaffner et al. 2001; Dellapenna et al. 2003; Dickhudt et al. 2009; Cartwright et al. 2011; Kraatz 2013).

Numerical studies examining sediment dynamics in the York have represented cohesive sediment in a variety of ways. Initial efforts neglected flocculation (Lin and Kuo 2003; Shen and Haas 2004). More recently, models accounted for flocculation using a positive relationship between settling velocity and SSC (Gong and Shen 2009), or defining multiple size classes whose settling velocities were informed by bulk measurements (Fall et al. 2014). An adjustment to the equation of state for SSC has been used to account for buoyancy affects (Gong and Shen 2009). Bed consolidation over time has been incorporated using a depth-varying critical shear stress for erosion (Rinehimer 2008; Gong and Shen 2009; Fall et al. 2014). When compared to observations, model estimates from Fall et al. (2014) showed a mismatch in SSC and bulk settling velocity ($W_{\text{bulk}}$), predominately overestimating both parameters. These models represented realistic domains that carried high computational costs to represent the three-dimensional structure of the York River estuary. However, these models could only incorporate select cohesive processes. A simplified test case using a less complex model domain would have lower computational costs while accounting for first-order hydrodynamic processes, but would be able to implement more complex cohesive processes. For example, estuarine test cases have been used to examine the performance of different turbulence closure models, the effect of tidal straining on
suspended sediment transport, and sediment transport in the bottom boundary layer

2 Dissertation Objectives and Outline

Combining numerical modeling with observations, this dissertation investigated the roles of various cohesive sediment processes in the distribution of sediment in the York River estuary. Idealized or simplified spatial model domains were adopted, while the cohesive processes were represented using recently developed routines, including the flocculation model, FLOCMOD (Verney et al. 2011), and a bed consolidation model (Sanford 2008). Both the flocculation and bed consolidation model have recently been added to the COAWST sediment transport routines (Sherwood et al. 2018). Additionally, observations of the water column suspended sediment properties and water column structure from the York River Claybank site were used to constrain the numerical models. Chapters 2 – 4 describe the approach that will be used to address the main research objectives:

a) Evaluate the performance of the cohesive sediment routines; determine the effects of flocculation, bed consolidation, and sediment-induced density gradients on sediment distribution within an idealized, partially mixed estuary; and explore the sensitivity of the flocculation module to the number of sediment sizes used in the model.

b) Examine the importance of floc dynamics, relative to other transport processes (advection diffusion, settling, and erosion) in controlling the distribution and
transport of SSC in estuaries, and evaluate the degree to which an equilibrium floc size model represents the particle size distribution.

c) Examine the sensitivity of flocculation dynamics to the variability in the fractal dimension ($n_f$), collision efficiency ($\alpha$), and breakup efficiency ($\beta$); determine the best values for $n_f$, $\alpha$, and $\beta$ that best represent the floc characteristics at the Claybank site of the York River estuary; and evaluate the role of flocculation in comparison to other transport mechanisms on SSC over a spring-neap cycle.

Chapter 2 used an idealized two-dimensional (vertical and longitudinal) estuarine model to evaluate the difference in sediment distribution in the dynamic ETM region versus a downstream location in the estuary that had lower SSC and turbulence. The effects of flocculation, bed consolidation, and sediment-induced density gradients on sediment distribution were examined by a set of test cases that removed individual processes. Lastly, the sensitivity of the SSC and median floc size to the reduction of the number of floc sizes used to represent the floc population was explored. Note that Chapter 2 has been published in the *Journal of Marine Science and Engineering* (Tarpley et al. 2019).

Chapter 3 extended the capabilities of the idealized two-dimensional model from Chapter 2, and used the model results to quantify the effect of flocculation on local sediment exchange between size classes in comparison to other mechanisms, namely advection, diffusion, erosion and settling. Additional analysis compared the modeled median diameter to an estimation of a median equilibrium floc diameter to evaluate the
ability of the equilibrium formulation to represent the floc population under varying hydrodynamic conditions.

Chapter 4 used a one-dimension (vertical) model derived from observations from the Claybank region of the York River estuary to evaluate the sensitivity of a population balance flocculation model, FLOCMOD, to parameterization of the collision/breakup efficiency and fractal dimension. Observations of SSC and grain size distribution were used to parameterize FLOCMOD to represent the floc population in the York River estuary Claybank site. Finally, this combination of best-fit parameters was applied to a model that simulated conditions in the York during a spring-neap cycle.
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Tidal Variation in Cohesive Sediment Distribution and Sensitivity to Flocculation and Bed Consolidation in An Idealized, Partially Mixed Estuary

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Chapter 2: Tidal Variation in Cohesive Sediment Distribution and Sensitivity to Flocculation and Bed Consolidation in An Idealized, Partially Mixed Estuary

Abstract

Particle settling velocity and erodibility are key factors that govern the transport of sediment through coastal environments including estuaries. These are difficult to parameterize in models that represent mud, whose properties can change in response to many factors, including tidally varying suspended sediment concentration (SSC) and shear stress. Using the COAWST (Coupled Ocean-Atmosphere-Wave-Sediment Transport) model framework, we implemented bed consolidation, sediment-induced stratification, and flocculation formulations within an idealized two-dimensional domain that represented the longitudinal dimension of a micro-tidal, muddy, partially mixed estuary. Within the Estuarine Turbidity Maximum (ETM), SSC and median floc diameter varied by a factor of four over the tidal cycle. Downstream of the ETM, the median floc size and SSC were several times smaller and showed less tidal variation (~20% or less). The suspended floc distributions only reached an equilibrium size as a function of SSC and shear in the ETM at peak tidal flow. In general, flocculation increased particle size, which reduced SSC by half in the ETM through increased settling velocity. Consolidation also limited SSC by reduced resuspension, which then limited floc growth through reduced SSC by half outside of the ETM. Sediment-induced stratification had negligible effects in the parameter space examined. Efforts to lessen the computation cost of the flocculation routine by reducing the number of size classes proved difficult; floc size distribution and SSC were sensitive to specification of size classes by factors of 60% and 300%, respectively.

Keywords: COAWST; numerical model; flocculation dynamics; cohesive sediment
1 Introduction

1.1 Motivation

Estuaries are valuable coastal ecosystems that provide habitat and nursery services to many fishery species, including finfish, crustaceans, and mollusks. In estuaries, freshwater interacts with saline water and mixing can be dominated by waves, tides, riverine input or any combination [1,2]. This leads to complex hydrodynamic conditions with a broad range in spatial and temporal variability [3,4], such as those driven by tidal asymmetries, spring-neap cycles, and seasonal fluctuations in river discharge [5]. The Estuarine Turbidity Maximum (ETM) is a key feature of partially mixed estuaries that occurs at the convergence of freshwater and seawater, which can trap sediment leading to a peak in suspended sediment concentration (SSC), and moves with changes in hydrodynamic conditions [6]. Thus, understanding the processes that are critical to maintaining healthy estuarine environments is challenging. Muds that are comprised of higher percentages of clays and silts typically dominate estuarine suspended sediments, and the distribution of these sediments impacts water quality, contaminant transport, and navigation [6]. Elevated SSC in surface waters limits light availability for phytoplankton and submerged aquatic plants [7,8]. It should be noted that this study does not address sandy sediments nor the effects of sand on the behavior of muddy sediments. In macrotidal estuaries, sediments within the channel bed are often dominated by sands [9,10] and the fate of sand is also essential to the evolution and stability of deltaic estuaries [11–13]. Thus, this study most directly applies to regions upstream from the mouths of micro- to low-mesotidal estuaries, where the
surficial sediments in the main channel are dominated by mud. Such systems are especially common along the US Atlantic coast and include, for example, the Satilla [14], Ashepoo [15], James [16], York [17], Rappahannock [18], Potomac [19], Delaware [8], and Hudson [20].

The cohesive nature of mud allows sediment to be transported as aggregated particles; these aggregates can absorb contaminants thereby influencing the dispersal of contaminants [21]. Recent research in response to the Deepwater Horizon spill in the Gulf of Mexico showed that the aggregation processes of muds was important for predicting the fate of hydrocarbon contaminants in marine systems, as it can combine with suspended sediment to form “OMAs” (oil-mineral-aggregates) that settle to the seafloor [22,23]. Additionally, the formation of fast-settling flocs (aggregated muddy particles; [24]) reduces SSC in surface waters. Other human activities, such as dredging to maintain shipping channels in estuaries, change the distribution of sediment. As long as dredging remains a practice, an understanding of how mud is transported is required to determine ideal locations for dredge materials that lowers environmental impacts, limits channel infilling and reduces the overall costs [25,26]. Therefore, innovative methods for predicting cohesive sediment transport are needed and would improve our understanding and ability to reduce human impacts in these systems.

In 2010, 39 percent of the U.S. population lived in coastal regions; this number and the resulting human impacts are expected to increase [27]. However, since 2010 in Virginia, USA alone, more than $350 million has been invested in reducing nonpoint source pollution and improve water quality [28]. Regulatory managers that are
responsible for allocating funds to handle environmental issues use numerical models to provide insight into the impacts on coastal aquatic systems due to changes in land development [29,30], nutrient loads and their reduction [31], climate change [32], as well as numerous other factors. In addition, these models allow scientists to test hypotheses over a variety of temporal and spatial scales, and isolate the impacts of individual processes that cannot be separated in observations [33]. For the Chesapeake Bay, USA, in particular, models have aided in the development of reduced nutrient loads needed to improve water quality and the evaluation of the confidence of these estimates [31,34,35].

1.2 Flocculation, Bed Consolidation, and Sediment-Induced Stratification

The flocculation or deflocculation of fine-grained sediments (i.e., the aggregation or dissaggregation of muddy sediment within the water column) leads to variability in suspended sediment properties such as floc size, shape, and density; producing settling velocities that can range over orders of magnitude [36,37]. For example, flocs observed by a video settling camera in surface waters of the York River estuary, USA, had equivalent spherical diameters that ranged from ~30–500 μm, with settling velocities ranging from ~0.06–3 mm s⁻¹, and exhibited a systematic decrease in floc densities with increasing diameter [38]. Other studies have measured floc sizes greater than 1000 μm [39]; specifically, in the Tamar estuary floc diameters were measured as large as 2200 μm [40]. These properties influence the vertical distribution and the residence time of flocs in the water column as well as their horizontal transport. The local conditions such
as the amount of biological secretions present, SSC of both muds and sand, salinity, and hydrodynamics impact floc properties [6,41,42].

Modeling the transport of flocs has been approached in several different ways, from using constant settling velocities obtained from observations for a single size or set of size classes [43–45] to predicting median size or other statistical properties of the size distribution including shifts in the size distribution with a set of population balance equations [46–52]. An equilibrium floc theory predicts median floc sizes using the SSC and shear rates [46,53], whereas other models are more process oriented, but require the user to define additional parameters such as the size and density of primary particles, (i.e., the smallest particles that make up the flocs), the floc fractal dimension (a parameter that describes the characteristic porosity of the flocs as a function of their diameter), and aggregation and break-up efficiencies [49,54]. However, these floc properties can be altered when deposited to the bed by bed consolidation, but the floc size and settling velocity can adjust to the SSC and turbulence within minutes after resuspension [55,56]. The proper estimation of erosional, depositional, and lateral fluxes for cohesive environments requires evaluation of the contribution of aggregation, as well as bed consolidation.

An unconsolidated and easily erodible muddy bed readily supplies sediment to the water column; but over time, the bed may de-water, consolidate, and become less erodible [57,58]. Bed characteristics other than water content such as clay mineralogy, silt-to-clay ratio, sand fraction and organic content can further alter the erodibility of a muddy bed [58–60]. The consolidation of the bed, and in some cases the fraction of
sand, increase with depth into the bed and can limit the supply of sediment to the water under increased bed stress [59,61,62]. The erosion of mud from the bed is not well correlated with the size of the component particles [58]; thus, numerical models use other techniques for representing the erodibility of the bed in fine-grained environments. The erosion rate is decreased [63,64], or the critical shear stress for erosion may be increased with increased bed density, depth into the bed, and/or age of the bed layer [65,66].

The presence of elevated SSC near the sediment bed creates vertical density stratification [67,68], i.e., sediment-induced stratification, that can dampen turbulence, reducing the bed stress and reducing the upward mixing process while diminishing the amount of sediment eroded and the sediment-carrying capacity of the fluid [69]. If SSC is limited, then the potential for longitudinal transport may be reduced. Reduction of the sediment carrying capacity due to elevated SSC is often incorporated into numerical models by adding parameters into the turbulence closure scheme that reduce mixing with elevated SSC [66,67,70] or reduce the applied bed stress in concert with increases in SSC [71,72]. A more fundamental approach is to add a formulation that incorporates density changes due to SSC into the equation of state (the function that quantifies fluid density) [73,74], and use the combination of water density and SSC stratification in a turbulence closure model to determine the eddy diffusivity. This requires that the hydrodynamic model have sufficiently high vertical resolution to represent the large gradients in SSC that produce the density-induced stratification found near the bed [74].
The implementation of these cohesive sediment processes into numerical models can be challenging, because several of the model coefficients have a large range of possible values [48,58]. Some parameterizations can be informed by local observations; for example, previous implementations of a bed consolidation formulation have fit model parameters based on erosion microcosm field measurements [75,76]. However, in many cases, parameterization of cohesive sediment models remains difficult. Additionally, inclusion of these cohesive processes can significantly add to the computational cost of a sediment transport model. Thus, due to computational limits, many implementations of sediment transport for muddy environments in the past have used simplified forms for flocculation and bed erodibility despite the potential reduction in the model skill and challenges in parameterizing cohesive formulations.

1.3 COAWST

The Coupled Ocean-Atmospheric-Wave-Sediment Transport model (COAWST), incorporates hydrodynamics from the Regional Ocean Modeling System (ROMS) and the Community Sediment Transport Modeling System (CSTMS; [73]). ROMS is a terrain-following, free-surface, hydrostatic primitive equation numerical model. ROMS simulates hydrodynamics by solving equations for continuity and conservation of mass and momentum using hydrostatic and Boussinesq assumptions with various initial and boundary conditions defined by the user. It has a large user community and has been described in detail elsewhere, see [73,77,78]. The CSTMS calculates erosion and deposition to the sediment bed and suspended transport of sediment. Sediment is removed from the bed at the user defined rate when the applied stress is greater than...
the critical shear stress for erosion. The transport of suspended sediment in the water column is estimated by solving the same advection-diffusion equations as used by the hydrodynamic model for salinity and temperature but with an added source/sink term to allow exchange with the sediment bed for individual sediment classes. Specifically, each sediment class has predefined hydrodynamic properties including particle density, settling velocity, and critical shear stress for erosion that have not accounted for cohesive processes until recently; for more details see [73]. Recent CSTMS developments have added cohesive modules for flocculation and bed consolidation; and its seabed layering routines now also account for cohesive, non-cohesive or mixed sediment beds [53].

The new flocculation routine (FLOCMOD) is a population balance module, and the bed consolidation routine increases the critical shear stress for erosion with depth into the sediment bed [53]. FLOCMOD requires flocculation growth and breakup parameters, primary particle size, and fractal dimension [49]. Flocculation parameters are typically chosen to follow field or laboratory studies that provide expected ranges for the associated parameters [38,79,80]. Sediment is entrained into the water column from the bed in CSTMS when the applied bed stress exceeds the critical shear stress for erosion [73,81,82]. The cohesive bed consolidation module specifies additional sediment erodibility parameters that change with depth [65]. In the York River estuary, a field study aided in defining the exponential increase of critical shear stress for erosion with depth into the bed due to consolidation [60]. However, model estimates were particularly sensitive to values that are difficult to obtain from field observations, such
as the initial and equilibrium critical shear stress profiles, and the consolidation and swelling timescales [45]. The effect of density-induced stratification from gradients in SSC in CSTMS is implemented using the same approach as [73,74].

The addition of these cohesive sediment routines provides a more complete representation of the processes that are important for suspended transport of muds. The flocculation routine provides a means of examining impacts that are difficult to measure in situ. However, as yet few studies have capitalized on the implementation of a floc population balance model such as FLOCMOD within a community sediment transport model to evaluate the role of cohesive processes in muddy estuaries.

1.4 Objective and Outline of the Study

The objective of this study is therefore to evaluate the performance of the cohesive sediment routines developed in the COAWST modeling system and examine the impact of these cohesive processes on sediment distribution within an idealized, partially mixed estuarine simulation. The sensitivity of the flocculation module to the number of sediment sizes was also examined, because the computational costs increase with the number of sizes. To that end, the goal of this study is to answer the following questions:

i. Considering sediment-induced stratification, flocculation dynamics, and bed consolidation, how do these processes impact sediment distribution along a partially mixed estuarine model?

ii. How does using fewer sediment sizes constrain our ability to represent sediment dynamics in a cohesive sediment environment?
To address these research questions, an idealized model domain was used to assess the effectiveness, sensitivity to parameterization, and computational costs of the CSTMS flocculation and other cohesive sediment formulations. The simplified, idealized domain was chosen because it carries lower computational costs than the more realistic three-dimensional simulation, allowing us to complete systematic testing in a more feasible time frame. Additionally, idealized models can provide insight on first order impacts and interactions without confounding factors such as complex bathymetry and highly variable forcing functions.

Section 2 details the numerical methods and sediment characteristics utilized in this study and the experiments performed. The results and discussion are presented in section 3, and suggestions for the future handling of flocculation are provided in section 4. Finally, the study’s conclusions are outlined in section 5.

2 Materials and Methods

2.1 York River Estuary, Virginia, USA

The York River estuary [17], which inspired the idealized model geometry utilized in this study, extends northeast from the lower Chesapeake Bay (where salinities are typically \(~26 \text{ g kg}^{-1}\)) to the confluence of the Pamunkey and Mattaponi rivers, with a total length of \(~60 \text{ km}\) (Figure 1). The depths in the main channel range from \(~20 \text{ m}\) at the mouth to \(~6 \text{ m}\) at the head of salt (\(~1 \text{ g kg}^{-1}\) isohaline; Figure 2; [83]). The York is a microtidal, partially mixed estuary that becomes relatively more well-mixed as its depth decreases and tidal energy increases towards its head [83]. Under typical conditions, tidal current magnitude is on the order of \(50 \text{ cm s}^{-1}\) at 1 meter above the bed (mab) in
the ETM region [17]. The sediment bed in the main channel is dominated by mud with percentages often exceeding 80% [84]. Total suspended solids within the ETM of 250 mg L\(^{-1}\) have been measured during slack at 1 mab [83]. For suspended flocs in the York that follow a fractal relationship in size and density distribution, [38] found the median values for the fractal dimension, primary particle size, and primary particle density to be 2.4, 1.7 microns, and 1900 kg m\(^{-3}\), respectively.

Figure 1. Map of the York River estuary, Virginia, USA.

Figure 2. Observations of (left) salinity and (right) SSC along the York River estuary near slack tidal flow on September 12, 1996, adapted from Figure 5c of [83] with permission from RightsLink: Springer Estuaries, Sept. 19, 2019.
2.2 Model Description

Our implementation of COAWST used components of CSTMS [73] and hydrodynamics associated with ROMS [77,85]. Unlike most previous implementations of the CSTMS, ours utilized the flocculation dynamics module, the bed consolidation/swelling routine, and sediment–induced stratification. We neglected the impacts of sand (non-cohesive sediment) because the York River channel is dominantly mud [84]. The flocculation dynamics were represented by a set of differential equations based on population balance equations described in detail elsewhere [48,49,53]. These equations allow the exchange of sediment mass between the defined size classes, depending on the rate of turbulent shear and the sediment concentrations. Bed consolidation was accounted for by increasing the critical shear stress for erosion with depth into the sediment bed, with model parameters based on erosion experiments [60,65,86]. To implement this within the cohesive version of the CSTMS, the user must define initial and equilibrium profiles for critical shear stress for erosion. The effective instantaneous profile of the critical shear stress can be altered by erosion or deposition, but is then nudged toward the equilibrium profile to simulate consolidation or swelling [53,65]. The adjustment for sediment-induced stratification is computed as in [73].

2.3 Model Configuration

A model with the following idealized two-dimensional domain was designed to represent the longitudinal dimension of a micro-tidal, partially mixed estuary. The model represented salinity-driven estuarine circulation, but neglected across-channel variation. The primary features of the idealized simulation were similar to the main
channel of the York (see Section 2.1), and the sediment characteristics were based on observed values from this system [17,38]. The idealized estuary was 180 km in total length, and the water column was partitioned into 40 vertical layers (Figure 3). A 60-km-long area of interest was in the center of the grid, with a buffer of about 60 km on either end (please note that in the figures, “0 km” marks the seaward end of the area of interest). The horizontal resolution was 500 m, and the vertical resolution varied with depth and ranged from 0.053–0.79 m, with higher resolution near the surface and the bed. Our analysis focused on the area of interest that encompasses the estuarine system with water depths of ~18 m at the seaward end to the head of salt at the landward end with a depth of 6 m. The full model grid included buffer regions to either side, to minimize the effects of boundary conditions within the area of interest. The model applied includes salinity dependence for flocculation. A natural system is likely to have different floc properties in the riverine portion due to an absence of salinity. The “riverine” section of our domain lies within the upstream buffer zone, outside our region of interest.

The tides were driven at the ocean boundary with a period of 12 hours and a microtidal range of 0.75 m at the mouth that increased to ~1 m at the head, as observed in the York River estuary [17], which produced tidal velocities similar to those observed in the York. The salinity at the seaward boundary was based on salinity measurements near the mouth of the York River estuary, which is open to the Chesapeake Bay. It was held constant in time, but varied in the vertical; specifically it was 26 psu near the bed and decreased to ~14 psu at the surface. Freshwater entered the grid at the upstream
river boundary with a discharge of 70 m$^3$ s$^{-1}$. On average, the salinity ranged between 0 and 25.5 psu in the area of interest. The temperature was held constant at 10 °C. The sediment model included 11 sediment floc size classes, with particle size diameters logarithmically spaced between 1 and 1024 μm, which represented the median diameter for each size class. These particle diameters span the range reported by [38]; from the inferred primary particle size through the largest flocs observed (~500 μm). We added an additional size class with a particle diameter of 1024 μm in order to account for larger flocs near the bed. The settling velocity ($w_{s,i}$) and density ($\rho_{f,i}$) of each class were calculated using a modified Stokes’ settling equation assuming a fractal dimension of 2.4, and a primary particle density and diameter of 2000 kg m$^{-3}$ and 1 μm, respectively (based on observations from the York River estuary [38]; Equations (1) and (2); Table 1). For definitions of the variables in the equations below, see Table A in the appendix.
Figure 3. Idealized estuary model grid including the buffer zone on both ends of the estuary. Black lines show water column grid cells; colors show the time-averaged modeled salinity (blue to yellow colors). Brown layer under the water column represents the sediment bed grid cells.

Table 1. Sediment model size classes for floc diameters ($D$), along with corresponding floc density ($\rho_f$) and settling velocity ($w_s$). All eleven size classes were represented in the reference case and the sizes included in the reduced floc cases are indicated in columns 5 and 6.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$D$ (μm)</th>
<th>$\rho_f$ (kg m$^{-3}$)</th>
<th>$w_s$ (mm s$^{-1}$)</th>
<th>3 Class Case</th>
<th>5 Class Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2000</td>
<td>0.00054</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1663</td>
<td>0.0014</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>1441</td>
<td>0.0038</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
<td>1294</td>
<td>0.0099</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>16</td>
<td>1198</td>
<td>0.026</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>32</td>
<td>1134</td>
<td>0.069</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>64</td>
<td>1092</td>
<td>0.18</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>8</td>
<td>128</td>
<td>1064</td>
<td>0.48</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>9</td>
<td>256</td>
<td>1046</td>
<td>1.27</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>10</td>
<td>512</td>
<td>1033</td>
<td>3.35</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>11</td>
<td>1024</td>
<td>1026</td>
<td>8.84</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

\[ \rho_{f,i} = \rho_w + (\rho_p - \rho_w) \left( \frac{D_p}{D_{f,i}} \right)^{3-n_f} \]  

(1)

\[ w_{s,i} = \frac{g(\rho_{f,i} - \rho_w)D_{f,i}^2}{\rho_w \cdot \nu} \]  

(2)

In the equations above, $\rho_w$ is the water density, $\rho_p$ is the primary particle density, $D_p$ is the primary particle diameter, $D_{f,i}$ is the diameter of the floc in size class $i$, $n_f$ is the fractal dimension, $g$ is the acceleration due to gravity, and $\nu$ is the kinematic viscosity.

No sediment was discharged from the river, and none left the domain through the river boundary, despite the gradient boundary condition. Table 2 lists the open boundary conditions used. Other critical components to the sediment transport model included a logarithmic drag formulation with a constant hydraulic bottom roughness, for simplicity ($z_{0b} = 5 \times 10^{-5}$ m [45,75]), and we used the $k-\epsilon$ turbulence closure model [87]. The model setup was designed to approximately reproduce tidal fluctuations in velocity and SSC as
observed in the York River estuary [17]. A time step of 30 s and the numerical schemes listed in Table 3 were utilized.

<table>
<thead>
<tr>
<th>Process</th>
<th>River (East)</th>
<th>Ocean (West)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D Momentum</td>
<td>Clamped</td>
<td>Flather</td>
</tr>
<tr>
<td>3D Momentum</td>
<td>Gradient</td>
<td>Gradient</td>
</tr>
<tr>
<td>Salinity/Temp</td>
<td>Clamped</td>
<td>Radiation/Nudging</td>
</tr>
<tr>
<td>Sediment</td>
<td>Gradient</td>
<td>Gradient</td>
</tr>
<tr>
<td>Free Surface</td>
<td>Gradient</td>
<td>Chapman Implicit</td>
</tr>
</tbody>
</table>

Table 2. Open boundary conditions.

<table>
<thead>
<tr>
<th>Process</th>
<th>Numerical Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Advection of momentum (Vertical, 3D)</td>
<td>4th order, centered</td>
</tr>
<tr>
<td>Advection of momentum (Horizontal, 3D)</td>
<td>3rd order, upstream</td>
</tr>
<tr>
<td>Advection of tracers</td>
<td>HSIMT¹</td>
</tr>
<tr>
<td>Vertical Sediment Settling</td>
<td>PPM²</td>
</tr>
</tbody>
</table>

¹ Higher-order spatial interpolation at the middle temporal level [88].
² Piecewise parabolic method [89].

2.4 Model Experiments

All model simulations presented here used the following procedure. The model was initialized with vertically homogenous salinity contours ranging from 0–26 evenly spaced surrounding the area of interest in the model domain (−22 to 65 km) and the water column was at rest ($u = 0 \text{ m s}^{-1}$). The model was run for 90 days to allow the water column properties to adjust to the tidal conditions. The velocity and salinity fields output at the end of the 90-day run were used to initialize a 45-day run that included sediment transport and the routines for sediment-induced stratification, bed consolidation and swelling, and flocculation dynamics. In the 45-day run, the water column was initialized with no sediment in suspension, and the sediment bed was initialized with equal proportions by mass of all the floc size classes, with an initial critical shear stress of
erosion profile based on data from the York River estuary taken in April 2006 following [45]. The final sediment bed characteristics, suspended sediment concentrations, velocity, and salinity fields from this 45-day run were then used as the initial conditions for a set of 30-day long case runs. Sediment was eroded from the bed in the same size class it was deposited for all runs that included flocculation dynamics. Additionally, when the bed consolidation routine was used, the consolidation timescale was 1 day, the swelling timescale was 100 days, and the equilibrium critical shear stress profile was based on data from the York River estuary taken in September 2006, also following [45]. Cases that neglected the bed consolidation routine used the default (non-cohesive) erosion formulation that calculates an active layer thickness [73].

Table 4 lists the case runs, the cohesive processes incorporated into each, and is summarized here. The reference case run incorporated the three cohesive processes described above, i.e., flocculation, bed consolidation, and sediment–induced stratification. The along estuary velocity (u) and shear rates (G) were used to show changes in hydrodynamic conditions that would transport sediment or influence floc size. The SSC, the floc size distribution in suspension and the sediment bed, and weighted settling velocity by mass were used to evaluate sediment distributions and reasoning behind changes in sediment distributions. The weighted settling velocity by mass ($w_{s\text{, mass}}$) provided insight on how quickly sediment will settle based on the amount of each floc size that was in suspension. For the reference case, the median floc diameter ($D_{50}$) by mass was also compared to $D_{50}$ estimated by an equilibrium theory to examine the influence of SSC and shear rate on floc size.
The impact of individual cohesive processes on sediment distribution was then examined by completing additional case runs, each of which removed one of the processes from the implementation. The average depth-integrated suspended mass and average sediment size distribution from the case runs were used to assess changes in sediment distribution compared to the reference case. To evaluate the relative importance of flocculation and bed consolidation, the weighted settling velocity by mass and the average change in suspended masses for the case runs that neglected these processes were compared to estimates from the reference case. The gradient Richardson number was used to compare the suspended sediment impacts on density-induced stratification relative to salinity alone (Equations (3) and (4)).

<table>
<thead>
<tr>
<th>Case Name</th>
<th>Sed. Strat.</th>
<th>Consolidation</th>
<th>Flocculation</th>
<th>No. of Sed. Classes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>11</td>
</tr>
<tr>
<td>No Floc.</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>11</td>
</tr>
<tr>
<td>No Strat.</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>11</td>
</tr>
<tr>
<td>No Consol.</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>11</td>
</tr>
<tr>
<td>3 classes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>3</td>
</tr>
<tr>
<td>5 classes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>5</td>
</tr>
</tbody>
</table>

Sensitivity to the number of sediment size classes was also evaluated. The number of sediment classes was reduced to five and three sizes from the eleven size classes in the reference case. The classes chosen for the test cases were selected in an attempt to maintain the size range while using fewer size classes. The run time, the depth averaged suspended sediment mass, the average size distribution, median size and mode, as well as the average mass weighted settling velocity were compared to reference case.
\[ Ri_{grad} = \left( \frac{N}{\frac{du}{dz}} \right)^2 \]  

\[ N^2 = -g(s - 1) \frac{dC}{dz} - g \frac{\partial \rho_w}{\partial z} \]  

In the equations above, \( N \) is the buoyancy frequency, \( u \) is the along estuary velocity, \( z \) is the depth, \( g \) is the acceleration due to gravity, \( s \) is sediment density divided by the water density, \( C \) is SSC, and \( \rho_w \) is the water density. Two Richardson numbers \( (Ri_{grad}) \) were calculated: one included the contribution of suspended sediment in the buoyancy frequency \( (N) \), and the other did not. See Table A in the Appendix for a definition of symbols. For the version of the \( Ri_{grad} \) that neglected sediment–induced stratification, only the second term in Equation 4 was used in the calculation of \( N \).

3 Results and Discussion

3.1 Reference Case

The reference case model that incorporated cohesive sediment processes (flocculation, bed consolidation, and suspended sediment stratification) showed distinct patterns in the suspension and transport patterns linked to changes in hydrodynamics along the estuary. Compared to other locations along the estuary, the up-river boundary of salt intrusion had the strongest vertical salinity gradient, and the near-bed, tidally averaged along-estuary currents converged at this location, as expected for a partially mixed estuary. Also, this convergence trapped and accumulated sediment in the region and created an Estuary Turbidity Maximum (ETM; Figure 4a, 5a). Throughout the
estuary, the suspended sediment concentration peaked near the bed and decreased with height above the bed (Figure 4a, 5a). Several processes limited the diffusion of sediment into the upper water column, including reduced mixing across the halocline, and median floc sizes whose relatively fast settling velocities hindered their upward mixing. Shear rates were greatest near the bed and near the ETM region, especially during flood tide (Figure 4b, 5b). At a height of 0.19 mab, maximum tidal shear reached 10 s$^{-1}$, which is comparable to the shear rate of 12 s$^{-1}$ for maximum tidal flow produced in the laboratory for a previous zero-dimensional application of FLOCMOD [49].

Looking at the lower half of the water column where both concentrations and shear were relatively high, the larger sizes formed by aggregation were found near the bed where there was enough shear to keep them in suspension. This was evident from a larger $w_{s,\text{mass}}$ near the bed versus smaller settling velocities in the upper layers of the water column (Figure 4c, 5c).

The bathymetric change in the upper estuary added some complexity but also relevant realism for this application relative to the CSTMS/COAWST model domains used by [87] and [53]. Specifically, the bathymetric step helped constrain the along-channel location of the maximum in tidal velocity and vertical mixing, along with the resulting salinity front and ETM, to be in the general vicinity of the transition from the deeper estuary to the shallower river, as seen in partially mixed estuaries such as the York, James, and Rappahannock ([17,90]). Nonetheless, the resulting SSC in the reference simulation was on the same order of magnitude and the ETM was roughly the same distance from the estuary mouth as the model results from [87]. The ETM in [53]
typically occurred ~20 km from the mouth and SSC was up to 400 mg L$^{-1}$ higher than the concentrations shown here. These differences were not surprising, given that the present model used parameterizations chosen for the York River. Specifically, compared to [53], we used a larger fractal dimension, a smaller primary particle size, and lower floc particle densities. This study also used a different equilibrium critical shear stress for erosion, and longer consolidation and swelling timescales for the bed consolidation parameterization.

Figure 4. Suspended sediment concentrations (mg L$^{-1}$; a), the shear rate (s$^{-1}$; b) and the mass-weighted settling velocity (mm s$^{-1}$; c) along the idealized estuary near slack tidal flow. The arrows in (a) represent the direction and magnitude of the along estuary flow velocity and the solid red lines represent salinity contours (1, 5, 10, 20).
Figure 5. Suspended sediment concentrations (mg L\(^{-1}\); \(a\)). the shear rate (s\(^{-1}\); \(b\)) and the mass-weighted settling velocity (mm s\(^{-1}\); \(c\)) along the idealized estuary during flood tidal flow. The arrows in (\(a\)) represent the direction and magnitude of the along estuary flow velocity and the solid red lines represent salinity contours (1, 5, 10, 20).

The median floc sizes, \(D_{50}\), predicted from FLOCMOD within the ETM were interpreted in the context of an equilibrium floc size theory that postulates that a floc distribution at equilibrium will exhibit a linear relationship between \(D_{50}\) and the ratio of SSC by mass (\(C\)) to the square root of the shear rate (\(G\)) [46,53]. To explore this with our model results, the ETM \(D_{50}\) was calculated as the diameter at which 50% of the suspended flocs were smaller by mass and compared to \(C/G^{1/2}\) (Figure 6). Hourly data for the last ten days of the model run were analyzed to avoid effects of model spin-up. Throughout much of the water column in the ETM, model results for periods with relatively high shear rates (i.e., between 4–12 s\(^{-1}\)) did indeed display a linear relationship between \(D_{50}\) and \(C/G^{1/2}\) consistent with an equilibrium floc distribution.
(Figure 6). Data from 0.70 mab and higher in the water column, during times with shear rates between 4 s\(^{-1}\) and 12 s\(^{-1}\), and SSC exceeding 100 mg L\(^{-1}\) were used to fit an equilibrium line (inset in Figure 6). These conditions were assumed to be mostly likely at equilibrium.

At times when the model produced a \(D_{50}\) that fell well above or below the equilibrium line in Figure 6, the modeled floc size was interpreted as larger or smaller than the equilibrium, which indicated that another process was likely influencing the size of the flocs in suspension. The median floc size in most of the water column alternated between lying near the predicted equilibrium size to being finer-grained than the equilibrium. In contrast, the model output that most consistently fell above the equilibrium line was for the very near-bed grid cell at 0.036 mab (triangles in Figure 6). These deviations from equilibrium were caused by non-local process such as settling from the upper water column and sediment input via seabed resuspension or advection; or local processes that lead to relatively long time scales for aggregation and disaggregation.
Figure 6. The ratio of SSC (C) to the square root of the shear rate (VG) versus the $D_{50}$ by mass for the last 10 days of the reference case for the ETM. The colors correspond to depth in the water column (blue being near the bed; red being near the water surface). The blue triangles represent the first grid cell above the sediment-water interface (~0.036 mab). The red line represents the best fit during times with shear rates between 4–12 s$^{-1}$; the slope and intercept are provided in the top left corner. The inset in the top right shows the subset of data used for the equilibrium regression.

Next, we explored time-dependent variability within the ETM region for the reference case starting with the hydrodynamic and sediment conditions nearest the seafloor (0.036 mab). The tidal velocities reached around 40 cm s$^{-1}$ during peak flood, when the near-bed conditions for the shear rates were about 225 s$^{-1}$, and SSCs were ~800 mg L$^{-1}$ (Figure 7a–c). Both the peaks in the shear and SSC corresponded with the velocity maximum (Figure 7a–c) and the larger particles in suspension, with the very largest seen at peak flood (Figure 7d). An examination of floc size distributions (Figure 7d,g) revealed that during peak tidal flow, the median floc size, at ~190 μm, exceeded the equilibrium and there were larger floc sizes on the sediment bed surface as finer grains had been winnowed (Figure 7f). The flow velocity and shear was again elevated during ebb flow but remained less energetic than during flood. These currents were
strong enough to erode sediment from the bed, and produced an ETM floc size
distribution that included larger size classes as during flood flow, but were slightly
smaller (not shown). The larger particles in the near-bed suspension during peak flows
may be attributed in part to erosion of larger aggregates from the bed, as well as
enhanced mixing and elevated SSC that promoted floc growth (Figure 7). However,
during slack flow the near-bed $D_{50}$ equaled the equilibrium at ~70 μm (Figure 7g). As
velocity decreased the larger, faster-settling floc sizes settled, leaving smaller sizes in
suspension. Also, the sediment bed became enriched in the fractions of smaller floc
sizes, as bed stresses decreased and the medium fractions could settle to the bed
without being resuspended (Figure 7i). A two-dimensional idealized model utilizing the
Chesapeake Bay ETM as a prototype predicted comparable near-bed SSC in the ETM of
~200 mg L$^{-1}$ near slack and 400 mg L$^{-1}$ during flood flow, and the median floc size during
flood was ~150 μm, but the largest flocs were predicted during slack flow [91].

Higher in the water column (0.90 mab) at the ETM, the fluctuations in velocity were
larger, but the shear and SSCs were smaller compared to near the bed (Figure 7a–c). The
floc size distribution had a smaller concentration of the mid-sized sediment classes,
which produced a larger $D_{50}$ than near the bed. Unlike the near-bed, $D_{50}$ at 0.90 mab
equaled the predicted equilibrium $D_{50}$ of ~256 μm at peak flow (Figure 7e), and was
smaller at ~90 μm than equilibrium at slack water (Figure 7h). At slack flow, the $D_{50}$ at
0.90 mab was similar to the value in the near-bed grid cell, as larger floc sizes had
settled. The SSC at 0.90 mab was on average ~2 times smaller than at 0.036 mab (Figure
6c), whereas $G^{1/2}$ at 0.90 mab was ~7 times smaller than at 0.036 mab (Figure 7b). Thus,
differences in $C/G^{1/2}$ and the equilibrium $D_{50}$ very near the bed versus higher in the water column were driven more by differences in shear rate than by differences in SSC. Overall, the ETM concentrations and floc sizes simulated in this study were smaller than those predicted at 0.80 mab in the idealized ETM model for the Chesapeake Bay [91].

![Figure 7](image)

**Figure 7.** The hydrodynamic and sediment conditions for a tidal cycle in the ETM, including the (a) along estuary velocity (flood positive), (b) square root of the shear rate, and (c) the SSC near the bed (~0.036 mab; black lines) and 0.90 mab (red lines). The near-bed sediment size distribution at max flood (d) and slack after flood (g), and the distribution at 0.90 mab at max flood (e) and slack after flood (h). The mass fraction of the sediment classes in the bed at max flood (f) and slack after flood (i). In panels d, e, g, and h, the black dashed lines represent the $D_{50}$ by mass, and the dashed red line the estimated equilibrium $D_{50}$ by mass.

The conditions in the lower reaches of the estuary differed from the ETM in that the tidal velocities, the square root of the shear, and SSC respectively stayed below 40 cm s$^{-1}$, ranged between 2–10 s$^{-1/2}$ and ranged between 50–90 mg L$^{-1}$ in the bottom 1.75 m (Figure 8a–c). These SSC values were similar to concentrations predicted in the
downstream portion of an idealized estuary in [87]. The tidal fluctuation in velocity was
greater at 1.75 mab than directly above the bed, but the shear rate showed greater tidal
fluctuation and magnitude near the bed (Figure 8a,b). The SSC, the floc distribution, and
$D_{50}$ showed minimal tidal variation in the bottom 1.75 m (Figure 8c–e,g,h). Near the bed
(~0.078 mab), the floc size was equal or near the predicted equilibrium floc sizes both
near slack and peak flood flow. Higher in the water column (1.75 mab), the modeled
median diameters were smaller than the equilibrium floc sizes. The SSC to the square
root of shear rate ratio was larger higher in the water column, leading to a larger
predicted equilibrium floc size than was calculated by the time-dependent model. Case
studies from [92] also showed situations where the floc size was over predicted by the
[46] model. The floc size within the sediment bed downstream did not change over the
tidal cycle (Figure 8i).
Figure 8. The hydrodynamic and sediment conditions for a tidal cycle, including the (a) along estuary velocity (flood positive), (b) square root of the shear rate, and (c) SSC near the bed (~0.078 mab; black lines) and 1.75 mab (red lines) at the downstream location outside of the ETM. The near-bed sediment size distribution at max flood (d) and slack after flood (g) and the distribution at 1.75 mab at max flood (e) and slack after flood (h). The mass fraction of the sediment classes in the bed at max flood (f) and slack after flood (i). In panels d, e, g, and h, the black dashed lines represent the $D_{50}$ by mass and the red dashed lines represent the estimated equilibrium $D_{50}$ by mass.

The results from the reference case demonstrate the variability of floc size under simplified tidal conditions, specifically within the ETM region. The results highlight that the assumption of an equilibrium floc size may not be valid here, because suspended floc sizes within the ETM often deviated from the equilibrium values. As also shown, the floc size predicted by the flocculation routine for the water column outside the ETM was fairly constant though it did not equal the equilibrium floc size. Therefore in the lower reaches of the estuary, a simulation with an appropriately chosen constant floc size and
settling velocity could likely yield similar predictions of SSC as the present flocculation routine.

3.2 Sensitivity Tests

The impacts of flocculation, bed consolidation, and suspended sediment induced stratification to the distribution of sediment in the idealized estuary was further explored by comparing the results from the reference case to the test cases that neglected each of these processes (Table 4).

3.2.1 Impacts of Flocculation vs. No Flocculation

The role of flocculation was evaluated by comparing results from the reference case, which included flocculation to the “no floc” case (Table 4). Including flocculation dynamics shifted the size distribution of suspended matter to the larger size classes relative to the no flocculation case, as seen in the size distribution for the ETM (Figure 9a,b). The time-averaged $D_{50}$ by mass in the ETM size distribution increased to 123 μm with flocculation, compared to 55 μm in the no flocculation case. Overall, the effect of flocculation was most significant in the upstream portion of the estuary, where flocculation in the reference run decreased the depth-integrated suspended mass by ~2.5 times in the ETM, compared to the no flocculation run (Figure 10). The size of sediment in suspension increased even though flocculation reduced the SSC, producing a higher $w_{s, mass}$ in the ETM relative to the no flocculation run (Figure 11a,b). Flocculation increased particle size and as a result increased the settling velocities of the suspended
sediment in the ETM. This limited the transport of sediment out of the ETM, and increased deposition there.

Figure 9. The time-averaged near-bed (0.036 mab) floc size distribution in the ETM region for the (a) reference, (b) no flocculation, (c) no consolidation, and (d) no stratification cases. Grain size (in microns) shown for each floc size class. Dashed vertical lines represent the $D_{50}$ by mass for each case.

Figure 10. Time-averaged depth-integrated suspended sediment mass in the idealized estuary for the reference (black line; incorporates all cohesive processes), and cases that neglected flocculation (red line), sediment-induced stratification (blue line), or bed consolidation (green line). The reference case (black line) and no sediment-induced stratification (blue line) nearly overlay one another.
Figure 11. The average mass weighted settling velocity ($w_{s,\text{mass}}$) along the estuary for the (a) reference simulation, (b) no flocculation run, and (c) no bed consolidation cases.

For individual size classes, the difference in suspended mass between the reference and no flocculation cases showed that in the ETM (found at ~45–55 km), flocculation moved mass from the smaller size classes ≤64 μm into larger classes ≥256 μm (Figure 12). In the lower estuary (≤ ~30 km), including flocculation generally removed mass from the smallest size classes of 1–16 μm in diameter (blue in Figure 12a,b); but increased suspended mass in the median sizes (red in Figure 12c,d). These larger particles with higher settling velocities concentrated closer to the bed, so that flocculation reduced SSC in the surface waters of the lower estuary (Figure 12).
Figure 12. The time-averaged difference (the reference case minus the no flocculation case) in the suspended sediment mass for sediment size classes. Panel (a) shows the sum of size classes with diameters 1–8 μm because the pattern was similar; panels (b-h) show a single size class with the diameters indicated in the bottom right corner. Red indicates that including flocculation increased the concentration; blue indicates that flocculation decreased the concentration.

3.2.2 Impacts of Bed Consolidation vs. No Consolidation

The time-averaged size distribution from the ETM when bed consolidation was included showed the $D_{50}$ by mass was reduced to 123 μm, compared to 170 μm when bed consolidation was neglected (Figure 9c). The depth-integrated suspended mass was reduced throughout most of the estuary; ETM concentrations were ~1.5 times smaller in the reference case than those calculated in the no consolidation case (Figure 10). The settling velocities ($w_{s,mass}$) were lower when bed consolidation was included compared to the case that neglected bed consolidation (Figure 11a,c). The reference run with consolidation showed that relative to no consolidation, suspended mass was removed
from the larger size classes (128–1024 μm), and suspended mass was added to the smaller sizes in most of the estuary (Figure 13). Throughout the area of interest, bed consolidation reduced bed erosion, lowering the SSC and the probability of flocculation to occur, which shifted the size distribution to smaller sizes compared to the no consolidation case (Figure 13).

**Figure 13.** The time-averaged difference (the reference case minus the no consolidation case) in the suspended sediment mass for sediment size classes. Panel (a) shows the sum of size classes with diameters 1–8 μm because the pattern was similar; panels (b-h) show a single size class with the diameters indicated in the bottom right corner. Red indicates that including consolidation increased the concentration; blue indicates that it decreased the concentration.

### 3.2.3 Impacts of Sediment-Induced Stratification

Density-induced stratification due to gradients in SSC did not significantly impact sediment patterns; the size distribution of suspended sediment was similar to the distribution calculated when sediment-induced stratification was removed, the time
averaged $D_{50}$ was 123 μm for the reference case compared to 116 μm for the case that neglected sediment-induced stratification (Figures 9d). The depth-integrated suspended sediment mass throughout the estuary for the reference case was nearly identical to the no stratification case (Figure 10). These results indicate that the SSC gradients estimated in this set of model runs were not sufficient to induce significant stratification. The gradient Richardson number ($R_{i,grad}$; Equations (3) and (4); [93]) was calculated for 0.5 and 1.0 mab throughout the area of interest. Suspended sediment on average contributed minimally to the $R_{i,grad}$. When the $R_{i,grad}$ exceeded the critical value of 0.25, SSC contributed 2.5% to the $R_{i,grad}$ at 0.5 mab, and 1.8% at 1 mab. Please note that the density of the flocs decreased with size, as was observed in the York River estuary (Table 1; [38]). Suspended sediment-induced stratification could be more important in situations where the density of large flocs did not decrease, where higher stresses or higher erodibility led to higher SSC near the bed, or where stronger temperature/salinity stratification more significantly enhanced sediment-induced stratification.

To summarize Sections 3.2.1–3.2.3, flocculation dynamics were especially important in the ETM, while bed consolidation impacted suspended sediment throughout the estuary. Based on these results, future modeling studies in cohesive environments should consider using flocculation if variability in SSC and shear rate is comparable or stronger than the ETM modeled here. However, changes in erodibility due to consolidation is important for most studies in regions with muddy or mixed-sediment beds. For this implementation, density-induced stratification due to SSC gradients was less important for suspended sediment dynamics. The SSCs in this study were < 1000 mg
L$^{-1}$ and floc densities were $\leq 2000$ kg m$^{-3}$; thus sediment-induced stratification could be neglected in studies with similar sediment dynamics. However, if a user is unsure, it is best to incorporate density-induced stratification from sediment, as this routine has a low computational cost in COAWST and may impact sediment distributions and mixing.

3.2.4  Sensitivity to the Floc Size Distribution

The final set of cases evaluated the sensitivity of model estimates to the number of size classes used to represent the floc population. Results showed that the calculations of SSC were sensitive to the number of size classes used. Reducing the number of sediment sizes from eleven classes in the reference case to five or three increased the amount of suspended sediment throughout most of the estuary (Figure 14). The case using only three size classes produced depth-integrated suspended sediment that exceeded those from the case that neglected flocculation; the peak concentration in the three size class case was approximately 30% higher than the no flocculation case (Figure 14).
Figure 14. Time-averaged depth-integrated suspended sediment mass along the idealized estuary for the reference case (black line), which used 11 sediment size classes, and model runs using 5 (red) or 3 (blue) sediment size classes.

The modal and $D_{50}$ floc size in suspension by mass were sensitive to the resolution of the floc size distribution. When five size classes were used, suspended mass near the bed in the ETM had a modal size of 64 μm, whereas the reference run had a modal size diameter of 128 μm (Figure 15a,b). The $D_{50}$ by mass of the five-size class run was 74 μm compared to the reference case $D_{50}$ of 123 μm. For the three-size class run, the floc $D_{50}$ near the bed in the ETM was similar to the 5-size class run at 72 μm. However, the modal size was similar to the reference case at 128 μm, but there was much more suspended mass for the three-class case compared to the reference case (Figure 15). The changes to suspended size distribution likewise reduced the weighted setting velocities calculated for the three and five class cases, compared to the reference case (Figure 16). The case with only three size classes had the smallest $w_{s, mass}$ of the cases considered (Figure 16c).

Figure 15. The time-averaged floc size distribution near the bed in the ETM region for the reference run with 11 sediment classes (a), 5 sediment size classes (b) and 3 sediment size classes (c). The dashed line represents the $D_{50}$ by mass for each case.
Figure 16. The average mass weighted settling velocity ($v_{s,\text{mass}}$) along the estuary for cases with varying number of sediment classes; results for (a) 11 (reference), (b) 5, and (c) 3 sediment classes.

The computational expense of the flocculation module was related to the number of size classes used. The maximum number of size classes used in this study was eleven because the computational expense to use more was prohibitive. Including flocculation dynamics in the reference model that had eleven sediment classes increased the computational time by a factor of ~130 (run time of ~128 h with flocculation and ~1 h without). Using five or three size classes increased the cost by factors of ~31, and ~13.4, respectively, compared to not using flocculation dynamics. Finding the optimal set of floc sizes may take several test runs to determine the best configuration as shown in previous studies [49]. Size distributions from our test cases indicated that representing the particles that are abundantly found in suspension (i.e., sizes 16–512 μm in our idealized estuary) is more important than maintaining the complete possible size range. This set of sensitivity shows that to apply the flocculation model in other environments,
using a one- or two-dimensional domain would be useful for designing an appropriate floc distribution and optimal number of sediment classes to represent. Additionally, the availability of observation-based detailed information on the floc size distribution is important for designing the size distributions for FLOCMOD. The flocculation routine was found to be sensitive to the characteristics assigned to size classes, therefore care should be taken in assigning floc properties. For these reasons, it remains challenging to select an optimal size distribution and associated sediment characteristics of sediment size classes that optimize the results while limiting computational costs.

4 Key Implications and Future Directions

The case presented in this study showed that sediment size distributions vary along a representative muddy, partially mixed estuary. Our results showed that the processes of bed consolidation and flocculation modified the sediment erodibility and settling velocity within the idealized estuary over tidal timescales. However, many sediment transport models hold these sediment characteristics constant when modeling an entire estuarine system, which can lead to under- or overestimates of SSC. The cohesive process sensitivity tests indicated that it was important to include bed consolidation in estimating the SSC along the estuary. Flocculation was important in areas of the estuary with tidal variability, that has a range similar to or greater than 300 mg L\(^{-1}\) and 8 s\(^{-1}\) in SSC and shear rate, respectively, as was the case for 0.90 mab in the ETM of this idealized estuary. However, due to the sensitivity of the flocculation routine to the size class distribution and other sediment characteristics, observational data are still needed to appropriately constrain the resulting SSC. Additional modeling studies are warranted
to help determine the optimal sediment parameters for FLOCMOD. Since the flocculation routine is computationally expensive, a set of one-dimensional runs that more systematically vary the sediment size classes and properties may be useful for parameterizing FLOCMOD for natural estuaries.

There are motivations for using FLOCMOD in regional scale domains despite the computational expense. Employing FLOCMOD in regional studies is now relatively straightforward, because the module has been coupled with the CSTMS [53]. The population balance equations fit well within the CSTMS piecewise parabolic settling scheme [73], chosen to reduce limitations by the CFL (Courant Friedrichs Lewy) stability criteria. Coupling less computationally expensive flocculation routines, such as those that track changes in effective floc settling velocity [46,94], would require structural change to the vertical advection scheme used within the CSTMS, which assumes that the settling velocity of each particle class remains constant throughout the water column.

One approach to assessing the impact of flocculation for a location while maintaining a modest computational expense is to apply FLOCMOD within a small one-dimensional vertical domain, with realistic physics and bed dynamics. This could be a reasonable method for evaluating flocculation dynamics for an area of interest such as the York River estuary ETM. In the York River estuary, flocculation dynamics seem more important within regions with elevated SSC, compared to the rest of the estuary. Further work on reducing the computational cost of the flocculation routine by reducing the number of vertical water column layers, or modifying the FLOCMOD convergence
criteria, could make a three-dimension model more cost effective and provide added insight on the distribution of flocs under more realistic and complex bathymetric conditions.

The flocculation formulation may also be useful for examining the formation, dispersal, and fate of oil-mineral aggregates. Parameterization of FLOCMOD could be modified to represent the properties of oil-mineral aggregates using data from laboratory experiments. For example, the growth and breakup parameters in Equations (7)–(12) from [49] may be modified to account for hydrocarbon content. This would allow the sediment transport routines within the CSTMS to be used to examine the dispersal of oil from a spill. However, this does not account for the impact of the bacterial communities that are attracted to oil–mineral aggregates and breakdown the oil, and excrete exopolymeric substances (EPS; [95]), which potentially changes the characteristics of the settling aggregates. Linking FLOCMOD to the HydroBioSed CSTMS module that has been used to account for biogeochemistry [96] may provide an avenue for incorporating microbial degradation with the flocculation process. This would be useful for tracking the formation, transformation, and transport of oil–mineral aggregates.

5 Conclusions

The idealized model developed in this study reproduced the key physical features of an estuary such as estuarine circulation and the formation of an ETM through flow convergence and sediment trapping. The flocculation model adequately represented the dynamics throughout the entire estuary, and the results demonstrated that sediment
conditions in the ETM were more variable over the tidal cycle with SSC ~3–10 times
greater and median diameters ~2–8.5 times larger than downstream. In the ETM, the
distribution of floc sizes fluctuated with the shear rate and SSC; the largest flocs in
suspension were seen during flood tide, and these tended to deposit to the bed during
slack flow. An equilibrium floc theory was applied to the modeled conditions that were
assumed to be near-equilibrium (ETM, above the bed, and peak flow conditions) to
derive a relationship between equilibrium floc diameter, SSC, and the shear rate. The
analysis indicated much of the estuary was not at equilibrium but that other processes
were impacting the floc size over much of the tidal cycle throughout the estuary.
Additional analysis is needed to determine which other processes are influencing floc
size and at which stage of the tidal cycle and where in the estuary are these other
processes more dominate.

The impact of individual processes and user-defined floc size characteristics were
evaluated through a series of case studies that individually excluded bed consolidation,
flocculation, or sediment-induced stratification, and varied the number of floc sizes
used. Flocculation dynamics had the largest impact on SSC within the ETM region where
both suspended sediment and turbulence varied in time and space. Flocculation
reduced the average depth-integrated suspended mass by ~50% within the ETM.
Outside of the ETM, bed consolidation had the largest impact and similarly decreased
the average depth-integrated suspended mass by ~50%. Sediment-induced density
stratification had a much smaller impact on the distribution of sediment than either
flocculation or bed consolidation. The vertical gradients in the suspended
concentrations within the idealized estuary did not inhibit mixing based on the SSC contributions to the gradient Richardson number. The use of fewer size classes, to reduce computational expense, resulted in estimates of sediment concentration that increased by as much as ~3.5 times, and an estimated median floc size that decreased by as much as ~1.7 times relative to the reference case. The flocculation routine was sensitive to the number of floc size classes used and is also expected to be sensitive to the characteristics (i.e. settling velocity, critical shear stress) assumed for the floc classes.

The reference run in this study, though it represented an idealized estuarine configuration, was parameterized using observational data from the York River estuary. Other applications of the cohesive sediment model for a different location would require some insight into how to effectively parameterize these routines. The use of both observed SSCs and floc sizes helped us to constrain model parameters because multiple possible model configurations can yield similar SSC. Measurements of the suspended sediment size distribution based on in situ camera systems, laser instruments, and/or laboratory experiments can be especially useful for constraining fractal dimension and primary particle size and density [25,38,40,97–99]. Erodibility estimates obtained under variable environmental conditions, either through erosion experiments or calibrated estimates from a high sample frequency acoustic instrument [60,100] can provide constraints for the bed consolidation parameters.

Our study showed that sediment transport calculations in partially mixed, muddy estuaries may be equally sensitive to incorporating flocculation and bed consolidation.
However, the inclusion of flocculation using a population-based floc model added significantly to the computational cost of our coupled sediment transport–hydrodynamic model. This may prove challenging for applying the population-based flocculation model to a regional-scale model domain, but the aggregation and disaggregation processes significantly impacted suspended sediment concentrations, and suspended grain size distribution.

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Author Contributions: The lead author, Danielle Tarpley, developed the model setup, implemented the cohesive sediment routines in the model, designed the model experiments and led the analysis of the results as part of her Doctoral Dissertation. The second and third authors, Drs. Courtney Harris and Carl Friedrichs, served as Ms. Tarpley’s major advisors during this work, and supervised the effort. Dr. Christopher Sherwood contributed to the development of the model, particularly the flocculation routine and provided guidance on the application of the flocculation routine.

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Conflicts of Interest: The authors declare no conflict of interest.
**Appendix A**

**Table A.** List and description of the variables and units used in equations.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$</td>
<td>Total suspended sediment concentration (kg m$^{-3}$)</td>
</tr>
<tr>
<td>$C_i$</td>
<td>Suspended sediment concentration for sediment class $i$ (kg m$^{-3}$)</td>
</tr>
<tr>
<td>$D_{50}$</td>
<td>Median floc size (microns) by mass</td>
</tr>
<tr>
<td>$D_{f,i}$</td>
<td>Diameter of the floc particle (m) for size class $i$</td>
</tr>
<tr>
<td>$D_p$</td>
<td>Diameter of the primary particle (m)</td>
</tr>
<tr>
<td>$\rho_{f,i}$</td>
<td>Density of the floc (kg m$^{-3}$) for size class $i$</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>Density of primary particle (kg m$^{-3}$)</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>Density of the water (kg m$^{-3}$)</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>Density of quartz sediment (kg m$^{-3}$)</td>
</tr>
<tr>
<td>$G$</td>
<td>Shear rate (s$^{-1}$)</td>
</tr>
<tr>
<td>$n_f$</td>
<td>Fractal dimension (non-dimensional)</td>
</tr>
<tr>
<td>$N$</td>
<td>Buoyancy frequency (s$^{-1}$)</td>
</tr>
<tr>
<td>$n$</td>
<td>Grid layer number or cell number in $x$-direction</td>
</tr>
<tr>
<td>$s$</td>
<td>Sediment density divided by the water density</td>
</tr>
<tr>
<td>$t$</td>
<td>Time (s)</td>
</tr>
<tr>
<td>$u$</td>
<td>Flow velocity in $x$-direction (m s$^{-1}$)</td>
</tr>
<tr>
<td>$v$</td>
<td>Kinematic viscosity (m$^2$ s$^{-1}$)</td>
</tr>
<tr>
<td>$w_{s,i}$</td>
<td>Settling velocity for sediment size class $i$ (m s$^{-1}$)</td>
</tr>
<tr>
<td>$w_{s,\text{mass}}$</td>
<td>Mass settling velocity (m s$^{-1}$)</td>
</tr>
<tr>
<td>$x$</td>
<td>Distance in the along estuary direction (m)</td>
</tr>
<tr>
<td>$z$</td>
<td>Distance in the vertical direction (m)</td>
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References


Processes Impacting Floc Size Over a Tidal Cycle in a Partially Mixed, Idealized Estuary: A Numerical Study
Abstract
Coastal environments, such as estuaries, are complex systems that exchange sediment and other constituents between the land and the open ocean. Estuaries, in particular, are especially complex because their local hydrodynamics are affected by tides, waves, freshwater discharge, and density gradients. Additionally, the less energetic estuaries tend to have predominantly muddy sediment that has a cohesive behavior. The processes impacting the transport of cohesive sediment include resuspension, flocculation, disaggregation, settling, advection, and diffusion; and these processes operate over temporal scales ranging from seconds (turbulent motions), to hours (tides), to days (spring-neap cycles), to seasons (sediment supply), and beyond. A range of methods is available for modeling the transport of muddy sediment through these environments. Steady-state or equilibrium models for flocculated sediment diameter have been developed that are computationally efficient, but whether an equilibrium model is appropriate will depend on the timescale for floc dynamics in comparison to other transport processes. Population balance flocculation models, such as FLOCMOD, are able to simulate dynamic variability in sediment size distributions, but these types of flocculation models are computationally expensive. An idealized two-dimensional (along-estuary and vertical) model was used to represent a longitudinal section of an estuary over a tidal cycle to evaluate the conditions under which equilibrium floc size is reached, and the timescales associated with floc dynamics. Built within the Regional Ocean Modeling System (ROMS), this idealized 2D model accounts for freshwater flow,
tides, estuarine circulation, sediment deposition and resuspension, and floc dynamics using FLOCMOD. Local changes in mass concentration for individual size classes due to flocculation were compared to the effects of transport and erosion. Flocculation and vertical diffusion were the dominant processes contributing to changes in sediment mass concentrations throughout the water column, except near the sediment-water interface, where erosion was also a major contributor. The median floc diameter predicted by FLOCMOD was compared to an equilibrium diameter calculated as a simple function of sediment concentration and shear rate. In the estuarine turbidity maximum (ETM), the floc size reached equilibrium very near the bed during slack flow, but not during peak flow when erosion increased the supply of large flocs. In the overlying water of the ETM, equilibrium was reached during peak flow. Downstream, away from the ETM, the floc size did not reach equilibrium in the lower half of the water column as shear rates were low at this location. In the model, the near-bed velocity was more useful than the depth-averaged velocity for understanding the SSC and floc dynamics.

1 Motivation and Background

Coastal environments are heavily impacted by human activities and at the same time coastal economies often depend on healthy coastal habitats to sustain commercial and recreational activities. One aspect governing the health of habitats such as oyster reefs or sea grass beds is the amount of sediment suspended in the water column that can, for example, block light to the sea grass beds or settle and bury the sea grasses and oyster reefs. Most of the sediment suspended in coastal environments is made up of fine-grained particles or muds that are composed of silts and clays. These muddy
materials have a cohesive nature that affects their dynamics, especially in brackish and saline environments.

1.1 Flocculation of Cohesive Sediment

The cohesive nature of mud causes sediment particles to flocculate, or stick together, and produce aggregates called “flocs” in the water column. Flocculation is influenced by physical drivers such as salinity, suspended sediment concentration (SSC), and turbulence; and by biological factors such as secretions from phytoplankton (Droppo 2001). Flocculation does occur in fresh water when biological components cause the particles to be “sticky” (Dyer 1989; Droppo and Ongley 1992; Droppo et al. 1997). However, aggregation more readily occurs at salinities greater than 1-2 g kg\(^{-1}\) as the salt ions interact with the electrostatic charges associated with clay-sized particles to facilitate the formation of flocs (Krone 1978). The likelihood of particles colliding and adhering to one another increases with the number of particles in suspension, or the SSC (Dyer 1989; Mehta 1989; van Leussen 1994). Turbulence in the water column also brings sediment particles together and increases the probability that flocculation will occur. However, at elevated levels of turbulence, the bonds holding flocs together can be broken leading to the disaggregation of the flocs (Winterwerp 1998; Fugate and Friedrichs 2003). The amount of turbulence needed to disaggregate flocs depends on the strength of the flocs, which varies due to their mineralogy and biological components (Burd and Jackson 2009; Cross et al. 2013; Fettweis et al. 2014). The factors influencing the growth and breakup of flocs vary seasonally and spatially, as well as
tidally, in estuarine and coastal environments (van Leussen 2011; Manning and Schoellhamer 2013; Fettweis and Baeye 2015).

The flocculation process not only changes the size, shape, and density of the particles in suspension, but also the rate at which sediment settles through the water column. The settling velocity of aggregated flocs increases with floc size, and variability in local conditions can lead to the continuous cycling of larger and smaller flocs being suspended (Dyer and Manning 1999). The settling velocity directly impacts the amount of sediment that is transported vertically and horizontally. Less sediment transport occurs when flocs have higher settling velocities, which causes them to settle out of the water column faster and be transported closer to the seabed where current velocities are usually lower (Dyer 1989; Mcanally and Mehta 2002). For example, the ability of an estuarine turbidity maximum (ETM) to retain and trap sediment is reduced when flocs have excessively slow settling velocities (Sanford et al. 2001). Therefore, the fate of sediment in muddy environments is linked to the settling velocity.

Aggregation and disaggregation occurs throughout muddy estuarine environments and leads to particulate matter that have wide ranges in size and settling velocity (Dyer 1989; Mehta 1989). Transport processes for suspended sediment include advection, diffusion, settling, and erosion; and flocculation processes influence the settling and transport of sediment. However, the temporal and spatial importance of flocculation dynamics on the settling and transport of sediment in estuaries, in comparison to other transport mechanisms, has rarely been systematically studied.
1.2  Modeling flocculation

Quantifying the transport of cohesive sediment in estuaries with numerical models requires the determination of sediment characteristics and the variability of these characteristics through time and space. Observations have shown that populations of flocs have a range of sizes, densities, and settling velocities (Dyer and Manning 1999; Fugate and Friedrichs 2003; Smith and Friedrichs 2011; Chapalain et al. 2018). Estimating sediment fluxes and transport is often simplified by using a single sediment class, however, using a constant settling velocity for a floc population to represent an average, best fit, or bulk value (Cancino and Neves 1999; Lin and Kuo 2003; Huijts et al. 2006; Sanford 2008; Talke et al. 2009) can over- or under-estimate the settling flux by more than 50% or as little as 5% depending on the value used (Manning and Dyer 2007; Lee et al. 2011; Lee et al. 2012). The use of two or more sediment classes with different, but constant settling velocities can represent a bimodal population and provide insight on large-scale depositional patterns and storm impacts (Lee et al. 2011; Ralston et al. 2013; Moriarty et al. 2014; Palinkas et al. 2014; McSweeney et al. 2017). However, this approach may not represent small-scale local interactions well, and local SSC estimates can be inaccurate (Fall et al., 2014; Manning and Dyer, 2007).

Allowing the diameter and settling velocity to vary with local dynamics may better represent a floc population. Winterwerp (1998) developed a dynamic single-class floc model that varied the floc diameter and settling velocity assuming the floc size was governed by shear rate and SSC. In this model, the time required to equilibrate to the median floc size was linearly proportional to the SSC divided by the square root of the
shear rate \( (G) \). The model introduced additional parameters that represented the rates of aggregation \( (k_A) \) and disaggregation \( (k_D) \) that could be used to estimate the timescale for flocculation (Winterwerp 1998; Winterwerp 2002). Several studies have indicated, however, that the maximum floc size was limited by the Kolmogorov microscale, which is proportional to the smallest turbulent eddies (Fugate and Friedrichs 2003; Bowers et al. 2007; Braithwaite et al. 2012). The Winterwerp (1998) single size-class model does not limit floc size based on the Kolmogorov microscale, and it is not known whether including this effect to the model dynamics would represent the sediment flux in an estuary as well as a multi-class flocculation model.

Dynamic floc models with multiple size classes, which allow the amount of mass in a floc size to vary with turbulence and SSC, provide the ability to represent a distribution of floc sizes, but also increases the number of model coefficients and computational costs (Verney et al. 2011; Tarpley et al. 2019). Several dynamic floc models have been based on a set of population balance equations (PBE) in which sediment is exchanged between floc sizes in concert with changes in local hydrodynamics and SSC (Maggi et al. 2007; Lee et al. 2011; Verney et al. 2011; Shen and Maa 2015). These PBE models define a set number of floc sizes and exchange particles between the sizes based on the turbulence, SSC, and aggregation and disaggregation efficiencies. The assumptions of these models often included a constant fractal dimension (this describes the ratio of the void space to particulate matter based on the size of the flocs), specified aggregation and disaggregation efficiencies, and constant settling velocities for each floc size (Lee et al. 2011; Verney et al. 2011). Comparisons of PBE results to settling column and
laboratory experiments have shown that a minimum of two floc classes is required to represent a bimodal population (Lee et al. 2011), and to represent the full floc distribution requires 7 to 14 floc sizes (Verney et al. 2011). The PBE model known as FLOCMOD (Maerz et al. 2011; Verney et al. 2011) is distributed with the Coupled Ocean-Atmosphere-Wave-Sediment Transport (COAWST) modeling system, making this flocculation model available for various applications (Sherwood et al. 2018).

The published applications of FLOCMOD, to date, have been limited to small model grid domains. For example, FLOCMOD was implemented in a “zero-dimensional” simulation for comparison to laboratory data, and the sensitivity of the model was examined (Verney et al. 2011; Maerz et al. 2011). Additionally, Sherwood et al. (2018) used a zero-dimensional model to compare FLOCMOD results to laboratory data, and a one-dimensional (vertical) model with FLOCMOD for a series of exploratory test cases. Progress toward the implementation of FLOCMOD at regional spatial scales, such as to represent a full estuarine environment, is underway but has not been published partially due to the computational demands of FLOCMOD.

Implementing FLOCMOD within an idealized 2D model of an estuary can yield insight into how flocculation impacts sediment transport along an estuarine transect while maintaining a reasonable computational cost. Toward this, the sensitivity of the distribution of cohesive sediment to flocculation in an idealized estuary was examined using FLOCMOD in Chapter 2 (i.e. Tarpley et al. 2019). Results from this study showed that the SSC and shear rate were higher in the ETM compared to the lower reaches of the estuary. Within the ETM, the small and medium floc sizes aggregated to form large
flocs during peak flow when the SSC and shear rate were highest. Downstream from the ETM, in the lower reaches of the estuary, the reduced shear rate and SSC produced smaller flocs. Also, the downstream region showed minimal variability in the floc size and SSC throughout the tidal cycle, but higher tidal variability in the shear rate. Thus, the SSC was the limiting factor controlling the floc size in the lower region of the estuary (Tarpley et al. 2019). Additionally, the SSC was reduced in the middle to surface waters of the estuary through the addition of flocculation to the model (Tarpley et al. 2019).

This study used a similar model implementation as Chapter 2 (i.e. Tarpley et al. 2019), but extended the analysis to specifically examine the spatial difference in the equilibrium floc size compared to the modeled median diameter; consider the factors that prevent the median diameter from reaching equilibrium; and quantify the impact of flocculation relative to transport processes such as advection, diffusion, erosion, and settling. This paper further extended the earlier analysis by identifying locations within the estuary for which flocculation has a large impact relative to other processes, and evaluating when it is advantageous to use a dynamic floc model in a cohesive estuary. This study examined spatial differences along the estuary, and considered temporal variability over the flood-ebb tidal cycle.

1.3 Objective and outline

The objective of this study was to understand the importance of floc dynamics, relative to other processes, in controlling the distribution and transport of SSC in estuaries. The flocculation model, FLOCMOD, was used in an idealized estuary model to compare the influence of flocculation on suspended sediment relative to transport
processes (advection, diffusion, settling, and resuspension), and to evaluate the degree to which an equilibrium floc size model represents sediment distribution. To that end, this study addressed the following questions:

a) How does the amount of mass transferred between floc sizes due to aggregation or disaggregation compare to the local change in the sediment mass within size classes due to advection, vertical diffusion, settling, and erosion from the sediment bed?

b) How does mass transfer between floc size classes and resulting suspended floc size distributions vary at different locations in an idealized estuary?

c) Under what conditions, and to what degree, does a population balance model produce a different estimate for the median floc diameter compared to a simple relationship for equilibrium floc size?

The idealized domain used in this study retained the key features of an estuary, such as density driven circulation and the formation of an ETM; but at a lower computational cost than would be needed to simulate dynamics in a more realistic representation that resolved spatial complexity for a specific field site in a three-dimensional model (Tarpley et al. 2019). The population balance flocculation model used in this study was computationally expensive; but the idealized model approach allowed us to examine the first-order impacts and flocculation dynamics in an estuary with a manageable computational cost. The model description and data analysis applied are outlined in
Section 2. The results from the idealized estuary analysis are provided in Section 3, and then discussed in Section 4. A summary and the conclusions are presented in Section 5.

2 Methods

2.1 Model Framework

The model was developed using the Coupled Ocean-Atmospheric-Wave-Sediment transport modeling system (COAWST version 3.5) and was designed to mimic key features and dynamics of the York River estuary, VA, USA. A detailed description of the model setup was provided in Chapter 2 (i.e. Tarpley et al. 2019), and is briefly summarized here. The model domain was 180 km in length, with an area of focused interest in the middle of the domain that is about the length of the York (60 km in length), and includes the ETM (Figure 3.1) and head of salt (1 g kg\(^{-1}\) salinity contour). The bathymetry of the main channel of the York River estuary was simplified for the model grid, with a smooth sloping bottom between the minimum depth at the head of the estuary (6 m) and the maximum depth at the mouth of the estuary (20 m). The salinity range represented in the model was the same as that commonly seen in the York River estuary (1-26 g kg\(^{-1}\)), and the tidal height (0.5-0.8 m) and tidal current magnitudes (<1 m s\(^{-1}\)) were likewise similar to those observed in the York. The SSC magnitude at 1 mab in the modeled ETM was also comparable to that measured in the York River estuary ETM (400 mg L\(^{-1}\); Friedrichs, 2009; Lin and Kuo, 2001).

Observations from surface waters of the York from Fall (2020) were used to constrain the model settings for fractal dimension, and primary particle size and density. We defined 11 floc sizes with diameters ranging between 1-1024 μm, with a fractal
dimension of 2.4. The primary particle diameter was 1 μm and density was 2000 kg m$^{-3}$.

Similar to observations from the York River estuary, the floc settling velocities increased while densities decreased with increasing size (Fall 2020). As expected by FLOCMOD, the floc densities ($\rho_{f,i}$; Equation 3.1) and settling velocities ($w_{s,i}$) used as input were chosen to be consistent with the modified Stoke’s Equation 3.2 (Winterwerp 1998):

**Equation 3.1:**  
$$\rho_{f,i} = \rho_w + (\rho_p - \rho_w) \left( \frac{D_p}{D_{f,i}} \right)^{3-n_f}$$

**Equation 3.2:**  
$$w_{s,i} = \frac{g(\rho_{f,i} - \rho_w)D_{f,i}^2}{\rho_w \cdot \nu}$$

where, $\rho_w$ is water density, $\rho_p$ is primary particle density, $D_p$ is primary particle diameter, $D_{f,i}$ is diameter of the floc in size class $i$, $n_f$ is fractal dimension, $g$ is acceleration due to gravity, and $\nu$ is kinematic viscosity. These equations assume flocs follow a fractal fit; and the fractal dimension, and the primary particle size and density are constant.

Within the framework of COAWST, the Regional Ocean Modeling System (ROMS) and the Community Sediment Transport Modeling System (CSTMS) were used to represent hydrodynamics and sediment transport, respectively. This study expanded on the reference case developed in Chapter 2 (i.e. Tarpley et al. 2019) where the characteristics of cohesive sediment in the previous and current study were accounted for by using modules for flocculation dynamics (FLOCMOD), bed consolidation, and sediment-induced stratification. The results from a 30-day reference run from Chapter 2 (i.e. Tarpley et al. 2019) were used to initialize a 3-day simulation in which results were recorded every 5 minutes for this study.
The evaluation of the role of flocculation was accomplished by analyzing the terms of the transport equation (Equation 3.3).

**Equation 3.3:**

\[
\frac{\partial C_i}{\partial t} = -\nabla_H UC_i + \frac{\partial K}{\partial z} \frac{\partial^2 C_i}{\partial z^2} - \frac{\partial(w - w_{s,i})C_i}{\partial z} + f\left(C_i, C_j, G, \ldots\right) + S_i
\]

<table>
<thead>
<tr>
<th>Horizontal Advection</th>
<th>Vertical Diffusion</th>
<th>Vertical Adv. &amp; Settling</th>
<th>Flocculation</th>
<th>Erosion / Deposition</th>
</tr>
</thead>
</table>

In Equation 3.3, \(C_i\) is SSC for floc size class \(i\), \(t\) is time, \(U\) is along estuary flow velocity, \(z\) is depth, \(K\) is vertical diffusion coefficient, \(w\) is vertical flow velocity, \(w_{s,i}\) is settling velocity for floc size class \(i\), \(f\) is the flocculation function, \(G\) is shear rate, and \(S_i\) is a source or sink of sediment from the bed due to erosion or deposition. To analyze the relative importance of each term in Equation 3.3, ROMS was modified to output their values. This allowed us to quantify mass exchanges among size classes for each of the processes. Specifically, the CSTMS solves Equation 3.3 by updating the SSC field after calculations that account for each of these terms in the following order. First, flocculation exchanges sediment mass between floc size classes. Next, transport for each size class is calculated for settling, then erosion or deposition, and lastly advection and diffusion. Our model output included the sediment mass transfer for each of these terms, calculated as the amount of mass in the suspended sediment field after the update minus the amount of suspended sediment field before the update (effectively a \(\Delta C_i\)). Therefore, a positive value in the \(\Delta C_i\) indicated that the concentration of floc class \(i\) increased during a time step. (See Appendix B for additional details and the
modifications made to COAWST to incorporate these variables). Erosion or deposition only altered the suspended sediment field in grid cells located directly above the sediment bed-water interface. Modifications to the code were not needed to quantify the advection and diffusion terms, as they are available in ROMS’ diagnostic output. The transport rate due to vertical diffusion in bottom grid cells was inferred by subtracting changes associated with the other processes (horizontal and vertical advection, settling, and erosion or deposition) from the calculated $\partial C/\partial t$ in post-processing.

2.2 Quantifying the Effect of Flocculation

Of special interest was comparing the magnitudes of the terms in Equation 3.3, especially the magnitude of the flocculation term, the $f(C_i, C_j, G, \ldots)$ that represented the mass exchanged between floc size $i$ and $j$ via aggregation and disaggregation. It is a function of SSC of the floc sizes ($C_i$ and $C_j$), shear rate ($G$), and other parameters (a full description is provided in Verney et al. (2011). The relative importance of each process was quantified as the proportion that each term contributed to the total change in concentration. Specifically, the magnitude of each term (in mass per unit volume per time step) was divided by the sum of the magnitude of all the terms. Equation 3.4 uses flocculation as an example for this relative fraction calculation. The denominator represents the total mass change for size class $i$, and was the magnitude of the right-hand side of Equation 3.3.
Equation 3.4:

\[
\text{Rel. Frac.} = \frac{|f(C_i, C_j, G, \ldots)|}{\left| -\nabla_H U C_i \right| + \left| \frac{\partial}{\partial z} K \frac{\partial C_i}{\partial z} \right| + \left| -\frac{\partial}{\partial z} (w - w_{s,i}) C_i \right| + \left| f(C_i, C_j, G, \ldots) \right| + |S_i|}
\]

where the variables in the relative flocculation fraction (Rel. Frac.) in Equation 3.4 are the same as those defined for Equation 3.3. This analysis of the relative transport fractions focused on two regions that represented the extremes within the estuary.

First, the ETM is subjected to strong turbulence and elevated SSC, and was located in the shallowest part of the grid (depth of 6 m). Secondly, the deeper downstream region (depth of ~13 m) was subjected to reduced turbulence and SSC. Additionally, a size distribution of the mass exchanged by flocculation was examined for these regions over the tidal cycle to determine the degree to which aggregation, disaggregation, or both caused changes to the floc size distribution.

2.3 Comparison of FLOCMOD to Equilibrium Floc Size

An equilibrium floc distribution is expected to asymptotically occur under steady conditions and can be characterized by an equilibrium floc size. Winterwerp’s (1998, 2002) theory from his single floc class model suggests that the steady-state equilibrium floc diameter is largely a function of SSC divided by the square root of the shear rate (\(G\)). According to Winterwerp (2002), the equilibration time is shortest when both SSC and shear rate are highest, like the conditions found within the ETM in our idealized model. Thus, model output from the ETM region was assumed to be nearest to the equilibrium and used to derive a relationship for equilibrium floc size for the idealized estuary conditions. Model data for ETM grid cells higher than ~70 cmab that had a shear rate
between 4-12 s\(^{-1}\) and SSC > 100 mg L\(^{-1}\) were assumed to best represent equilibria (Figure 3.2). Model data from these conditions were used determine the best-fit relationship between the expected equilibrium floc size and the ratio of the SSC/VG. Even in the ETM, equilibrium conditions did not occur throughout the full tidal cycle, leading to times in which the median floc size was not in equilibrium with G and SSC.

The relationship between the equilibrium floc distribution and the local, instantaneous distribution was quantified by comparing two representative diameters over the entire tidal cycle for all water column layers. The first was D\(_{50}\), the mass-weighted median diameter of the local, instantaneous size distribution generated by FLOCMOD. The second was D\(_{eq}\), the equilibrium diameter calculated from the local SSC/VG ratio using the linear fit determined (Figure 3.2). Times during the tidal cycle and locations in the water column where the D\(_{50}\) notably deviated from the expected equilibrium (D\(_{eq}\)) were identified. Differences in local conditions, such as erosion, settling, advection, and vertical diffusion were examined to explain these departures from the predicted D\(_{eq}\).

To further interpret model results, we used the theoretical flocculation timescale, T\(’\), from the Winterwerp (1998, 2002; Equation 3.5), which calculates a single theoretical timescale for aggregation and disaggregation.

**Equation 3.5:** \[ T’ \approx \frac{1}{k_BG^{3/2}D_{eq}} \]

here, T\(’\) depends on a disaggregation (k\(_B\)) coefficient; and will vary with the shear rate, G, and D\(_{eq}\). To estimate T\(’\) from Equation 3.5, we used the value of D\(_{eq}\) predicted by the best-fit line in Figure 3.2 along with the value of k\(_B\)=1.40x10\(^3\) s\(^{1/2}\) m\(^{-2}\) provided by
Winterwerp (2002), which was based on fitting his model to laboratory data. Unlike Winterwerp’s model, FLOCMOD does not have a single coefficient that controls disaggregation. $T'$ was calculated using the 5 minute output from the idealized estuary model by applying Equation 3.5 (Winterwerp, 2002) to each model grid cell for a 24-hour period ($n=288$) and the median value for $T'$ was calculated for each grid cell using the data from the 24-hour period.

3 Results

3.1 Floc Size and Mechanisms Driving Changes in Floc Size in the ETM

The comparison of the median diameter ($D_{50}$) relative to the equilibrium floc size ($D_{eq}$) in the ETM region showed the relationship between the two values evolved over the course of the tidal cycle. Additionally, the grain size distribution in the bottom-most grid cell evolved differently from the grain size distributions in the overlying water. For reference, the ETM region was ~6 m deep, the SSCs ranged between 200-800 mg L$^{-1}$, $VG$ ranged between 1-15 s$^{-1/2}$, and over the tidal cycle the along-estuary velocity magnitude fluctuated between approximately +/- 0.5 m s$^{-1}$ in the bottom meter of the water column. At slack flow (Figure 3.3a,d), the modeled $D_{50}$ was nearly equal to $D_{eq}$ at ~3 cmab (5.96 m depth; blue triangles), but was smaller than $D_{eq}$ throughout the rest of the water column. During the transition into peak flow (Figure 3.3b,e), $D_{50}$ values were closer to $D_{eq}$ over most of the water column but still notably smaller; except very near the bed where $D_{50}$ was slightly larger than $D_{eq}$. During the transition to flood flow (Figure 3.3b), the model showed closer agreement between $D_{50}$ and $D_{eq}$ than during the transition to ebb flow (Figure 3.3e). During peak flood (Figure 3.3c), $D_{50}$ was within 32
μm of $D_{eq}$ for the majority of the water column, except for very near the bed where $D_{50}$ exceeded $D_{eq}$. During peak ebb (Figure 3.3f), $D_{50}$ was near the equilibrium size for a majority of the water column; however, for several locations in the bottom meter the $D_{50}$ remained finer than the equilibrium (blue colored points).

The amount of mass transferred locally into or out of a floc size by aggregation or disaggregation was examined and compared to transport mechanisms that drive local changes in concentrations. Specifically, for the lower water column of the ETM, the relative fractions for the terms in the transport equation (Equation 3.3) were examined, starting with the model grid cell nearest the bed (~3 cmab; Figure 3.4). During periods spanning slack before flood to peak flood flow (Figure 3.4a-c), the comparison showed that flocculation, settling, erosion, and vertical diffusion played key roles in varying the floc concentrations. At slack flow (Figure 3.4a), flocculation contributed ~5-30% to the mass transfer in the ETM very near the bed for each floc size. As will be discussed in more detail below, most of the transfer involved floc break-up. Vertical diffusion was the second largest driver contributing ~20-80%, and settling was the next largest for the medium to large flocs (>32 μm) at ~2-45%. Lastly, horizontal advection accounted for 0-10% of the suspended mass transferred, while vertical advection and erosion were not important at slack flow (Figure 3.4a). As the current increased toward peak flood flow (Figure 3.4b,c), the contribution of flocculation to mass transfer increased slightly to range between ~2-50% in the transition and ~0-50% at peak flood flow. The second largest contributor under increased flow was vertical diffusion followed by erosion from the bed. Vertical diffusion ranged from ~20-70% in the transition, and ~15-70% at peak
flood flow. The contribution of erosion for some sizes was as high as 50% for the transition and peak flood flows. At this very near-bed location, horizontal advection and settling played smaller roles than the other processes in the mass transfer with contributions less than 20% and 10%, respectively for all floc sizes (Figure 3.4b,c).

The influence of flocculation on floc size was examined in more detail by analyzing the flocculation term from Equation 3.3, starting with very near the bed (~3 cmab) in the ETM where the rate of change was the highest in the estuary (Figure 3.4d-f). Flocculation was not responsible for much mass transfer here during slack flow (Figure 3.4d), but transferred much more mass during the transition toward flood and at peak flood flow very near the bed (Figure 3.4e,f). Very near the bed, sediment mass was removed from larger floc sizes (≥128 μm) and added to the smaller sizes (Figure 3.4e,f); demonstrating that disaggregation was important here except during slack flow. As for the comparison of the $D_{50}$ to $D_{eq}$, the two converged during slack flow (Figure 3.4d). As the flow increased toward peak flood flow, $D_{50}$ increased and was larger than the predicted $D_{eq}$ by ~32 μm in the transition and ~130 μm at peak flood flow (Figure 3.4e,f).

The relative contributions of the different processes to local mass transfer between floc sizes for slack before ebb through peak ebb flow very near the bed in the ETM (Figure 3.5a-c) were generally similar to those shown for flood (Figure 3.4a-c). While the relative fraction of mass transfer due to erosion was similar, the total amount of mass eroded from the bed was five times greater under peak flood compared to peak ebb (not shown).
Similar to slack before flood, the amount of mass transferred due to flocculation at slack before ebb was minimal compared to peak ebb flow (Figure 3.5d), very near the bed in the ETM. The amount of mass transferred between size classes by flocculation increased with the increasing flow toward ebb (Figure 3.5d-f), but the magnitudes were about one-third of that seen during peak flood very near the bed (Figure 3.4d-f). Similar to peak flood flow, larger flocs disaggregated during peak ebb flow, as shown by the mass being removed from larger floc sizes into the medium floc sizes (Figure 3.5f).

Again, the modeled $D_{50}$ equaled the equilibrium diameter for slack flow very near the bed (Figure 3.5d). Whereas, the $D_{50}$ nearly equaled $D_{eq}$ at peak ebb flow (Figure 3.5d-f) compared to $D_{50}$ being much larger than $D_{eq}$ during peak flood (Figure 3.4d-f).

The relative mass transfers show different patterns slightly higher in the water column at ~37 cmab (5.63 m deep) in the ETM with horizontal advection affecting floc concentration, and the effect of flocculation less important than at the very near-bed (Figure 3.6). The relative mass fraction increased for vertical diffusion, settling and horizontal advection compared to ~3 cmab, and the dominant processes transferring sediment mass at ~37 cmab were flocculation, vertical diffusion, settling, and horizontal advection (Figure 3.6). At this height in the water column, the fraction of mass transferred by flocculation was greatest during slack flow, ranging between ~3-70%; and decreased with increasing flow to <10% at peak flood flow (Figure 3.6a-c); both floc growth and break-up were occurring during peak flood flow. Vertical diffusion transferred ~1-90% at slack flow to ~55-90% during peak flood flow. The settling relative fraction was 0-60% at slack and 0-30% during peak flood flow, and horizontal advection
contributed 0-30% at slack to 0-40% during peak flow (Figure 3.6a-c). Vertical advection contributed less than 3% at slack flow and had no influence in the transition and at peak flow (Figure 3.6a-c). The relative fractions of the mass transfer analysis from slack to ebb at this location (not shown here) were similar to those shown for slack to flood flow.

Similar to the near-bed, the change in mass due to flocculation was minimal during slack, however, the amount of mass transferred by flocculation in the ETM was more than five times greater at ~3 cmab that at ~37 cmab. Under peak flood flow there was removal of mass from the 16-64 μm and 1024 μm floc sizes into the 128-512 μm floc sizes. Therefore, both the aggregation of smaller flocs and the disaggregation of the largest flocs occurred at ~37 cmab (Figure 3.6d-f). Slack before ebb was similar to slack before flood in the amount of mass that was transferred due to flocculation. The amount of mass moved between floc sizes due to aggregation increased as flow increased toward peak ebb flow but was at a lower magnitude than during flood flow and there was no evidence of disaggregation during ebb flow. The resulting $D_{50}$ due to aggregation and disaggregation at ~37 cmab converged with $D_{eq}$ during peak flood (Figure 3.6e-f) but not during ebb (Figure 3.6h-i). The largest difference between $D_{50}$ ($D_{50}$ ~100 μm) and $D_{eq}$ ($D_{eq}$ ~256 μm) occurred during slack flow (Figure 3.6d,g).

However, as the flow velocity increased from slack to peak flow, $D_{50}$ shifted closer to $D_{eq}$ (Figure 3.6d-i). During peak ebb flow, $D_{50}$ was ~60 μm smaller than $D_{eq}$.

Moving higher in the water column, the mass transfer terms at ~90 cmab (depth of 5.10 m; Figure 3.7) in the ETM showed that diffusion, advection and settling were larger contributors to local mass exchange between size classes than was flocculation, as was
the case at ~37 cmab. The relative effect of flocculation was similar to ~37 cmab but the effect of horizontal advection and settling increased compared to ~37 cmab.

Flocculation accounted for ~3-30% of the mass transferred at slack flow and less than 10% at peak flood flow, while vertical diffusion accounted for ~1-75% at slack and 0-90% at peak flood flow (Figure 3.7a-c). In terms of flocculation, aggregation was dominate and discussed in more detail below (Figure 3.7d-i). The proportion of the mass reallocated by settling was as high as 90% at ~90 cmab and was greatest for floc sizes >128 μm during slack before flood. As flow increased to peak flood, the proportion of mass transferred by settling remained high for the larger flocs (Figure 3.7a-c). The mass fraction transferred by horizontal advection increased compared to ~37 cmab, ranging from 0-40% at slack and 0-90% at peak flood flow. Vertical advection contributed less than 1%, if at all, from slack to flood flow (Figure 3.7a-c). As seen closer to the bed, there was little to no difference in the mass transfer fractions from slack to ebb in comparison to slack to flood flow at ~90 cmab (not shown).

The magnitude of mass exchanged in the ETM due to flocculation decreased with height above the bed (Figures 3.4f, 3.6f, and 3.7f); and accounted for less than 0.02 mg L\(^{-1}\) s\(^{-1}\) for each floc size at ~90 cmab (Figure 3.7d-i). Minimal mass was transferred due to flocculation at slack before flood and ebb, at ~90 cmab (Figure 3.7d,g). The sediment mass moved due to flocculation at ~90 cmab was from aggregation in which sediment was removed from the medium floc sizes to the larger floc sizes (256-1024 μm). The comparison between \(D_{50}\) and \(D_{eq}\) showed trends over the tidal cycle at ~90 cmab that
were similar to those at ~37 cmab, i.e., \( D_{50} \) was smaller than the \( D_{eq} \) during slack and ebb flow, but reached equilibrium during peak flood flow.

3.2 \textit{Floc Size and Mechanisms Driving Changes in Floc Size Downstream of the ETM}

The conditions in the downstream region (13.12 m deep, see Figure 3.1) of the estuary were generally less energetic and had lower SSC than calculated for the ETM; specifically, SSC ranged between 60-80 mg L\(^{-1}\), the \( \sqrt{G} \) ranged between 1-10 s\(^{-1/2}\), and the peak tidal velocity was approximately 0.4 m s\(^{-1}\) in the bottom 2 m of the water column. At the downstream location, throughout the tidal cycle, \( D_{50} \) approached \( D_{eq} \) in the bottom grid cell (~7 cmab; Figure 3.8, blue triangles) and in the top several meters of the water column (red/orange colors). For the rest of the water column, however, \( D_{50} \) was smaller than \( D_{eq} \) throughout the tidal cycle. However, as velocity increased during flood and ebb flow, \( D_{50} \) in the lower 2 m of the water column shifted closer to \( D_{eq} \) (Figure 3.8).

At the downstream location very near the bed (~7 cmab; depth of ~13.05 m), the relative transfer of sediment mass within size classes showed that flocculation, vertical diffusion, and settling dominated the transport equation. At this location, the average relative fraction of changes driven by flocculation at slack accounted for ~15-50% for all but one floc size (Figure 3.9a). At peak flow, the relative fractions contributed by flocculation were generally smaller, but did reach ~50% for medium sizes (Figure 3.9b). However, at peak flood flow relative mass transfer due to flocculation was less than 10% for the several floc sizes that had little to no sediment in suspension (1-8 μm and 256-1024 μm, Figure 3.9b). Vertical diffusion accounted for a significant amount of mass
transport at this location; accounting for ~40-90% at slack and ~35-50% at peak flood flow (Figure 3.9a,b). Erosion did not contribute to mass transfer at slack but contributed ~15-50% at peak flood, even in the smallest floc sizes (1-8 μm). Lastly, settling and horizontal advection played smaller roles in the transfer of mass. Settling mainly impacted floc sizes ≥128 μm, and the relative fraction for horizontal advection was greater than 10% floc sizes ≤128 μm, but only during slack flow when SSC was low and transport of sediment from other processes was greatly reduced (Figure 3.9a,b). Most of the time flocculation here reduced sediment mass from floc sizes 32-128 μm and added to the 16 μm floc size, showing disaggregation was occurring (Figure 3.9d). The exception was during slack, when aggregation occurred but at a much slower rate of change than during peak flood flow (Figure 3.9c,d). Additionally, the magnitude of the change in mass due to flocculation (Figure 3.9c,d) was smaller at the downstream location than calculated for the ETM, and mainly impacted floc sizes of 16-128 μm in the downstream region. D_{50} and D_{eq} were within ~10 μm of each other over the tidal cycle (Figure 3.9c,d) and D_{eq} stayed between 16-32 μm from slack to peak flow (Figure 3.9).

In the downstream region, but higher above the bed at ~105 cmab, the relative fractions of mass transferred by the various mechanisms were as follows (Figure 3.10a,b); at slack and peak flood, respectively, flocculation accounted for ~5-40% and ~3-20%, vertical diffusion contributed ~5-80% and ~50-80%, and, for sizes >8 μm settling transferred ~0-90% and ~0-40%. At slack flow, the horizontal advection proportion of mass transferred was ~0-40% and decreased to ~1-30% at peak flood flow. Similarly, the vertical advection contribution was greater at slack at ~0-10% and dropped to <3% at
peak flood flow (Figure 3.10a,b). Aggregation of the 16 μm floc size by flocculation, which removed mass from this size and added mass to the 32-128 μm floc sizes, occurred throughout the entire tidal cycle (Figure 3.10c,d). The amount of mass transferred by flocculation was ~3 times larger during peak conditions than slack flow (Figure 3.10c,d), but about 20 times less than those calculated for ~7 cmab (Figure 3.9c,d) in the lower estuary or at ~90 cmab in the ETM (Figure 3.7c,d). D_{50} remained below D_{eq} throughout the tidal cycle by ~100 μm and ~40 μm at slack flow and peak flood flow, respectively.

3.3 Estimate of the Amount of Time Required for Floc Size to Reach Equilibrium

The timescale for flocculation (T'; Equation 3.5) in hours was estimated, the median values for each grid cell are shown in Figure 3.11a. In a large portion of the estuary, the median exceeds 100 hours, which is much longer than timescales of tidal fluctuations. One exception was the very near-bed layer, where relatively short amounts of time were needed to reach equilibrium by aggregation and/or disaggregation (Figure 3.11a). Also, much of the water column in the ETM region and shallow portions of the estuary (depth <6 m) also had relatively short median timescales (<10 hours; blue colors) to reach equilibrium through aggregation and disaggregation (Figure 3.11a).

The average fractional difference between D_{50} and D_{eq} showed that, on average, D_{50} was close to the equilibrium value near the water surface, at the sediment-water interface and in the ETM (Figure 3.11b). The average magnitude in the fractional difference between the D_{50} and D_{eq} was <0.25 near the sediment bed throughout the estuary except in the ETM where the average fractional difference was ~0.4 (Figure
3.11b). The average fractional difference between the modeled $D_{50}$ and $D_{eq}$ increased to $\geq 2$ above the near-bed layer and through the bottom boundary layer except for the ETM where the fractional difference was $< 1$ in the bottom boundary layer. In the surface waters, the fractional difference between the two diameters was $< 0.5$.

The timeseries of $T'$ for the ETM (Figure 3.12a,b) illustrated the tidal variation of $T'$ and showed that the longest timescale occurred during slack flow when SSC and shear rate were reduced. In the bottom meter of the water column, $T'$ was shortest during peak flood flow, reaching as low as $\sim 4$ sec at $\sim 3$ cmab (Figure 3.12a), and lengthened during slack flow to as much as $\sim 1.3$ hours at $\sim 90$ cmab (Figure 3.12a,b). Over the full tidal cycle, in the ETM the $T'$ was $< 14$ minutes very near the bed, and $T' \leq 1.3$ hours at $\sim 90$ cmab (Figure 3.12a,b). $D_{50}$ was at times greater than $D_{eq}$ (Figure 3.12; red shading), converged to near $D_{eq} (+/- 15\%)$ (Figure 3.12; blue shading), or was less than $D_{eq}$ (Figure 3.12; green shading). The difference between $D_{50}$ and $D_{eq}$ was lowest very near the bed in the ETM around slack flow and during elevated flow surrounding peak flood and ebb flow at $\sim 90$ cmab (Figure 3.13a,c). While $D_{50}$ was frequently larger than $D_{eq}$ very near the bed in the ETM (Figure 3.12c), the two typically increased and decreased at the same time over the tidal cycle. At $\sim 90$ cmab (Figure 3.13b), when $D_{50}$ did not converge to $D_{eq}$, $D_{50}$ was smaller than the $D_{eq}$ and tended to decrease when $D_{eq}$ increased. Within the ETM very near the bed, $D_{50}$ equilibrated with the SSC/VG when the flocculation timescale was the longest (\sim 2-3 minutes), and when $T'$ was approximately $< 6$ minutes at $\sim 90$ cmab (Figure 3.12b-c).
The shortest $T'$ in the downstream region was very near the bed during peak flood flow where $T'$ was $\sim 2.1$ minutes and $T'$ remained below $\sim 1.2$ hours at slack flow (Figure 3.13a), which was similar to the $T'$ values estimated at $\sim 90$ cmab in the ETM (Figure 3.12b). At $\sim 105$ cmab the minimum of $T'$ was $\sim 1.7$ hours at peak flow and stayed $\leq 10$ hours over the full tidal cycle (Figure 3.13b). In the downstream region, $D_{50}$ at times converged to $D_{eq}$, was near $D_{eq}$ ($+/ -15\%$) (Figure 3.13; blue shaded region), or was less than $D_{eq}$ (Figure 3.13; green shaded area). Similar to very near the bed in the ETM, very near the bed in the downstream region (Figure 3.13c) $D_{50}$ and $D_{eq}$ increased and decreased at the same time, but $D_{50}$ remained smaller than the $D_{eq}$. The difference between $D_{50}$ and $D_{eq}$ in the downstream region at $\sim 105$ cmab (Figure 3.13d) increased when $D_{eq}$ increased, since $D_{50}$ varied little over the tidal cycle. Overall, the $D_{50}$ did not equilibrate with the $SSC/\sqrt{G}$ ratio when the flocculation timescale was $> 6$ minutes (Figure 3.12a,b and 3.13a,b).

4 Discussion

The analysis of the output from idealized estuarine model was focused on the bottom meter of the water column in the ETM and at the downstream location (see Figure 3.1). The results highlighted variability in the importance of flocculation within the ETM, for example the relative transfer rate was greater during flood than during ebb flow, and the difference between $D_{50}$ and $D_{eq}$ was greater during ebb than flood flow at $\sim 90$ cmab in the ETM. These differences are discussed further in Section 4.1. Additionally, the modeled $D_{50}$ approached $D_{eq}$ under specific conditions, which was expected for the grid cells in the ETM that were used to produce the equilibrium
relationship. Here, we discuss the processes that affect floc size for conditions when the population balance model’s (i.e. FLOCMOD’s) median diameter was dissimilar to Winterwerp’s (2002) equilibrium size. This analysis provided insight on when a simple equilibrium model would be inaccurate, and modifications that could be made to derive an equilibrium relation that better represented the floc population.

4.1 Flocculation Dynamics during flood versus ebb flow

The trends in the relative fraction of mass transport by advection and diffusion were similar between flood and ebb flow, except that the contribution of horizontal advection was slightly reduced during ebb flow (Figures 3.4, 3.5). In contrast, in the ETM, flood and ebb flows differed in the magnitude of the rate of mass transferred by flocculation, and in the degree to which $D_{50}$ approached $D_{eq}$. The depth-averaged along-estuary velocity was $\sim 10$ cm s$^{-1}$ faster during ebb flow than flood flow (Figure 3.4g). However, in the bottom meter of the water column, peak ebb flow was slower than peak flood flow by $\sim 10$ cm s$^{-1}$ (not shown). The SSC, and shear rate in the bottom meter of the ETM were lower during ebb flow than flood but the ratio of SSC/$\sqrt{G}$ was similar at flood and ebb flow; and flocculation exchanged less mass between floc sizes during ebb than flood flow. Additionally, the timescale for flocculation was slightly longer during ebb than flood flow. $D_{eq}$ predicted during ebb flow was similar to flood flow, based on the similar SSC/$\sqrt{G}$. The slower near-bed flow during ebb reduced erosion from the bed resulting in a lower SSC, combined with lower shear, this reduced the rate of aggregation and disaggregation, and led to a smaller $D_{50}$. Therefore, the difference between $D_{50}$ and $D_{eq}$ was smaller during ebb flow in the near-bed location of the ETM. However, the
difference in the diameters was larger during ebb at ~90 cmab because the local hydrodynamics produced a smaller $D_{50}$. Thus, the slower near-bed velocities led to flocculation, resuspension, and horizontal advection to be less important during ebb flow. Also, this illustrates that the near-bed conditions may be more relevant to sediment transport processes than depth-averaged velocities.

4.2 Equilibrium conditions versus Non-equilibrium Conditions

When FLOCMOD produced $D_{50} \approx D_{eq}$, this implied that the floc population had reached equilibrium with the available suspended sediment and shear rate. Within the ETM, modeled $D_{50}$ converged with $D_{eq}$ very near the bed around slack, and higher in the water column (~37 cmab and ~90 cmab) during peak flood flow (Figures 3.4-3.7, 3.12). At the ETM during slack flow very near the bed, the effects of flocculation were minimal; vertical diffusion and settling governed the amount of SSC, and caused $D_{50}$ to merge with $D_{eq}$ (Figure 3.4a, 3.5a). Higher in the water column of the ETM, flocculation was able to balance the combined effects of vertical diffusion, settling and horizontal advection during peak flood flow (Figure 3.6, 3.7). The model also showed $D_{50} \approx D_{eq}$ during most of the tidal cycle in the downstream region in the near-bed location (Figure 3.9, 3.13). Despite the longer flocculation timescale in the downstream region, flocculation nearly balanced the vertical diffusion and settling during slack flow, and balanced the vertical diffusion and erosion during peak flow (Figure 3.9, 3.13). The $\sqrt{G}$ was greater than 4 s$^{-1/2}$ over the full tidal cycle very near the bed in the downstream region. Therefore, the higher shear rate near the bed likely played a key role in allowing
flocculation to occur causing the FLOCMOD $D_{50}$ to approach equilibrium near the bed at the downstream location.

The modeled $D_{50}$ was not in equilibrium with the SSC and shear rate in the ETM very near the bed during flood flow. It also did not reach $D_{eq}$ in the ETM at locations higher in the water column (~37 cmab and ~90 cmab) during slack and ebb flow. At the downstream location at ~105 cmab, $D_{50}$ diverged from the $D_{eq}$ throughout the entire tidal cycle. The conditions leading to non-equilibrium behavior in the model were different in the near-bed layer than higher in the water column.

Very near the bed, flocculation, vertical diffusion, and erosion were the main processes that contributed to the mass balance of sediment in the ETM during flood flow, when the near-bed $D_{50}$ did not reach equilibrium. Keep in mind that both the flocculation and vertical diffusion were two key contributors in the ETM near-bed when the $D_{50}$ was in equilibrium at slack flow (Figures 3.4-3.5). The timescale for flocculation was less than a minute (Figure 3.12), and flocs were being disaggregated as shown by the transfer of sediment mass from the largest floc sizes to the medium floc sizes (Figures 3.4-3.5,d-f). The sediment mass being eroded from the bed was predominantly in the larger floc sizes (>128 μm; Figure 3.4-3.5,a-c). Thus, the erosion of larger flocs outpaced the breakup of the flocs (Figure 3.4c,b), allowing $D_{50}$ to remain larger than $D_{eq}$. During peak ebb very near the bed, erosion of large flocs contributed a similar relative fraction to sediment mass transfer, but the overall amount of erosion and SSC was lower than during flood. This allowed $D_{50}$ to shift closer to equilibrium during peak ebb flow but not enough for $D_{50}$ to converge with $D_{eq}$, thus erosion still outpaced
flocculation. In contrast, at the downstream location near the bed under both peak ebb and flood flow, $D_{50}$ was near equilibrium despite erosion being a major contributor to the mass transfer. The difference in the downstream region was that erosion accounted for ~40% of the sediment mass transport in the smaller floc sizes (1-16 μm) as well as ~35-50% in the largest floc sizes (256-1024 μm). Whereas, in the ETM very near the bed, erosion delivered mainly floc sizes >64 μm. Therefore, the system did not reach equilibrium in regions where erosion of flocs significantly larger than $D_{eq}$ was a major source of SSC to the near-bed region.

In the ETM higher in the water column (~37 cmab and ~90 cmab), the equilibrium floc relation predicted a floc size larger than $D_{50}$ when turbulence was reduced near slack flow, and during the ebb flow. The SSC and shear rate both decreased during slack flow; however, the decrease in the shear rate was more significant than reduction in the SSC, causing the $SSC/VG$ and $D_{eq}$ to increase at both heights. At ~90 cmab the settling of sediment further reduced SSC. During peak ebb flow, the SSC was ~25% and $SSC/VG$ was ~25% lower compared to peak flood flow in the ETM, (not shown), leading to a smaller $D_{eq}$ during ebb flow. Despite the smaller $D_{eq}$, the model produced a $D_{50}$ that was smaller than the equilibrium floc size at ~37 and ~90 cmab in the ETM. At these heights, transport processes, namely vertical diffusion, horizontal advection, and settling, reduced SSC, leading to a slight increase in the flocculation timescale during ebb flow, and a reduced estimated of $D_{50}$. Thus, the rate of mass transfer due to flocculation was too small to compensate and $D_{50}$ remained smaller than $D_{eq}$. Therefore, at these heights,
the equilibrium floc relation did not provide an accurate estimate of floc size because the SSC/\(\sqrt{G}\) ratio remained too large for the \(D_{50}\) to converge to the \(D_{eq}\).

5 Summary and Conclusions

The idealized model, configured to represent the main features of the York River estuary, accounted for flocculation via a population balance model, FLOCMOD, and suspended sediment transport processes including erosion, advection, diffusion, settling. Flocculation was an important contributor in the transport of suspended sediment throughout the idealized, partially mixed estuary. Flocculation caused as much or more change to concentrations of individual size classes as advection and settling. Erosion, vertical diffusion and flocculation were responsible for the majority of the change in sediment concentrations in the very near-bed region. Directly above the sediment-water interface, erosion accounted for more of the mass balance than flocculation in floc sizes >128 \(\mu\text{m}\) in the ETM, and flocs sizes 1-8 \(\mu\text{m}\) and 256-1024 \(\mu\text{m}\) in the downstream region. Very near the bed, flocculation transferred more mass than erosion for floc sizes 16-64 \(\mu\text{m}\) in the ETM and for floc sizes 16-128 \(\mu\text{m}\) in the downstream region. Slightly higher above the bed, \(\sim 37\ \text{cmab to}\ \sim 90\ \text{cmab}\), vertical diffusion and flocculation were the dominant mechanisms effecting the sediment mass concentrations across all size classes. Settling was typically a major contributor to the local transfer of mass for only the largest floc sizes during slack very near the bed, and throughout the tidal cycle slightly higher in the water column.

The relative importance of aggregation and disaggregation varied over the tidal cycle and with location in the idealized estuary. Throughout the estuary, the very near-bed
region had the highest SSC and shear rates, which led to the disaggregation of the largest flocs (>256 μm in the ETM, and 32-256 μm downstream of the ETM) throughout the tidal cycle. These large flocs were supplied to the very near-bed via resuspension during peak flows (Figures 3.4c, 3.5c) from the material that had previously settled during slack conditions (Figures 3.4a, 3.5a). In the ETM, there was a transitional location in the water column (~37 cmab) that had intermediate SSC and shear rates when aggregation of the smaller flocs, and disaggregation of the larger ones transferred mass into the medium floc sizes (128-512 μm). SSC and shear rates were reduced slightly higher in the water column (~1 mab), leading to the aggregation of smaller flocs in suspension (16-128 μm in the ETM and 16 μm downstream) into the larger floc sizes (256-1024 μm in the ETM and 32-128 μm downstream) throughout the tidal cycle. Near-bed current velocities were slower in the ETM during ebb flow compared to flood. These weaker near-bed currents led to lower SSC and less exchange due to flocculation, but a median floc size that was nearer to the equilibrium than during peak flood flow.

Above ~70 cmab in the ETM at time periods with SSC > 0.1 kg/m³ and 4< G<12 s⁻¹, the modeled D₅₀ generally followed a linear relationship with SSC/√G, as predicted with equilibrium floc theory, and this was used to identify an equilibrium floc size (Dₑq), dependent on SSC and √G. However, the modeled D₅₀ often differed from the Dₑq. For example, very near the bed when elevated erosion rates entrained large flocs from the bed, and also when turbulent stresses were reduced in the lower water column (<1 mab). An equilibrium timescale for flocculation was also derived following floc theory. However, criteria that would indicate conditions for which the modeled D₅₀ converged
to the $D_{eq}$ were not straightforward. Very near the bed in the ETM, the supply of large flocs via bed erosion outpaced the breakup of the large flocs, even though the disaggregation timescale was <1 minute. Away from the sediment-water interface, where the timescale of flocculation was still short, $D_{50}$ approached and often converged with the $D_{eq}$ at peak flood flow. Generally, the equilibrium floc relation best represented $D_{50}$ for locations away from the immediate vicinity of the sediment-water interface, and when flocculation timescales were on the order of minutes. Very near the sediment bed, the equilibrium floc relation represented the floc population when erosion was minimal or when finer flocs were part of the eroded distribution; but at peak flows very near the bed in the ETM, modeled $D_{50}$ did not equilibrate to a simple equilibrium relationship with SSC/VG.

For future research we suggest changes in the population balance floc model based on the results from this study. Knowledge of the timescale for flocculation could be used to reduce the computational cost of the population balance floc model. For example, FLOCMOD might be used only very near the bed, and for conditions when the flocculation timescale is less than 5 minutes, which is relative short compared to the tidal timescale. The exact criteria may need to be adjusted for different study locations. This modification would require that FLOCMOD implementations include the additional disaggregation parameter, $k_B$, from Winterwerp (2002), to enable FLOCMOD to estimate the flocculation timescale, shown in Equation 3.5.

The results from this study showed that the floc distribution did not follow the theoretical equilibrium relationship in the water column below the pycnocline when
turbulence was low, or near the bed when bed erosion supplied larger flocs. The activation of FLOCMOD is recommended when the area of interest is very near the bed with shear rates and SSC similar to the ETM in this study, or slightly higher in the water column with shear rates and SSC similar to those shown in the ETM during slack and ebb flow. For the deeper regions of the estuary, activation of FLOCMOD is recommended for the lower half of the water column, except for very near the bed. For other conditions similar to top several meters of the water column or during peak flood flow in the lower water column of the ETM, the relation of $D_{eq}$ to the $SSC/\sqrt{G}$ could be applied.
Figure 3.1: Model setup of the idealized estuary. The water column is represented by 40 layers, stretched to have high resolution in the near-bed and surface waters. Color represents the time-averaged SSC. The sediment bed is represented by 10 layers initially containing 1 m thick of sediment (brown layer at base of model grid).
Figure 3.2: The model data from the ETM used to produce the best-fit equilibrium floc size curve (red line). These data fit the following criteria: 4<\text{G}<12, \text{C}>0.1 \text{ kg m}^{-3}, \text{ and } >\sim 70 \text{ cmab.}
Figure 3.3: Comparison of $D_{eq}$ (black lines) to modeled $D_{50}$ (colored points) from 4 horizontal grid cells in the ETM region, as a function of SSC/VG. Panels a-c show slack before flood to peak flood; while Panels d-f show slack before ebb to peak ebb (bottom row). Black dashed lines are +/- 32 μm from $D_{eq}$. Triangles mark data from the lowest grid point in the water column (~3 cmab).
Figure 3.4: For the ETM very near the bed (~3 cm ab), (a-c): the relative mass transfer fractions for slack before flood to peak flood; (d-f): the mass transfer rates between floc sizes for slack before flood to peak flood. Positive values indicate flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{eq}$, respectively. (g): Depth-average velocity (black line). Red dots identify times within tidal cycle for panels a-f.
Figure 3.5: For the ETM very near the bed (~3 cmab), (a-c): the relative mass transfer fractions for slack before ebb to peak ebb; (d-f): the mass transfer rates between floc sizes for slack before ebb to peak ebb. Positive values indicate flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{eq}$, respectively. (g): Depth-average velocity (black line). Red dots identify times within tidal cycle for panels a-f.
Figure 3.6: For ETM at ~37 cmab, (a-c): the relative mass transfer fractions for slack before flood to peak flood, (d-f): the mass transfer rates between floc sizes for slack before flood to peak flood, and (g-i): the mass transfer rates between floc sizes for slack before ebb to peak ebb. Positive values in (d-i) indicate that flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{eq}$, respectively. Insets to the right show depth-averaged velocity (black lines), and identify times within tidal cycle for panels a-i (red dots).
Figure 3.7: For ETM at ~90 cmab, (a-c): the relative mass transfer fractions for slack before flood to peak flood, (d-f) the mass transfer rates between floc sizes for slack before flood to peak flood, and (g-i): the mass transfer rates between floc sizes for slack before ebb to peak ebb. Positive values in (d-i) indicate that flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{eq}$, respectively. Insets to the right show depth-averaged velocity (black lines), and identify times within tidal cycle for panels a-i (red dots).
Figure 3.8: Comparison of $D_{eq}$ (black lines) to modeled $D_{50}$ (colored points) from 4 horizontal grid cells in the downstream region, as a function of $SSC/\sqrt{G}$. (a): slack before flood, (b): peak flood. Black dashed lines are +/- 16 $\mu$m from $D_{eq}$. Triangles mark data from the lowest grid point in the water column (~7 cmab).
Figure 3.9: For the Downstream location very near the bed (~7 cmab). Top row: The relative mass transfer fractions for (a) slack before flood and (b) peak flood. Bottom row: The mass transfer rates between floc sizes for (c) slack before flood and (d) peak flood. Positive values indicate flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{eq}$, respectively.
Figure 3.10: For the Downstream location at ~105 cmab. Top row: The relative mass transfer fractions for (a) slack before flood and (b) peak flood. Bottom row: The mass transfer rates between floc sizes for (c) slack before flood and (d) peak flood. Positive values indicate flocculation added mass to that size. Black and red dashed lines are $D_{50}$ and $D_{	ext{eq}}$, respectively.
Figure 3.11: (a) Median for the flocculation timescale ($T'$; top) calculated as described in Section 2.3. (b) The time-averaged percent difference between $D_{50}$ and $D_{eq}$ ($|D_{50} - D_{eq}|/D_{50}$). The thickness of the bottom-most (near-bed) grid cell is enlarged for visibility in both panels.
Figure 3.12: Timeseries of the flocculation timescale (T'; black line) in hours for the ETM (top row) at ~3 cmab (a) and ~90 cmab (b). Bottom row: Timeseries of D_{50} (solid black line) and D_{eq} (solid red line) for the ETM at ~3 cmab (c) and ~90 cmab (d). The tidal cycle shown is the same as in previous figures. The black dashed lines represent the timing of the peak flood, ebb and slack flow. The shaded regions represent time periods when D_{50} \approx D_{eq} \pm 15\% (blue), D_{50} > D_{eq} (red), and D_{50} < D_{eq} (green).
Figure 3.13: Timeseries of the flocculation timescale ($T'$; black line) in hours for the downstream region (top row) at ~7 cmab (a) and ~105 cmab (b). Bottom row: Timeseries of $D_{50}$ (solid black line) and $D_{eq}$ (solid red line) for the downstream region at ~7 cmab (c) and ~105 cmab (d). The tidal cycle shown is the same as in previous figures. The black dashed lines mark peak flood and slack, respectively. The shaded regions represent time periods when $D_{50} \approx D_{eq} \pm 15\%$ (blue), $D_{50} > D_{eq}$ (red), and $D_{50} < D_{eq}$ (green). Note: The vertical axis for panel b has a larger range.
References


Appendix B

The diagnostic variables (advection and vertical diffusion) were recorded in a separate model output file when the “define DIAGNOSTICS_TS” flag is set in the header file and the output flag in the sediment input file was turned on (”T”). Within the advection and diffusion routine, CSTMS calculates the transport flux of sediment mass due to vertical advection, horizontal advection and vertical diffusion for each grid cell for each floc size as shown in Equation 3.3 and is recorded in the model output as a transport rate in kg m\(^{-3}\) s\(^{-1}\). These transport rates were converted to mass per unit volume during post-processing by multiplying by the model time step (dt = 30 s).

As for the added variables, the units varied due to the methods used by CSTMS to calculate the various processes, thus, mass transfer for flocculation was recorded in kg m\(^{-3}\), while settling and erosion was recorded in kg m\(^{-4}\). The settling and erosion mass transfer output was divided by grid cell thickness (\(dz\)) in post-processing to convert to mass per unit volume.

The update in the sed_flocmod subroutine in the sed_flocs.F file to calculate the mass transferred due to flocculation (a similar modification was made in the xx and xx files for settling and erosion). Modifications are marked using my initials, drnt.

```
#include "cppdefs.h"

MODULE sed_flocs_mod

#if defined NONLINEAR && defined SEDIMENT && defined SUSPLOAD && defined SED_FLOCS
  !
  !svn $Id: sed_flocs.F 429 2009-12-20 17:30:26Z arango $
  !=======================================================================
  !  Copyright (c) 2002-2017 The ROMS/TOMS Group                         !
```

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This routine computes floc transformation.

References:


implicit none
PRIVATE
PUBLIC :: sed_flocmod
CONTAINS

SUBROUTINE sed_flocmod (ng, tile)
!
!************************************************
***********************
USE mod_param
USE mod_forces
USE mod_grid
USE mod_mixing
USE mod_ocean
USE mod_stepping
USE mod_bbl
USE mod_sedflocs

! Imported variable declarations.
!
integer, intent(in) :: ng, tile
!
! Local variable declarations.
!
#include "tile.h"
!
ifdef PROFILE
CALL wclock_on (ng, iNLM, 16)
#endif

CALL sed_flocmod_tile (ng, tile, 
& LBi, UBi, LBj, UBj, N(ng), NT(ng), 
& IminS, ImaxS, JminS, JmaxS, 
& nstp(ng), nnew(ng), 
& GRID(ng) % z_r, 
& GRID(ng) % z_w, 
& GRID(ng) % Hz, 
 ifndef BBL_MODEL

# ifdef BBL_MODEL
& BBL(ng) % bustrcwmax, &
& BBL(ng) % bvstrcwmax, &
& FORCES(ng) % Pwave_bot, &

# endif
& FORCES(ng) % bustr, &
& FORCES(ng) % bvstr, &
& MIXING(ng) % Akt, &
& MIXING(ng) % Akv, &
& MIXING(ng) % Lscale, &
& MIXING(ng) % gls, &
& MIXING(ng) % tke, &
& OCEAN(ng) % t, &
& SEDFLOCS(ng) % f_mass, &
& SEDFLOCS(ng) % f_diam, &

! drnt 10-8-19
& SEDFLOCS(ng) % floc_mass)

# ifdef PROFILE
CALL wclock_off (ng, iNLM, 16)
# endif
RETURN
END SUBROUTINE sed_flocmod

!***********************************************************************
SUBROUTINE sed_flocmod_tile (ng, tile, &
& LBi, UBi, LBj, UBj, UBk, UBt, &
& IminS, ImaxS, JminS, JmaxS, &
& nstp, nnew, z_r, z_w, Hz, &

# ifdef BBL_MODEL
& bustrcwmax, &
& bvstrcwmax, &
& Pwave_bot, &

# endif
& bustr, &
& bvstr, &
& Akt, Akv, Lscale, gls, tke, &
& t, &
& f_mass, f_diam, floc_mass)

!***********************************************************************

USE mod_param
USE mod_scalars
USE mod_sediment
USE mod_sedflocs

! drnt
USE bc_3d_mod, ONLY : bc_r3d_tile
USE exchange_3d_mod, ONLY : exchange_r3d_tile

# ifdef DISTRIBUTE
USE mp_exchange_mod, ONLY : mp_exchange3d, mp_exchange4d
# endif

! implicit none

! Imported variable declarations.
!
integer, intent(in) :: ng, tile
integer, intent(in) :: LBi, UBi, LBJ, UBj, UBk, UBt
integer, intent(in) :: IminS, ImaxS, JminS, JmaxS
integer, intent(in) :: nstp, nnew
!
ifdef ASSUMED_SHAPE
real(r8), intent(in) :: z_r(LBi:,LBj:,;)
real(r8), intent(in) :: z_w(LBi:,LBj:,0:)
real(r8), intent(in) :: Hz(LBi:,LBj:,;)
endif
!
ifdef BBL_MODEL
real(r8), intent(in) :: bustrcwmax(LBi:,LBj:)
real(r8), intent(in) :: bvstrcwmax(LBi:,LBj:)
real(r8), intent(in) :: Pwave_bot(LBi:,LBj:)
endif
!
real(r8), intent(in) :: bustr(LBi:,LBj:)
real(r8), intent(in) :: bvstr(LBi:,LBj:)
real(r8), intent(in) :: Akt(LBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: Akv(LBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: Lscale(LBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: tke(LBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: gls(LBi:,LBj:,0:UBk,3)
real(r8), intent(inout) :: t(LBi:,LBj:,UBk,3,UBt)
!
real(r8), intent(out) :: floc_mass(LBi:,LBj:,UBk,NCS)
!
ifdef BBL_MODEL
real(r8), intent(in) :: bustrcwmax(LBi:,LBj:,UBj:UBj)
real(r8), intent(in) :: bvstrcwmax(LBi:,UBi:,LBj:,UBj)
real(r8), intent(in) :: Pwave_bot(LBi:,UBi:,LBj:,UBj)
endif
!
real(r8), intent(in) :: bustr(LBi:,UBi:,LBj:,UBj)
real(r8), intent(in) :: bvstr(LBi:,UBi:,LBj:,UBj)
real(r8), intent(in) :: Akt(LBi:,UBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: Akv(LBi:,UBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: Lscale(LBi:,UBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: tke(LBi:,UBi:,LBj:,0:UBk,3)
real(r8), intent(in) :: gls(LBi:,UBi:,LBj:,0:UBk,3)
real(r8), intent(inout) :: t(LBi:,UBi:,LBj:,UBk,3,UBt)
!
real(r8), intent(out) :: floc_mass(LBi:,UBi:,LBj:,UBj,UBk,NCS)
!
real(r8), intent(in) :: f_mass(0:NCS+1)
real(r8), intent(in) :: f_diam(NCS)
!
real(r8), intent(out) :: floc_mass(LBi:,LBj:,UBj,UBk,NCS)
!
!
Local variable declarations.
! integer :: i, indx, ised, j, k, ks, itrc
!
! Variable declarations for floc model
!
integer :: iv1
real(r8), dimension(IminS:ImaxS,N(ng)) :: Hz_inv
real(r8) :: Gval,diss,mneg,dttemp,f_dt
real(r8) :: dt1,f_csum,epsilon8
real(r8) :: fm_tmp
real(r8) :: cvtotmud,tke_av, gls_av, exp1, exp2, exp3, uest2, effecz
real(r8), dimension(IminS:ImaxS,N(ng),NT(ng)) :: susmud
real(r8), dimension(N(ng),IminS:ImaxS,JminS:JmaxS) :: f_davg
real(r8), dimension(N(ng),IminS:ImaxS,JminS:JmaxS) :: f_d50
real(r8), dimension(N(ng),IminS:ImaxS,JminS:JmaxS) :: f_d90
real(r8), dimension(N(ng),IminS:ImaxS,JminS:JmaxS) :: f_d10
real(r8), dimension(1:NCS) :: cv_tmp,NNin,NNout
!
! f_mneg_param : negative mass tolerated to avoid small sub time step (g/l)
real(r8), parameter :: f_mneg_param=0.000_r8
#include "set_bounds.h"
epsilon8=epsilon(1.0)
!
epsilon8=1.e-8
!

! * Executable part
!
! J_LOOP : DO j=Jstr,Jend
!
! Extract mud variables from tracer arrays, place them into
! scratch arrays, and restrict their values to be positive definite.
DO k=1,N(ng)
    DO i=Istr,Iend
        Hz_inv(i,k)=1.0_r8/Hz(i,j,k)
    END DO
    END DO
DO ised=1,NCS
    indx = idsed(ised)
    DO k=1,N(ng)
        DO i=Istr,Iend
            susmud(i,k,ised)=MAX(t(i,j,k,nstp,indx),0.0_r8)
        END DO
    END DO
!
! min concentration below which flocculation processes are not calculated
!
! f_clim=0.001_r8
exp1 = 3.0_r8+gls_p(ng)/gls_n(ng)
exp2 = 1.5_r8+gls_m(ng)/gls_n(ng)
exp3 = -1.0_r8/gls_n(ng)
DO i=Istr,Iend
DO k=1,N(ng)

   f_dt=dt(ng)
   dttemp=0.0_r8

   ! concentration of all mud classes in one grid cell
   cvtotmud=0.0_r8
   DO ised=1,NC
      cv_tmp(ised)=susmud(i,k,ised)
      cvtotmud=cvtotmud+cv_tmp(ised)
   ENDDO

   NNin(ised)=cv_tmp(ised)/f_mass(ised)
ENDDO

DO iv1=1,NCS
   IF (NNin(iv1).lt.0.0_r8) THEN
      WRITE(*,*) '***************************************'
      WRITE(*,*) 'CAUTION, negative mass at cell i,j,k :', i,j,k
      WRITE(*,*) '***************************************'
   ENDIF
ENDDO

IF (cvtotmud .gt. f_clim) THEN

   # if defined FLOC_TURB_DISS && !defined FLOC_BBL_DISS
   #ALA dissipation from turbulence closure
   
   IF (k.eq.1) THEN
      tke_av = tke(i,j,k-1,nnew)
      gls_av = gls(i,j,k-1,nnew)
   ELSEIF (k.eq.N(ng)) THEN
      tke_av = tke(i,j,k,nnew)
      gls_av = gls(i,j,k,nnew)
   ELSE
      tke_av = 0.5_r8*(tke(i,j,k-1,nnew)+tke(i,j,k,nnew))
      gls_av = 0.5_r8*(gls(i,j,k-1,nnew)+gls(i,j,k,nnew))
   ENDIF

   ! exp1 = 3.0_r8+gls_p(ng)/gls_n(ng)
   ! exp2 = 1.5_r8+gls_m(ng)/gls_n(ng)
   ! exp3 = -1.0_r8/gls_n(ng)
   
   diss = gls_cmu0(ng)**exp1*tke_av**exp2*gls_av**exp3

   # elif defined FLOC_BBL_DISS && !defined FLOC_TURB_DISS
   
   #ALA dissipation from wavecurrent bottom stress
   
   ! NOT READY FOR PRIME TIME
   ! NEEDS VERTICAL DISTRIBUTION
   ! As first cut, use turbulence closure
   
   IF (k.eq.1) THEN
      tke_av = tke(i,j,k-1,nnew)
      gls_av = gls(i,j,k-1,nnew)
   ENDIF

END
ELSEIF (k.eq.N(ng)) THEN
  tke_av = tke(i,j,k,nnew)
  gls_av = gls(i,j,k,nnew)
ELSE
  tke_av = 0.5_r8*tke(i,j,k-1,nnew) +
& 0.5_r8*tke(i,j,k,nnew)
  gls_av = 0.5_r8*gls(i,j,k-1,nnew) +
& 0.5_r8*gls(i,j,k,nnew)
ENDIF

! MODIFIES THE BOTTOM LAYER TO INCLUDE WAVECURRENT STRESS
!
IF (k.eq.1) THEN
  # ifdef BBL_MODEL
  ustr2 = sqrt((bustrcwmax(i,j)**2.0_r8 +
& bvstrcwmax(i,j)**2.0_r8))
  effecz = (ustr2**0.5_r8)*Pwave_bot(i,j)*0.5_r8/pi
  diss = MAX((ustr2**(1.5_r8))/(vonKar*effecz),diss)
  # else
  ustr2 = sqrt((bustr(i,j)**2.0_r8 + bvstr(i,j)**2.0_r8))
  diss = MAX((ustr2**(1.5_r8))/(vonKar*(z_r(i,j,1)-zw(i,j,0))),diss)
  # endif
ENDIF

# ifdef BBL_MODEL
  ENDIF
# else
  diss = epsilon8
  IF (l_testcase) THEN
    IF (j.eq.1.and.i.eq.1.and.k.eq.1) then
      WRITE(*,*) 'VERNEY ET AL TESTCASE FOR FLOCS'
    endif
  ELSE
    WRITE(*,*) 'CAUTION :'
    WRITE(*,*) 'CHOOSE A DISSIPATION MODEL FOR FLOCS'
    WRITE(*,*) 'SIMULATION STOPPED'
    STOP
  ENDIF
# endif

CALL flocmod_comp_g(k,i,j,Gval,diss,ng)

DO WHILE (dttemp .le. dt(ng))
  CALL flocmod_comp_fsd(NNin,NNout,Gval,f_dt,ng)
  CALL flocmod_mass_control(NNout,mneg,ng)
  IF (mneg .gt. f_mneg_param) THEN
    DO WHILE (mneg .gt. f_mneg_param)
      f_dt=MIN(f_dt/2.0_r8,dt(ng)-dttemp)
      IF (f_dt.lt.epsilon8) THEN
        CALL flocmod_mass_redistribute(NNin,ng)
        dttemp=dt(ng)
        exit
      ENDIF
    CALL flocmod_comp_fsd(NNin,NNout,Gval,f_dt,ng)
  ENDIF
CALL flocmod_mass_control(NNout,mneg,ng)
ENDDO
ELSE
IF (f_dt.lt.dt(ng)) THEN
DO while (mneg .lt.f_mneg_param)
IF (dttemp+f_dt .eq. dt(ng)) THEN
CALL flocmod_comp_fsd(NNin,NNout,Gval,f_dt,ng)
exit
ELSE
dt1=f_dt
f_dt=MIN(2.0_r8*f_dt,dt(ng)-dttemp)
CALL flocmod_comp_fsd(NNin,NNout,Gval,f_dt,ng)
CALL flocmod_mass_control(NNout,mneg,ng)
IF (mneg .gt. f_mneg_param) THEN
f_dt=dt1
CALL flocmod_comp_fsd(NNin,NNout,Gval,f_dt,ng)
exit
ENDIF
ENDIF
ENDIF
ENDIF
ENDIF
ENDIF
ENDDO
ENDIF
ENDIF
dttemp=dttemp+f_dt
NNin(:)=NNout(:) ! up date new Floc size distribution
! redistribute negative masses IF any on positive classes,
! depends on f_mneg_param
CALL flocmod_mass_redistribute(NNin,ng)
IF (dttemp.eq.dt(ng)) exit
ENDDO ! loop on full dt
ENDIF ! only if cvtotmud > f_clim
!
! update mass concentration for all mud classes
DO ised=1,NCS
susmud(i,k,ised)=NNin(ised)*f_mass(ised)
ENDDO
ENDDO
ENDDO
!
! Update global tracer variables.
!
!-------------------------------------------------------------
!
DO ised=1,NCS
indx = ised
DO k=1,N(ng)
DO i=1str,1end
fm_tmp=t(i,j,k,nnew,indx)
t(i,j,k,nnew,indx)=susmud(i,k,ised)*Hz(i,j,k)
flocmass drnt 10-8-19

floc_mass(i,j,k,ised)=t(i,j,k,nnew,indx)-fm_tmp

! if floc_mass > 0 then t(new)>t(old) so flocillation added mass to that size class
! if floc_mass < 0 then the opposite occurred
ENDDO
ENDDO

END DO J_LOOP

! exchange
IF (EWperiodic(ng).or.NSperiodic(ng)) THEN
DO itrc=1,NCS
    CALL exchange_r3d_tile (ng, tile,
& LBi, UBi, LBj, UBj, 1, N(ng),
& floc_mass(:,:,,:,itrc))
END DO
END IF

! boundary condition
DO itrc=1,NCS
    CALL bc_r3d_tile (ng, tile,
& LBi, UBi, LBj, UBj, 1, N(ng),
& floc_mass(:,:,,:,itrc))
END DO

! distribute
# ifdef DISTRIBUTE
    CALL mp_exchange4d (ng, tile, iNLM, 1,
& LBi, UBi, LBj, UBj, 1, N(ng), 1, NCS,
& NghostPoints,
& EWperiodic(ng), NSperiodic(ng),
& floc_mass)
# endif
RETURN

! WRITE(*,*) 'END flocmod_main'
END SUBROUTINE sed_flocmod_tile

# endif

! END MODULE sed_flocs_mod
Flocculation in a Muddy Estuary: Parameterization of a Flocculation Model, and Application over a Spring-Neap Cycle in the York River Estuary
Chapter 4: Flocculation in a Muddy Estuary: Parameterization of a Flocculation Model, and Application over a Spring-Neap Cycle in the York River Estuary

Abstract

The York River estuary is dominated by fine-grained sediment, clays and silts, as are many other relatively low energy, partially mixed estuaries. In muddy estuarine environments, suspended sediment concentrations are influenced by the local hydrodynamics and by sediment characteristics such as particle size, density, and settling velocity. However, characterizing suspended muddy sediments is complicated since mud tends to be transported as aggregated particles (flocs) due to its cohesive nature. Therefore, numerical methods used to represent flocculation dynamics of cohesive sediment can also be complex and require multiple parameters. In this study, a one-dimensional (vertical) water column model was developed within the Coupled Ocean-Atmosphere-Wave-Sediment Transport (COAWST) modeling system to simulate the conditions for the middle reaches of the York River estuary, Virginia. The model represented suspended sediment dynamics, and flocculation processes were simulated using FLOCMOD. The sensitivities of the suspended sediment concentration (SSC) and floc size distribution to three parameters (i.e. fractal dimension, collision efficiency, and breakup efficiency) were examined. SSC was especially sensitive to parameterization in regions of higher concentrations such as the bottom meter of the water column. The median floc size was less sensitive and the width (spread) of the distribution was most sensitive to variability in the fractal dimension. Observations of SSC and floc size distributions were used to select the set of parameters that best represented the
sediment characteristics in the York. After parameterization, the one-dimensional model was used to simulate variability in sediment dynamics over a spring-neap cycle for the York River estuary site. Parameterizing FLOCMOD was challenging, however, and no single combination of parameters produced the best fit for both the SSC and floc size distribution. Therefore, the set of parameters that had a low average error for SSC, with reasonable error for the distribution mode and spread were chosen. The model was able to capture variability in SSC, floc distribution, and the sediment bed over the full spring-neap cycle. In the transition from spring to neap, the adjustment to reduced flow and increased stratification was quickest in the surface waters, followed by the very near-bed; whereas the lower water column (~1 meter above the bed) required more time to adjust. The effect of flocculation on mass concentration across multiple floc size classes was also compared to the effects of other transport mechanisms. In general, vertical diffusion, settling, and erosion affected floc mass exchange more strongly than flocculation. However, changes in floc size indicated that flocculation still played a key role in vertical sediment distribution and the size distribution of flocs.

1 Introduction

1.1 Background

Estuaries are complex environments that connect freshwater systems to the ocean, and as such exhibit substantial spatial gradients in salinity, temperature, suspended sediment concentrations (SSC), and biological activity. Due to its connection to both riverine and oceanic systems, the local hydrodynamics and SSC in an estuary are impacted by freshwater discharge in addition to tides, density and pressure gradients,
and wind waves. Therefore, vertical stratification, currents, and turbulent mixing can fluctuate over a variety of time scales from seconds (waves), to hours (flood-ebb flow), to days or weeks (spring-neap cycle), to seasons (discharge). Specifically, during the spring-neap cycle, the tidal amplitudes are greatest during spring tide leading to faster currents that enhance mixing and reduce vertical gradients in temperature, salinity, and SSC. In contrast, tidal amplitudes are smallest during neap tides that usually generate tidal velocities and mixing that are reduced during neap tides and can lead to differences in the size of sediment in suspension during neap tide in comparison to spring tide. However, modifications to this general trend may occur due to elevated river discharge, along estuary winds (Sharples et al. 1994; Scully et al. 2005), tidal straining (MacCready and Geyer 2010; Figueroa et al. 2019), or storm events (Brasseur et al. 2005; Ralston et al. 2013). This variability in the hydrodynamics affects the SSC and additionally, sediment characteristics in muddy estuaries.

Sediment in muddy estuaries is often transported in the form of flocs, aggregated particles, due to the cohesive nature of clay and silt particles, and these flocs exhibit a wide range of size, density, and settling velocity (Dyer 1989; Mehta 1989). The growth and breakup of flocs are influenced by SSC, salinity, turbulence, and the concentration of biological secretions such as exopolymeric (EPS) substances (Manning and Dyer 2002; Shen, Toorman, et al. 2018). Salinity >0.6-2.6 (McAnally and Mehta 2001) and elevated SSC, and EPS promote the aggregation or growth of flocs (Dyer 1989; Mehta 1989; van Leusen 1994; Droppo et al. 1997). However, while lower levels of turbulence promote the growth of floc size via aggregation, high shear rates and turbulence stimulate
disaggregation via the breakup of flocs (Winterwerp 1998; Fugate and Friedrichs 2003). The amount of turbulence needed to begin to tear flocs apart varies with the strength of the floc, which is influenced by the mineralogical and biological composition (Burd and Jackson 2009; Cross et al. 2013; Fettweis et al. 2014). Conditions that promote aggregation cause floc size to grow, which tends to increase their settling velocity; while disaggregation creates smaller diameter flocs with slower settling velocities (Dyer and Manning 1999; Droppo et al. 2000; Fall 2020). Additionally, observational evidence indicates that larger flocs tend to have decreased density compared to smaller flocs (Dyer and Manning 1999; Droppo et al. 2000; Fall 2020). Flocs with higher settling velocities are more likely to settle out of the water column to the sediment, which reduces SSC and the net transport of sediment (Dyer 1989; Mcanally and Mehta 2002). Therefore, as the local hydrodynamics vary in muddy systems, floc characteristics vary, which greatly impacts the net transport of sediment.

Models developed for muddy estuaries use a variety of methods to account for the variability in floc size. Some models use an average or bulk settling velocity with one or more sediment classes (Hill and McCave 2001; Ralston et al. 2012; Fall et al. 2014; Moriarty et al. 2014). Others track changes in the floc distribution by allowing exchange between multiple sediment classes that have a range in settling velocities (Maerz et al. 2011; Lee et al. 2012; Burd 2013; Shen and Maa 2016). Several models that account for the dynamic changes in flocculation by tracking the shift in the distribution are based on population balance equations (Xu et al. 2008; Verney et al. 2011; Shen and Maa 2015; Shen et al. 2018). One trade-off with using a more dynamic representation is that with
complexity often comes an increase in the number of numerical parameters that need to be specified for the model. For example, for a population balance flocculation model requires specification of a range of floc sizes, characteristics for each floc size (diameter, settling velocity, density), as well as parameters for the flocculation equations (described below). For flocculation, these parameters are often poorly constrained, with wide ranges reported in the literature (Dyer and Manning 1999; Fettweis 2008; Maerz et al. 2011; Mietta et al. 2011; Chapalain et al. 2018). Ideally, observations are available to help constrain the parameters, but these are often limited to small time- and space-scales, and not directly measured (Dyer and Manning 1999; Fugate and Friedrichs 2002; Cartwright et al. 2011; Manning and Schoellhamer 2013; Guo et al. 2017; Chapalain et al. 2018; Fall 2020).

The Coupled Ocean-Atmosphere-Waves-Sediment Transport (COAWST) modeling system now includes a population balance flocculation model, FLOCMOD, which uses the fractal dimension ($n_f$), collision efficiency ($\alpha$), and breakup efficiency ($\beta$) to describe the aggregation and disaggregation of flocs (Verney et al. 2011; Sherwood et al. 2018). Theoretically, $n_f$ has a range from 1-3, and $\alpha$ and $\beta$ have ranges from 0-1. Generally, the fractal dimension quantifies the shape and packing efficiency of a floc, with values near 3 indicating tightly packed spherically shaped flocs, and near 1 loosely bound and fragile flocs (Kranenburg 1994; Winterwerp 1998; Thomas et al. 1999). Observed values for $n_f$ range from 1.2-1.3 for freshwater flocs (de Boer et al. 2000), and in saline waters some studies reported a range of 1-3 (Dyer and Manning 1999) while others reported average values 2.0-2.5 (Kranenburg 1994; Chapalain et al. 2018; Fall 2020). However, numerical
studies often use \( n_f \) between 2.0-2.3 (Winterwerp 1998; Mietta et al. 2011; Shen et al. 2018; Sherwood et al. 2018). Reported values for \( \alpha \) based on observations range from 0.1-0.8 (Dam and Drapeau 1995), while numerical studies have used values 0.1-0.45 (Maerz et al. 2011; Verney et al. 2011; Shen et al. 2018; Sherwood et al. 2018). Little guidance is available for FLOCMOD’s breakup efficiency parameter, \( \beta \), since other models use a different representation for the disaggregation of flocs (Winterwerp 1998; Maerz et al. 2011; Mietta et al. 2011; Chai et al. 2018). In past studies that used FLOCMOD, \( \beta \) ranged from 0.05-0.34 (Verney et al. 2011; Sherwood et al. 2018).

Therefore, as shown by these examples the parameterization of flocculation models has been challenging. Laboratory studies are often used to parameterization flocculation models (Winterwerp 1998; Xu et al. 2008; Mietta et al. 2011; Verney et al. 2011; Keyvani and Strom 2014; Shen and Maa 2015; Chai et al. 2018; Sherwood et al. 2018), and fewer studies apply population based flocculation model to field site observations (Khelifa and Hill 2006; Son and Hsu 2011; Lee et al. 2014; Xu and Dong 2017; Shen et al. 2018). Ideally, choice of the flocculation parameters would be guided from observations of SSC and floc size distributions. In this study, observations from a muddy estuary, the York River, Virginia, were used to explore parameterizations for the flocculation model, FLOCMOD.

1.2 Site Description – York River Estuary

The York River estuary is a micro-tidal, partially-mixed estuary that is ~50 km in length extending from the confluence of the Pamunkey and Mattaponi Rivers to the Chesapeake Bay, VA, USA (Friedrichs 2009; Figure 4.1). Tidal currents approach 1 m s\(^{-1}\) in
the surface during spring tide, and flow is predominantly along the major axis of the estuary. In the middle reaches of the York, the estuary transitions from being more well-mixed to partially-mixed. Additionally, stratification in the middle reaches increase under elevated river discharges that typically occur during the spring season (Scully et al. 2005). A rapid change in the bathymetry occurs near Claybank, in the middle region of the York, and when the stratification is enhance with increased river discharge a convergence zone forms that traps sediment producing a secondary turbidity maximum (STM; Lin and Kuo 2001), as also seen in the Hudson River (Ralston et al. 2012). The ephemeral nature of the STM has made the Claybank region of the York River estuary an area of interest, and has long been an the area of focus for field observations (Sharples et al. 1994; Dellapenna et al. 1998; Friedrichs et al. 2008; Cartwright et al. 2009; Dickhudt et al. 2009; Ha et al. 2011; Rodríguez-Calderón and Kuehl 2013; Fall 2020). Fixed instrumentation was deployed in this region since 2006 through June of 2017. Specifically, data used in this study was from instrumentation deployed May 31 or June 1 of 2016 and retrieved July 27, 2016. The specific instrumentation from the 2016 deployment used for this study is described in Sections 2.1 and 2.2.

1.3 Objectives and outline

The objectives of this study were to examine the sensitivity of a population-based flocculation model, FLOCMOD, to variability in the fractal dimension \((n_f)\), collision efficiency \((\alpha)\), and breakup efficiency \((\beta)\), and use observed SSC and sediment size distributions to determine the values for \(n_f\), \(\alpha\), and \(\beta\) that best represented the sediment characteristics in the York River estuary. Using the best-fit parameters to characterize
the flocs, the study then examined the roles of flocculation and other transport mechanisms on temporal changes in SSC over a spring-neap cycle in the York River estuary. To these ends, this study addressed the following questions:

a) What is the sensitivity of the SSC, floc size distribution and median floc size to variability in the parameters ($n_f$, $\alpha$, and $\theta$) used for the flocculation routine?

b) What flocculation parameterization best represents suspended sediment concentrations and size distributions in the middle reaches of the York River estuary?

c) What processes are important for suspended sediment dynamics in the York River estuary during a spring-neap cycle? Specifically, how do transport terms (vertical diffusion, settling, erosion, and vertical advection) and flocculation impact vertical distribution of suspended sediment over the spring-neap cycle?

A one-dimensional (vertical) model was designed to represent the water column structure (salinity, temperature, and velocity) conditions for the middle reaches of the York River estuary. The sensitivity of modeled SSC and floc size distributions were investigated through a sensitivity study, and flocculation model parameters were chosen to represent the York River site sediment characteristics. Then, the model was run for a spring-neap cycle to evaluate the role of transport processes and flocculation in the vertical distribution of sediment. Unlike the idealized two-dimensional model used in Chapters 2 and 3, the results from this one-dimensional implementation can be directly compared to observations facilitating the parameterization of FLOCMOD to
represent the floc population in the middle reaches of the York River estuary.

Additionally, the model in this study was used to examine the temporal variability in flocculation dynamics in the estuary, specifically, over timescales encompassing the flood-ebb to the spring-neap tidal cycles. The observations used in the model setup and parameterization, the sensitivity of the SSC and floc distribution, the results of the parameterization, and a summary of the findings are provided in Section 2. The application of the one-dimensional model for a spring-neap cycle, results, and discussion are provided in Section 3. Lastly, the conclusions of the study are presented in Section 4.

2 Model Sensitivity and Parameterization for Observed York River Estuary Flocs

2.1 Observations used for model implementation and parameterization

The VIMS Coastal Hydrodynamics and Sediment Dynamics (CHSD) laboratory deployed instrumentation fixed to a piling and benthic platforms in the Claybank region (~30 km upriver of the mouth) of the York River estuary (Figure 4.1). The benthic instrumentation included an upward-looking Nortek Acoustic Wave and Current (AWAC) profiler and a tripod-mounted SonTek Acoustic Doppler Velocimeter (ADV). On the piling were four HOBO Conductivity and Temperature (CT) probes. The AWAC was deployed at 37°20'35.9” N and 76°37'35.7” W (Figure 4.1) and sampled every 15 minutes for 5 minutes at a 2 Hz frequency. The first bin in the AWAC profile was centered at ~90 cmab, and the centers of additional bins in the profile were spaced 25 cm apart. The CT probes were deployed on the piling at 37°20'35.1” N and 76°37'32.5” W at 120, 218, 308, and 405 cmab and sampled every 15 minutes. The tripod ADV was deployed at 37°20'34.3” N and 76°37'32.5” W at 53 cmab. The ADV was mounted in a
downward looking orientation and sampled every 15 minutes for 1.67 minutes at a 10 Hz frequency. The data from the AWAC and CT probes were used to implement a one-dimensional (vertical) model representation of the York River estuary, as described below in Section 2.4.

The CHSD’s profiling system was used to collect total suspended solids (TSS) and sediment size distributions at three depths in the water column over a 6-hour period from near slack before flood to near peak flood flow on June 7, 2016 in the Claybank region. The system was deployed off of a vessel that was allowed to swing on anchor. The samples were collected at approximately at 37°20.6’ N and 76°37.7’ W. The instrumentation and sampling gear on the profiling system included: a Sequoia Scientific Laser In-Situ Scattering and Transmissometry instrument Type C (LISST-100X), a high-definition Particle Imaging Camera System (PICS), a YSI6600 Conductivity, Temperature and Depth sensor (CTD), and a high-speed pump sampler with an intake hose at roughly the same height on the frame as the sample location for the LISST-100X. The sampling location for the LISST-100X and the PICS were close enough to assume the two instruments were sampling the same sediment particle population. The suite of instrumentation was lowered to each depth, was held there, and sampled for 2-3 minutes -- see Table 4.1 for sample times and relative depths (z/h). Pump samples were collected in 1-liter, dark plastic bottles, held on ice, and filtered for TSS upon returning to the laboratory. Vacuum filtering was used with a pre-weighted, 0.7 μm, 47 mm diameter glass fiber filter. The filters were rinsed with deionized water for salt removal, and then oven-dried for at least 24 hours at 103-105°C. The filters were weighed, dried,
and re-weighed until the consecutive weights were within 0.5 mg of each other to quantify the TSS (TSS will be referred to as SSC moving forward as these observations will be compared with the modeled SSC with the same units of mg L\(^{-1}\)). Note that the surface SSC sample from profile 2, later referred to as sample 2 was an outlier and removed from the analysis.

The LISST-100X has the capability to resolve diameters from 2.5-500 μm, while the PICS resolves particles whose diameters range from 30-1000 μm. LISST-100X data were processed assuming the particles had a random shape (Agrawal et al. 2008), and the volume fraction was averaged for the 2-3 minute time period at each depth. The volume fraction distributions from the two instruments were merged following procedures developed by Fall (2020). The \(D_{30}, D_{50},\) and \(D_{70}\) by volume were defined as the diameters at which 30%, 50%, or 70%, respectively, of the volume concentration had a diameter smaller or equal to that value. These characteristic diameters were calculated for the merged distributions and used to quantify the distribution’s dimensionless spread \(((D_{70}-D_{30})/D_{50})\). The distribution spread indicates how well “sorted” the floc population is, with large values indicating that the floc size distribution is spread across a wider range of floc sizes.

The distribution spread, mode, and the SSC were used to quantify the best-fit parameters for the flocculation model, FLOCMOD, when applied to the York River estuary suspended sediment. The relative error was used to compare the observations to the model results (Equation 4.1). The relative difference was used to choose between sets of parameters that produced similar relative error values (Equation 4.2).
**Equation 4.1:** \( \text{Rel. Error} = \frac{(\text{Model Value} - \text{Observation Value})}{0.5 \times (\text{Model Value} + \text{Observation Value})} \)

**Equation 4.2:** \( \text{Rel. Difference} = \frac{(\text{Model Value} - \text{Observation Value})}{\text{Observation Value}} \)

Relative error ranges between -2 and 2, where negative values indicate the model value was less than the observed (for -2 model << observed), positive values indicate the model value was greater than the observed (for +2 model >> observed), and values near zero indicate the model value was approximately equal to the observed.

### 2.2 Model Configuration

The quasi one-dimension model was developed within the Coupled Ocean-Atmosphere-Wave-Sediment transport (COAWST) modeling system, which uses the Regional Ocean Modeling System (ROMS) and the Community Sediment Transport Modeling System (CSTMS) to represent the hydrodynamics and sediment transport, respectively. The model setup was modified from the sed_floc_toy configuration that was distributed with the COAWST 3.5 version. The grid was a horizontally-uniform, 6x5 rectangular grid that is 40 m wide in the x-direction and 30 m wide in the y-direction. The water column was 5 m deep, partitioned into 40 vertical layers with a vertical resolution that ranged from 0.053-0.17 m (Figure 4.2). The stretching function used for the vertical grid (defined by a Vstretching of 3) had higher resolution near both the water surface and the sediment bed interface, and used a surface \( \theta_S \) of 2 and a bottom \( \theta_B \) of 4. The horizontal open boundary conditions were periodic in both the x- and y-directions. The advection schemes used were: MPDATA (Multi-Dimensional Positive-Definite Advection Transport Algorithm) for tracers (Smolarkiewicz and Margolin 1998);
third-order upstream bias and fourth-order centered for horizontal two-dimensional (depth-averaged velocity) and three-dimensional momentum (depth-resolved horizontal velocity), respectively; and fourth-order centered for vertical momentum (vertical velocity). The model time step was 2 seconds; this was needed to stabilize the momentum when nudging toward velocity observations for the two- and three-dimensional momentum. We used the $k$-$\Omega$ turbulence closure model (Warner et al. 2005) and the logarithmic drag formulation with a constant hydraulic bottom roughness ($z_{0b} = 5 \times 10^{-7}$ m). The hydraulic bottom roughness was adjusted until the modeled applied bed shear stress compared well with estimates from the tripod ADV.

The sediment dynamics were modeled using the cohesive sediment routines in COAWST that represent flocculation dynamics, bed consolidation/swelling, and sediment-density stratification (Sherwood et al. 2018). The bed consolidation/swelling routine estimates the effective instantaneous critical shear stress as a function of depth into the bed. This is adjusted to account for erosion and deposition, and also nudged over a defined timescale toward a user-defined equilibrium profile for the critical shear stress for erosion (Rinehimer et al. 2008; Sanford 2008; Tarpley et al. 2019). The SSC was included in the equation of state’s water density calculation (Shchepeletkin and McWilliams 2011) to account for the role that sediment-density gradients play in stratifying the water column (Warner et al. 2008). The population balance model, FLOCMOD, was used to represent aggregation and disaggregation (Verney et al. 2011). The sediment floc sizes were represented using 11 classes with diameters logarithmically spaced between 1–1024 μm, and settling velocities were calculated
using a modified Stoke’s equation (Equation 4.3; Winterwerp 1998). The floc densities were calculated following Equation 4.4 assuming a constant fractal dimension (Winterwerp 1998).

**Equation 4.3:** \[ w_{s,i} = \frac{g(\rho_{f,i} - \rho_w)D_{f,i}^2}{\rho_w \cdot \nu} \]

**Equation 4.4:** \[ \rho_{f,i} = \rho_w + (\rho_p - \rho_w) \left( \frac{D_p}{D_{f,i}} \right)^3 - n_f \]

where \( \rho_w \) is the water density, \( \rho_p \) is the primary particle density, \( D_p \) is the primary particle diameter, \( D_{f,i} \) is the diameter of floc size class \( i \), \( n_f \) is the fractal dimension, \( g \) is the acceleration due to gravity, and \( \nu \) is the kinematic viscosity.

**2.3 Model Implementation**

A 30-day spin-up run with idealized flow velocity, temperature, and salinity was generated to allow the sediment bed characteristics and SSC to adjust to tidal conditions. The initial SSC was zero for all floc sizes. The sediment bed was divided into 10 layers and was initialized as follows: the top 9 layers were each 0.01 m thick, the bottom layer was 0.91 m thick, and the mass fraction in the bed was the same for all floc sizes. For use during model spin-up, the velocity profile near slack before flood at 5:00am on June 7, 2016 was scaled-up using a sine curve with a 12-hour frequency to produce an idealized, tidally-varying velocity field with velocity magnitudes ranging from 0-0.94 m s\(^{-1}\). The temperature and salinity profiles for slack before flood (5:00am on June 7, 2016) were scaled by a similar sine curve to produce the idealized tracer fields for spin-up with ranges between 24.1-25.1 °C and 9.9-15.4 g kg\(^{-1}\) for temperature and
salinity, respectively. The sediment bed and SSC for all of the sensitivity runs were initialized with output for the final slack before flood flow near the end of the 30-day spin-up run.

The simulations for the sensitivity and parameterization of FLOCMOD were for a 30-hour period starting at slack before flood flow on June 7, 2016, and used the observations described in Section 2.1 to derive salinity, temperature, and along-estuary velocity profiles for every half-hour during the modeled period (Figure 4.2). The measured values sampled the water column from ~1 to 4.8 mab for the velocity and ~1.2 to 4 mab for the temperature and salinity. These were interpolated to the model grid points, which spanned from 0.03 m below the surface to 0.03 mab above the sediment bed. The along-channel velocity profiles from the AWAC were smoothed by fitting a linear curve to the data if the depth-averaged velocity was less than 0.55 m s\(^{-1}\) and by fitting a quadratic polynomial for profiles with a faster depth-averaged velocity. Using the smoothed curve and the assumption that the along-estuary velocity was equal to zero at 5×10\(^{-5}\) mab (the assumed hydraulic bottom roughness), the velocity was interpolated to the model vertical grid points.

The timeseries for the temperature and salinity from the four CT probes were smoothed to remove spikes in the data. In some instances, the observed salinity and temperature profiles were problematic, signaling potential errors in the measurements. For example, salinity might decrease or temperature might increase in the near-bed measurements. These were adjusted in these cases by setting the near-bed values equal to the measurements made directly above them. Since the CT probes did not span the
entire water column, the lowest and highest measurements were extrapolated as follows. For a near-bed value at z=5x10^{-5} mab, the temperature and salinity were assumed equal to the value measured by the lowest CT probe. For a surface value some stratification was assumed, based on comparing the average differences between the data from the CT probes closest to the surface of the water column to four profiles from a YSI Castaway CTD collected on June 7, 2016. Specifically, surface salinity was assumed to be 2.4 g kg\(^{-1}\) less than the value measured at the highest CT probe, and the temperature was assumed to be 0.2°C warmer than the value from the uppermost CT probe. A linear curve was fit for temperature and salinity for the near-bed through to the surface most CT probe, and a piece-wise cubic interpolation was fit between the data from the near surface probe to the assumed value for the surface salinity and temperature. Lastly, these fits for temperature and salinity were interpolated to the vertical grid of the model to obtain the forcing profiles for salinity and temperature.

As the model ran, the calculated velocity, salinity and temperature were nudged to the profiles interpolated from the data at nudging timescales of 5 and 10 minutes for the velocity, and salinity and temperature tracers, respectively. In this manner, a one-dimensional (vertical) model was developed with conditions that approximately represented the temperature, salinity, and velocity profiles that were measured at the Claybank site during the field deployment for the 30-hour period of interest.

A set of model runs with a range in parameter values that affect the results of FLOCMOD were explored to examine the flocculation model’s sensitivity and to choose flocculation parameters that represent sediment characteristics in the York River.
estuary. Specifically, FLOCMOD's fractal dimension ($n_f$), collision efficiency ($\alpha$), and breakup efficiency ($\beta$) were varied. The fractal dimensions ranged from 2.0-2.5 at increments of 0.1, $\alpha$ ranged from 0.1-0.5 at increments of 0.1, and $\beta$ ranged from 0.01-0.2 (0.01, 0.05, 0.1, 0.15, 0.2). Every combination of parameters in these ranges was examined, leading to a total of 150 individual model runs. Additional values for $\alpha$ and $\beta$ were explored when the results indicated an intermediate or higher value would better represent the sediment dynamics in the York. The floc density and settling velocity were adjusted following Equations 4.3 and 4.4 to maintain consistency with the $n_f$ used in each run. Table 4.2 shows the settling velocity of the 11 floc size classes with all 6 $n_f$'s explored in the sensitivity runs.

2.4 Sensitivity and Parameterization Results

Sensitivity tests showed that SSC, $D_{50}$, and the distribution spread varied over wide ranges in response to changes in $n_f$, $\alpha$, and $\beta$. Specifically, the SSC increased with decreasing $n_f$ and $\alpha$, and with increasing $\beta$ (Figure 4.3a,b), while the $D_{50}$ increased with increasing $\alpha$, and decreasing $n_f$ and $\beta$ (Figure 4.3c). In general, the range in the predicted SSC due to changes in the FLOCMOD parameters was smaller in the surface meter of the water column where SSC, $D_{50}$, and shear rates were typically lower, than in the bottom meter (Figure 4.3a,b). For example, the difference in the SSC for a run with $n_f=2.5$, $\alpha=0.1$, $\beta=0.01$ compared to a run with $n_f=2.5$, $\alpha=0.1$, $\beta=0.2$ was ~30 mg L$^{-1}$ in the surface and ~100 mg L$^{-1}$ in the bottom. However, the trends in the effects of varying the $n_f$, $\alpha$, or $\beta$ were the similar in the surface and bottom with one exception; at higher values of $\alpha$, changes to $n_f$ and $\beta$ had a smaller effect on the SSC in the surface waters (Figure 4.3a).
The model runs that had the lowest SSC had the largest $D_{50}$ in the bottom meter (Figure 4.3b,c). The distribution spread, which represented the variance around the mode of the floc size distribution, generally had values between 0.7 and 1 (Figure 4.3d). The spread was most sensitive to $n_f$ and $\theta$ for low values of $\alpha$ and became less sensitive to $n_f$ and $\theta$ as $\alpha$ increased (Figure 4.3d). At higher values of $\alpha$, the distribution spread was highest for intermediate values of $n_f$ and was relatively insensitive to $\theta$ (Figure 4.3d).

Following examination of the sensitivity, the results from these 150 model runs were compared to observed values to select the parameter values that provided the best representation of the floc characteristics for the York River estuary. To evaluate goodness of fit, we looked at the relative error (Equation 4.1) for several metrics: $D_{30}$, $D_{50}$, $D_{70}$, the distribution mode and spread, SSC, and the slope between the surface two and bottom two SSC samples. Of these, we found the SSC and the distribution mode and spread (Figure 4.4) to be most useful, and these three metrics were therefore used to select the best-fit parameters to represent the York River estuary. The relative difference (Equation 4.2) for the SSC was also examined (not shown).

Relative errors ranged from as low as 0.15, to as high as 1.5, and no single set of model parameters produced consistently lower relative error for all the three metrics considered (Figure 4.4). Several model runs with $n_f=2.1$ produced relatively low relative errors for the distribution spread, and in general the relative error for distribution spread increased with $n_f$ (Figure 4.4a). The model with $n_f=2.1$, $\alpha=0.3$, and $\theta=0.2$, “Case 1” was used to represent this subset of runs in additional analysis below. For the distribution mode, the model with $n_f=2.2$, $\alpha=0.2$, and $\theta=0.15$ had the lowest average
relative error, “Case 2”, but for most values of $\alpha$, relative error decreased with $n_f$ (Figure 4.4b). For SSC, model runs with $\theta=0.2$ produced the lowest relative error on average (Figure 4.4c). Models with $\alpha=0.1$ and $\theta=0.05$, and $\alpha=0.4$ and $\theta=0.2$ had the lowest average relative difference for SSC (not shown), but the runs with $\alpha=0.1$ and $\theta=0.05$ did not represent the size distribution (mode and spread) as well. Thus, models with $\alpha=0.4$ and $\theta=0.2$ were of interest, and those with $n_f=2.4$ had a low relative error for the SSC and size (mode). However, the model with $n_f=2.4$, $\alpha=0.3$, and $\theta=0.2$ had a lower average relative error for the size distribution spread. These two sets of parameters used the same $n_f$ (2.4) and $\theta$ (0.2), and only differed in $\alpha$ (either 0.3 or 0.4). Therefore, a model using the average of these values ($\alpha=0.35$), with $n_f=2.4$ and $\theta=0.2$ was run. It produced intermediate average relative errors for the SSC, size distribution mode, and spread (Figure 4.4; larger light green star). Thus, $n_f=2.4$, $\alpha=0.35$, and $\theta=0.2$ were the set of parameters chosen to best represent the York River estuary sediment distribution and will be referred to as the “reference run”. Note that this parameter selection used the relative errors averaged over all water depths (surface to bottom), in an effort to choose FLOCMOD parameters that performed adequately throughout the water column.

The above calculations considered relative error averaged over the full water column, but we also evaluated the model skill for surface samples only with the range of model parameters considered. The set of parameters chosen for the water column had relative errors from 0.21 to 0.6 for the surface samples (green stars in Figure 4.4d-f), but other sets of parameters produced lower relative errors for these samples. For example, the model run that used $n_f=2.3$, $\alpha=0.1$, and $\theta=0.05$ had the lowest average relative error.
for the surface SSC and distribution mode. While this model did not produce the lowest average relative error for the distribution spread in the surface water, model runs with lower relative error for the distribution spread produced much higher errors for SSC and mode than the run with $n_f=2.3$, $\alpha=0.1$, and $\beta=0.05$. Therefore, the model with $n_f=2.3$, $\alpha=0.1$, and $\beta=0.05$ was considered a better representation of flocs in the surface water of the York River estuary and will be designated “Case 3” (Table 4.3).

The relative error between modeled and observed for the reference run was compared to relative errors from other model runs that also used $n_f=2.4$ (Figure 4.5). The relative error for SSC samples for these select model runs showed, that when averaged over the water column, the mean relative error for SSC was ~0.4, and that the reference run (green star) produced one of the lowest values (Figure 4.5). However, when individual observations were considered, use of different $\alpha$ and $\beta$ values produced relative errors that ranged from near zero to as high as >1 (Figure 4.5). For the observations nearest the sediment bed (Figure 4.5c), the model with $\alpha=0.4$ and $\beta=0.2$ (yellow squares) had the lowest relative error. The relative error for the reference run (Figure 4.5c; green stars) provided the second-best relative error of SSC for the bottom samples. However, for the six observations from the middle water column (Figure 4.5b), the reference run (green stars) produced the lowest relative error for two of the six samples, and the second lowest for three others. The model run with $\alpha=0.4$ and $\beta=0.2$ (Figure 4.5b; yellow squares) produced the lowest relative error for three of the mid-water observations and the second-best for two. For the surface observations, however, no single choice of parameters provided a consistently low set of relative errors (Figure
The run that used $\alpha=0.40$ and $\beta=0.4$ had the lowest relative error for samples 3-6, but it had the highest relative error for first sample (Figure 4.5a; orange diamonds). While the reference run did not perform especially well for the surface samples, it did fall toward the middle of the group (green stars, Figure 4.5a). Therefore, while no set of parameters produced consistently low relative errors for SSC, the set of parameters chosen to represent the York River estuary sediment distribution performed reasonably well in the surface waters and very well in the middle and near-bed portions of the water column.

The full floc size distributions produced by the model were also evaluated to determine whether the distributions reasonably represented those from the York River estuary, and the sensitivity of the size distribution to parameter choices was explored. The size distributions that corresponded to the merged LISST and PICS distributions (N=10) produced by a select set of model runs (Figure 4.4f; circled symbols) were averaged and examined in Figure 4.6. These included runs that produced the lowest average relative error for the distribution spread and mode (Cases 1 and 2). The comparison of the modeled and observed average normalized volume fraction distribution showed that multiple combinations of $n_f$, $\alpha$ and $\beta$ produced size distributions that were similar to those produced by the reference run (Figure 4.6). The size distribution produced by the reference run (thick green lines) contained more small flocs than the observed data, both in terms of the mode (which was smaller by $\sim$16 $\mu$m), and the cumulative distribution (Figure 4.6). Case 2 had a mode slightly larger than the observations (by $\sim$16 $\mu$m) and provided the best fit to the cumulative distribution
(Figure 4.6; thick yellow lines). The other examples shown had low relative errors for at least one metric, but they did not represent the average distribution for the York River estuary samples as well as other parameter combinations (Figure 4.6). Models that had a low relative error for the distribution mode and spread showed reasonable fits to the average observed sediment size distribution samples.

Representing the vertical structure of SSC was as important as representing the size distribution, thus, we also evaluated the ability of the model to represent SSC profiles. The observed SSC samples (Figure 4.7) were compared with SSC profiles estimated from the same model runs that were shown in Figure 4.6. A few of these models produced sediment size distributions similar to the reference run, but they had a higher estimate for the SSC than the reference run, in general. The reference run underestimated the SSC in the upper water column but produced a similar value or overestimated the SSC near the bottom (Figure 4.6; thick green line). Case 2 (Figures 4.6 and 4.7; thick yellow line) had higher SSC than the reference run and overestimated most observed concentrations. Case 1 represented some of the SSC samples reasonably well but consistently over-estimated the near-bed samples (Figure 4.7; thin orange line). The model with \( n_f=2.5, \alpha=0.2, \) and \( \beta=0.2 \) (Figure 4.6; thin red line) had higher concentrations in the upper water column that were closer to 80% of the observed values in the surface in comparison to the reference run and had similar values as the reference near the bed.

2.5 Summary: Model Sensitivity and Parameterization

In summary, a one-dimensional (vertical) model was developed to represent conditions from the Claybank site of the York River estuary. This model was used to
examine the sensitivity of the modeled suspended sediment concentration and floc size distribution to variability in FLOCMOD parameters, namely the fractal dimension ($n_f$), collision efficiency ($\alpha$), and breakup efficiency ($\theta$). Toward this, over 150 model runs were evaluated, each using a different combination of $n_f$, $\alpha$, and $\theta$. Lastly, the modeled SSC and floc distribution metrics were compared to values obtained from field measurements from the same region of the York River estuary.

The suspended sediment concentration was sensitive to all three parameters while modeled $D_{50}$ and distribution spread were typically most sensitive to $\theta$ and to $n_f$, respectively (Figure 4.3). Changes in all three parameters produced variability in the SSC but this was more extensive in the bottom meter (depth 4-5 m) of the water column (Figure 4.3a-b). $D_{50}$ was most sensitive to changes in $\theta$ except for the smallest value of $\theta$ investigated in which $n_f$ also added to the variability in $D_{50}$ (Figure 4.3c). The size distribution spread was most sensitive to $n_f$, in general, except for the lowest value of $\alpha$ evaluated. In that case, the spread was also sensitive to the changes in $\theta$ (Figure 4.3d). Additionally, the interaction between metrics was apparent. For example, parameter combinations that produced a large $D_{50}$ also produced low SSC in response to associated floc settling (Figure 4.3b-c).

The modeled SSC and floc distribution metrics were also used to evaluate whether the model could reasonable represent the sediment concentrations and floc sizes for the Claybank site of the York River estuary. Specifically, we aimed to determine which combination of values for $n_f$, $\alpha$, and $\theta$ yielded the best estimates. The comparison of modeled SSC, floc sizes, and suspended sediment profiles to observations showed that a
single set of parameters was not obviously preferable across all sampling periods and metrics considered (i.e. SSC, and distribution mode, and spread). Thus, we chose a set of parameters ($\eta=2.4$, $\alpha=0.35$, and $\beta=0.2$) that provided a reasonable overall representation of sediment dynamics for York River estuary when considering all the conditions examined; this run was designated as the “reference run”. This set of parameters on average performed well in terms of SSC from slack to flood flow and throughout the water column (Figure 4.5), provided a modal floc diameter within 16 μm of the measured value (Figure 4.6), and produced SSC profiles that were within the bounds of the observed values (Figure 4.7).

3 Application for the York River Estuary for a Spring-Neap Cycle

The parameters used in the reference run in Section 2 were implemented in a 15-day, spring-neap cycle simulation for the Claybank site in the York River estuary. This longer model run was used to evaluate the variability of sediment transport and the influence of flocculation on suspended sediment over spring to neap conditions. Section 3.1 describes modifications made to the one-dimensional (vertical) model configuration, and Section 3.2 provides analysis of model output. The results of spring-neap variability in hydrodynamic and sediment dynamics are examined in Section 3.3, the mass exchange rates are explored in Section 3.4, and results are discussed in Section 3.5.

3.1 Modifications to Model Implementation

This study’s sensitivity analysis (Section 2) was based on modeling a 30-hour period beginning at slack before flood on the morning of June 7, 2016; to represent the spring-
neap cycle in the York River estuary, the model was implemented from June 1-15, 2016. The derivation of the along estuary velocity for this run remained the same as the method used for the sensitivity runs: 30-minute along-channel velocity profiles were acquired from the AWAC deployed in the Claybank region and are shown in Figure 4.8b. The u-velocity is positive for flood flow and negative for ebb flow and was slower during neap tide in comparison to spring tide (Figure 4.8b). The representation of the temperature and salinity for this application differed from Section 2’s sensitivity simulations. For the temperature, observations from the HOBO CT sensors from June 1, 2016 were used, but values were extrapolated to characterize water temperature above the uppermost sensor, while taking diurnal variations into account. Specifically, the HOBO CT temperature data were smoothed and vertical profiles for every 30 minutes were created. Temperatures for the surface waters were extrapolated as follows: from 9:00 am until 6:00 pm we assumed the surface waters above the uppermost sensor were warmer; whereas from 6:00 pm – 9:00 am the temperature profile above the uppermost sensor was assumed to be homogenous. The temperature profiles for this 24-hour period (June 1, 2016) were used for every day in the 15-day period.

The vertical resolution of the HOBO CT sensors was too low to properly represent the vertical salinity structure, and YSI Castway CTD profiles were not available for the full spring-neap cycle. Therefore, the salinity structure for the one-dimensional model was based on output from the idealized two-dimensional estuary developed in Chapter 2 (i.e. Tarpley et al. 2019). To generate the salinity structure, the hydrodynamic component of the idealized two-dimensional estuarine model was run for 90 days with
tidal heights that represented a combination of $M_2$ and $S_2$ tidal constituents. The amplitude and frequency for the $M_2$ constituent were 0.85 m and 12.42 hours, and for the $S_2$ constituent were 0.25 m and 12 hours. A freshwater discharge of 60 m$^3$ s$^{-1}$ produced stratification in the shallow section (depth = 6m) of the idealized estuary that was similar to the values observed in the middle reaches of the York. The 90-day run allowed ample time for model spin-up. The salinity for the last spring-neap cycle of the simulation was used to generate the salinity structure for the one-dimensional York River estuary application discussed in this section. The vertical structure of the salinity was maintained, but the depth-averaged values for the salinity were increased to match the range observed in the middle reaches of the York River estuary (9-16 g kg$^{-1}$).

Thus, these temperature and salinity values for the spring-neap cycle were used to calculate the density anomaly (density in kg m$^{-3}$ – 1000 kg m$^{-3}$), shown in Figure 4.8a. The density stratification during neap tide was greater than that during spring tide. Also, the density stratification was greater for flood tide than during ebb flow (Figure 4.8). This is because the river flow superimposed on the ebb tide at this relatively shallow location causes the depth-averaged current to be notably stronger on ebb than flood, leading to greater overall mixing on ebb.

3.2 Quantification of $D_{eq}$, Size Class Exchange, and Tidal Conditions of Interest

The results from the one-dimensional representation of the Claybank region of the York River estuary over a spring-neap cycle were used to explore the degree to which the modeled median diameter could be represented by an equilibrium floc diameter ($D_{eq}$) under these changing conditions. Also, the influence of flocculation on the
exchange of particles between size classes in comparison to other transport processes over timescales ranging from tidal to spring-neap was analyzed. The methods used in this analysis are described in the following paragraphs.

The equilibrium floc diameter predicted by a simple relationship between the SSC and shear rate ($G$) as shown in Winterwerp (1998, 2002) was compared to the modeled median diameter by volume ($D_{50}$). To derive the equilibrium relationship from the model results, the turbulent kinetic energy (tke) and the turbulence closure model parameters were used to calculate $G$. The shear rates along with the SSC by volume were then used to estimate a linear relationship between the SSC/$\sqrt{G}$ ratio and the median equilibrium floc diameter ($D_{eq}$). We used criteria similar to those employed in Chapter 2 (i.e. Tarpley et al. 2019) to identify times when the model most likely reached equilibrium. Specifically, model output that was ~80 cmab, had $4\leq G\leq 12$ s$^{-1}$, and SSC $\geq 0.08$ μL L$^{-1}$ were used to fit the equilibrium curve. The $D_{50}$ by volume concentration produced by the model at depths and times could then be compared to the predicted $D_{eq}$.

The model analysis for the spring-neap cycle also included quantifying the relative roles of flocculation and other transport mechanisms on changes in the local particle size distribution. The transport equation for our one-dimensional (vertical) model (Equation 4.5) relates the local rates of change in mass concentration in each size class due to vertical advection, vertical diffusion, settling, flocculation, and source/sink terms, and these rates were compared to each other. In Equation 4.5, $C_i$ is SSC for floc size class $i$, $t$ is time, $U$ is along estuary flow velocity, $z$ is the vertical coordinate, $K$ is vertical diffusion coefficient, $w$ is vertical flow velocity (positive upward), $w_{s,i}$ is settling velocity
for floc size class $i$, $f$ is the flocculation function, $G$ is shear rate, and $S_i$ is the source or sink of sediment from the bed due to erosion or deposition. Erosion and deposition only affected the mass concentration in the bottom-most grid layer directly above the sediment-water interface. As discussed in Chapter 3, new variables were added to CSTMS to track and record the exchange of mass per time step due to flocculation, erosion, and settling. The local changes in size class concentration due to advection and diffusion were already available as CSTMS output, in units of kg m$^{-4}$. In post-processing the exchange of mass was converted to mass concentration (kg m$^{-3}$), if needed, and then converted to a rate (kg m$^{-3}$s$^{-1}$) by dividing by the model time step ($dt = 2$ s). This provided the rates at which each mechanism in Equation 4.5 (i.e. vertical advection and diffusion, settling, flocculation, and erosion/deposition) contributed toward changes in concentration for each floc size class $i$. Horizontal advection was neglected in this analysis since the horizontal flux convergence is zero in the one-dimensional (vertical) model. Mass transport rates with positive values ($>0$) indicate the process increased concentration to an individual floc size class while negative values ($<0$) indicate that the process reduced concentration.

**Equation 4.5:**

$$\frac{\partial C_i}{\partial t} = -\nabla H U C_i + \frac{\partial K \partial^2 C_i}{\partial z^2} - \frac{\partial (w - w_{s,i})C_i}{\partial z} + f(C_i, C_j, G, ...)+ S_i$$

<table>
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<tr>
<th>Term</th>
<th>Description</th>
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<tr>
<td>Horizontal Advection</td>
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<td>Vertical Diffusion</td>
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<td>Vertical Adv. &amp; Settling</td>
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<td>Flocculation</td>
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<td>Erosion / Deposition</td>
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Over the 15-day spring-neap simulation, transfer rates were calculated at a 2-second timestep and were saved to model output every 5 minutes. The timeseries of the modeled $D_{50}$ by volume in the surface and very near-bed grid layers (Figure 4.9) showed three times within the spring-neap cycle that had distinct sediment characteristics: peak spring conditions, the transition from spring to neap, and peak neap conditions; thus these three periods were targeted for analysis. $D_{50}$ was largest during peak spring conditions in both the surface and near-bed. In the transition from spring to neap, the tidal fluctuations in $D_{50}$ quickly dissipated in the surface waters (Figure 4.9a), while near the bed the magnitude of the fluctuations in $D_{50}$ decreased more slowly (Figure 4.9b). During neap conditions, $D_{50}$ in the surface waters showed minimal change over the tidal cycle (Figure 4.9a), whereas near the bed tidal fluctuations were still notable, albeit significantly less than that seen during the transition period (Figure 4.9b). The responses in $D_{16}$ and $D_{84}$ were qualitatively similar as that for $D_{50}$ and were therefore not shown.

The results analyzed in Section 3.3 compare conditions over the spring-neap cycle by focusing on these three time periods.

3.3 SSC, Shear Rate, Floc Size, and Bed Erodibility Over the Spring-Neap Cycle

Timeseries of SSC, $VG$, the SSC/$VG$ ratio, and $D_{eq}$ for the three time periods showed tidal variability between flood and ebb and from spring to neap (Figure 4.10). During peak spring conditions, the SSC and $VG$ were highest, and sediment was mixed to the surface. Transitioning into neap conditions, however, the flow became less energetic, and the water column was more stratified, which led to little to no sediment in the surface 1-2 meters of the water column. Stratification also varied over the flood-ebb
tidal cycle, and during spring tide conditions flood flow had stronger stratification than ebb, leading to lower SSC and G in the surface waters (Figure 4.10a,b). Both SSC and G were reduced in the transition period, though G maintained a tidal signal during this time (Figure 4.10b,e). Sediment concentrations and G were the low during neap compared to the transition and spring conditions (Figure 4.10c,f). Also, a less consistent tidal signal in G was seen during peak neap conditions (Figure 4.10f). The SSC/VG ratio was largest during time periods when G reduced more quickly than SSC after peak flow (yellow colors; Figure 4.10g-i). During time periods when SSC and G increased simultaneously, the SSC/VG ratios were at their lowest, such as seen during ebb flow in spring conditions throughout the water column (Figure 4.10g). Also, a decrease in SSC more rapid than in G produced a lower SSC/VG ratio, as seen toward the end of neap conditions (Figure 4.10i; vertical blue band). The fluctuations in D_eq reflected the variability in SSC/VG, in that the predicted D_eq was largest when SSC/VG was greatest, as expected. At times this produced a larger D_eq during neap conditions than during the transition period (Figure 4.10k,l).

The timeseries of the fractional difference between D_50 and D_eq ((D_50-D_eq)/D_50) showed that D_50 was frequently less than D_eq (blue colors) except for in the upper water column, very near the sediment bed, and often around peak ebb flow (Figure 4.11; yellow to green colors). During spring conditions and through the transition period, D_50 was larger or merged with D_eq during ebb flow through the majority of the water column (Figure 4.11a-b). Whereas during flood flow, D_50 was greater than or merged with D_eq only in the surface 1-1.5 m (Figure 4.11a-b). During neap conditions, D_50 was
smaller than $D_{eq}$ over a majority of the tidal cycle in the lower half of the water column, except for very near the bed (Figure 4.11c). In the upper half of the water column during neap, the fractional difference was nearly zero or $<$0.2 (Figure 4.11c). Very near the sediment bed, $D_{50}$ was larger than $D_{eq}$ throughout the full spring-neap cycle, and the fractional difference was typically largest during slack flow (Figure 4.11a-c).

The response of sediment dynamics to the changing stratification and flow conditions that caused the variability in Figures 4.10 and 4.11 over the spring-neap cycle were examined in more detail at different depths within the water column (Figure 4.12). The SSC, $vG$, $D_{16}$, $D_{50}$, $D_{84}$, and $D_{eq}$ were examined over two-day periods during peak spring, the transition to neap, and peak neap conditions for three locations in the water column, the surface ($z/h=-0.006$), the lower water column ($z/h=-0.804$), and very near the sediment bed ($z/h=-0.994$; Figure 4.12).

Suspended floc concentrations and sizes tended to be highest overall during spring tide (Figure 4.12, left column). The timeseries of SSC showed concentrations in the surface waters highest during ebb flow for spring tide reaching $\sim130 \mu$L L$^{-1}$ (Figure 4.12a). The peak in SSC in the surface waters occurred when concentrations were greatly reduced in the lower column and very near the sediment bed (Figure 4.12g,m). Very near the bed, peaks in SSC occurred before peak flow, and the offset was greater during ebb flow in spring conditions, indicating a limiting factor (Figure 4.12m). The magnitude in $G$ was similar between flood and ebb flow during spring tide throughout the water column (Figure 4.12a,g,m). During spring at the surface, the floc sizes were all largest during ebb flow and increased slightly over the course of the ebb (Figure 4.12d).
However, in the lower column and very near the bed, the floc sizes tended to be largest during slack flow when $G$ was lowest (Figure 4.12j,p). In the surface water, $D_{50}$ was very near or merged with $D_{eq}$ from flood to ebb (Figure 4.12d). In the lower water column, the $D_{50}$ merged with $D_{eq}$ when the SSC was lowest while $G$ was higher than during slack flow; during other times in the flood-ebb cycle $D_{50}$ was smaller than $D_{eq}$ for spring tide (Figure 4.12j). Very near the bed, $D_{50}$ was larger than $D_{eq}$, and the largest difference was during slack flow (Figure 4.12p).

During the transition from spring to neap, sediment concentrations and $G$ decreased. The decrease was most evident and quickest near the surface, while the transition was slower in the lower water column ($z/h=-0.804$) away from very near-bed (Figure 4.12, middle column). Within the first 14 hours of the transition period, surface values of SSC decreased to nearly zero, and both SSC and $G$ ceased to show tidal fluctuations (Figure 4.12b). In the lower water column, SSC continued to show tidal fluctuations during the transition period, but fluctuations decreased until they were similar to SSC during neap conditions. In contrast, $G$ showed tidal fluctuations and remained relatively elevated with similar $\sqrt{G}$ values for flood flow during peak spring conditions (Figure 4.12g-i). Therefore, SSC adjusted to the reduced flow quicker than $G$ in the lower water column. Very near to the bed, SSC and $G$ were also lower toward the end of the transition period (Figure 4.12n). Early in the transition period very near the bed, SSC peaked before the peak in $G$. However, by the third ebb tide, SSC had reduced, and the peaks in SSC and $G$ coincided (Figure 4.12n; first peak in $G$ after the black dashed line). Similar to the SSC and $G$, the floc distribution adjusted quickly in the
surface, and $D_{50}$ merged with the equilibrium (Figure 4.12e). In the lower water column in the transition period, $D_{50}$ merged with $D_{eq}$ during ebb flow and remained smaller than $D_{eq}$ throughout the rest of the flood-ebb cycle, similar to the case during peak spring conditions (Figure 4.12j,k). The peaks in $D_{16}$, $D_{50}$, $D_{84}$, and $D_{eq}$ continued to occur during slack flow in the transition very near the bed, resembling the trends during spring tide (Figure 4.12q). Also, $D_{50}$ was larger than $D_{eq}$, but their difference became smaller toward the end of the transition to neap (Figure 4.12q).

During neap conditions in the surface waters, SSC, $G$, and floc sizes continued to display no tidal fluctuations, consistent with the conditions at the end of the transition to neap (Figure 4.12c,f). Conditions in the lower water column, however, continued to experience tidal fluctuations (Figure 4.12k,l). Peaks in SSC were similar during neap to those at the end of the transition period; however, $G$ was lower during neap than in the transition period in the lower water column (Figure 4.12h-i). There was less variability in the floc sizes during neap tide (Figure 4.12l); $D_{50}$ merged with $D_{eq}$ less frequently, but $D_{50}$ was most similar to $D_{eq}$ after peak flood flow in the lower water column during neap conditions (Figure 4.12l). Very near the bed, the peak in SSC was slightly lower during neap compared to the end of the transition period, which slightly reduced the difference between $D_{50}$ and $D_{eq}$ (Figure 4.12o,r).

The sediment bed conditions were also evaluated to examine the influence the bed had on the near-bed SSC by exploring variability in the bed shear stress, erodibility of the bed, and erosion/deposition from the bed (Figure 4.13). These showed both tidal fluctuations, but also an increase in bed erodibility during neap compared to spring tide
(Figure 4.13). Note that because our one-dimensional (vertical) model assumed uniform conditions, sediment could be exchanged between the sediment bed and the above water column, but the total sediment mass in the system remained constant. Over the spring-neap cycle, the applied bed stress was greatest, the erodibility was lowest and the least amount of sediment was in the bed during peak spring conditions (Figure 4.13). The applied bed stress decreased from peak spring to the end of the neap tide (Figure 4.13a). As the applied bed stress decreased, the difference in magnitude between flood and ebb flow increased, in which during neap the system had higher bed shear stresses during ebb flow that flood (Figure 4.13a). Compared to the initial bed conditions, the least amount of sediment was on the bed during peak spring tide (Figure 4.13c), when more sediment was suspended. In the transition period, the amount of sediment on the bed began to increase, and sediment on the bed peaked toward the end of peak neap conditions (Figure 4.13c). At the end of the model, 0.2 cm of sediment had been deposited from the overlying water column (Figure 4.13c). Sediment erodibility (Figure 4.13b) was calculated as the amount of sediment that could be eroded from the bed at an applied shear stress of 0.2 Pa (Fall et al. 2014). Erodibility began to increase during the transition from spring to neap, as sediment was deposited. The model assumes that freshly deposited sediment was easily erodible, thus, the bed erodibility increased with deposition and was highest at end of the transition to neap conditions, when the amount of recently deposited sediment was greatest (Figure 4.13b-c).
3.4 Mass Exchange Rates For Size Classes during the Spring-Neap Cycle

Quantifying the contributions to changes in concentration as a function of size class in Equation 4.5 revealed insights about the relative roles of flocculation and vertical transport over the spring-neap cycle. The mass balance terms were evaluated for surface water \((z/h=-0.006)\) over a tidal cycle during spring conditions and then for a tidal cycle during neap conditions. The mass balance terms were also quantified and examined for the lower water column \((z/h=-0.804)\) and the very near-bed \((z/h=-0.994)\) for a tidal cycle during spring tidal conditions.

In the surface waters over a spring tidal cycle, for all the floc sizes in suspension, vertical diffusion added mass concentration and settling removed mass concentration (Figure 4.14). The settling term is roughly proportional to the product of suspended concentration and settling velocity (Equation 4.5), thus, the highest mass transfer rates in the surface waters (Figure 4.14) tended to coincide with the peak in SSC. However, the settling term is further proportional to the \(w_s\times\text{SSC}\); thus, SSC is elevated when the settling term is larger. The highest rate of mass transfer in the surface water during spring tide occurred during and following ebb flow (Figures 4.14c-f). The vertical diffusion and settling nearly balanced each other, and they together dominated the transfer of sediment mass concentration (Figure 4.14). Nonetheless, some aggregation was also occurring when near-surface SSC was highest, causing mass to be removed from floc sizes 16-32 μm to floc sizes 64-256 μm, but at a much lower rate of \( \leq 2.5\times10^{-7} \) kg m\(^{-3}\) s\(^{-1}\), which is too small for the associated “floc” term to be seen in Figure 4.14.
In the surface waters over a neap tidal cycle, the sediment concentrations were near zero; therefore all rates of exchange were at least 2 orders of magnitude lower than during spring conditions (Figure 4.15). Additionally, the material suspended involved smaller floc size classes compared to spring conditions (16-32 μm; Figure 4.15). Vertical diffusion and settling were still the dominant mechanisms for transferring mass concentration, except for a small contribution from vertical advection. The upward diffusion and settling nearly balanced each other over the full tidal cycle.

Similar to the surface waters, vertical diffusion and settling were the two main processes transferring concentration in the lower water column \((z/h=0.804)\) during spring and neap conditions. However, unlike the surface, the transfer rates in the lower water column were an order of magnitude smaller than surface rates (Figures 4.14 & 4.16). At first this seems counterintuitive, since SSC is certainly not smaller in the lower water column. It is important to recall that the vertical diffusion, advection, and settling terms in Equation 4.5 depend on \(\partial / \partial z\) to create convergences that then drive \(\partial C / \partial t\). Since SSC is vertically well-mixed in the lower water column, \(\partial (C \, ws) / \partial z\) and \(\partial^2 C / \partial z^2\) can each be quite small. Also, unlike the near-surface case, the settling and vertical diffusion terms do not balance in the lower water column; instead vertical diffusion is often much larger than the settling term (Figure 4.16), it is this imbalance that allows \(\partial C / \partial t\) to be non-zero. Also, whereas vertical diffusion was always a source of sediment in the surface (Figure 4.14), in the waters in the bottom meter vertical diffusion could add to or reduce the concentration of individual floc sizes, depending on the tidal stage in the flood-ebb cycle (Figure 4.16). While aggregation was \(~1\) order of magnitude lower than
the vertical transport terms, it was relatively more important in the bottom waters than in the surface waters. Aggregation here removed mass from the smaller flocs (16-32 μm) and added mass to floc sizes 64-256 μm. The trends in transport rates during neap tide conditions were similar to spring, but were 2 times smaller and are not shown.

Very near the sediment bed, erosion, and vertical diffusion were the dominant processes transferring mass concentration during spring tide, and for much of the tidal cycle these two were nearly balanced (Figure 4.17). The mass transfer rates in the bottom-most grid cell were on the same order of magnitude as rates in the surface waters during spring conditions (Figures 4.14, 4.17). Unlike the surface, vertical diffusion reduced concentration from the floc sizes in suspension (16-512 μm), while erosion added to the concentration during spring tide (Figure 4.17). During spring tide very near the bed, settling played a small role, and when settling contributed, it typically added mass to the larger flocs in suspension (Figure 4.17). Disaggregation occurred very near-bed during spring tide, except during slack flow, and acted to remove sediment from floc sizes 64-256 μm and add it to floc sizes 16-32 μm. Disaggregation here was most significant during peak flow, when transfer rates were on the same order of magnitude as erosion and vertical diffusion (Figures 4.17). At slack flow, both aggregation and disaggregation occurred, which added mass to floc sizes 32-64 μm while removing it from the other sizes in suspension, but at rates at least 2 orders of magnitude slower than rates under higher flow (too small to see on Figure 4.17). Trends in the transfer of mass concentration very near the bed were similar during neap, except the rates were ~2 times lower compared to spring tide and are not shown. It is worth noting, however,
that disaggregation transfer rates were consistently smaller than vertical diffusion and erosion during neap tide.

3.5 Summary and Discussion for the York River Estuary Application

The model results for sediment transport and flocculation in the York River over the spring-neap cycle from this study were synthesized by characterizing conditions during three time periods: spring tide (Section 3.4.1), neap tide (Section 3.4.3), and the transition between them (Section 3.4.2).

3.5.1 Spring Tide

The sediment concentrations, \( G \), and transport rates were largest during peak spring conditions. Flocculation and vertical diffusion played key roles in the floc concentration and size distribution during peak spring conditions, especially during ebb tide. Sediment was eroded from the bed as flow increased (Figure 4.17), and concentrations reached their maximum before peak flow near the bed (Figure 4.12). With increasing turbulence, sediment was diffused upward (Figure 4.17), which reduced concentrations near the sediment bed (Figure 4.12). As flocs were eroded from the bed, they were disaggregated into smaller flocs whose slower settling velocities meant that they were more easily diffused upward. The reduction in SSC during peak ebb flow (Figure 4.12g,m) was a combination of the diffusion of sediment upwards as well as a reduction in erosion due to a limit in sediment availability (Sanford and Maa, 2001; Figure 4.17). The deeper layers of the sediment bed were more consolidated, had a higher critical shear stress for erosion, and limited the supply of sediment from the bed during peak
flow conditions (Figure 4.13). Toward the end of ebb flow in the surface waters, the SSC began to decrease, but the $D_{50}$ increased (Figure 4.12). Aggregation was occurring in the surface waters. Even though the mass transfer rates due to flocculation were an order of magnitude smaller than diffusion and settling, it was enough to increase $D_{50}$ in order to allow it to merge with $D_{eq}$ and slightly exceed $D_{eq}$ toward the end of ebb tide.

3.5.2 Transition from Spring to Neap Tide

Sediment concentrations and the floc distribution adjusted relatively quickly to the reduced flow and increased stratification conditions for neap tide in the surface and very near the sediment bed because both the SSC and $G$ reduced rather abruptly during the transition period (Figure 4.12b,h). In the lower water column ($z/h = 0.804$), the SSC responded to the reduced velocity as less sediment was entrained from the sediment bed. However, $G$ responded much more slowly and remained relatively elevated through the end of the transition, allowing floc sizes to gradually decline over transition period into neap tide (Figure 4.12h,k,l). However, the faster reduction in the SSC compared to $G$ in the transition period produced SSC/$G$ ratios that were smaller than during peak spring and neap conditions. This reduced $D_{eq}$, and as a consequence, the difference between $D_{50}$ and $D_{eq}$ was smaller in the lower water column during the transition period than during peak spring or neap tide (Figures 4.10j-l and 4.12h,k).

3.5.3 Neap Tide

Toward the end of the transition period into neap conditions, the SSC and applied bed stress were reduced, which allowed sediment to be deposited to the bed (Figures
4.12n,o and 4.13a,c). The bed consolidation routine used here designated that recently deposited sediment has a lower critical shear stress for erosion, which increased the erodibility of the sediment during neap relative to spring conditions. Therefore, the lower SSC during neap conditions was not a reflection of reduced sediment supply from the bed but was flow limited. Additionally, the lower SSC and $G$ caused mass transfer rates to be two orders of magnitude less in the surface (Figures 4.14-4.15) and be reduced by half both in the lower water column and very near the bed (not shown) during neap compared to spring tide. In the lower water column, this reduction in SSC and $G$, produced SSC/$\sqrt{G}$ ratios that were slightly larger compared to the end of the transition period, which, in turn, produced a larger $D_{eq}$ (Figure 4.10l). This led to a larger difference between $D_{50}$ and $D_{eq}$ during neap compared to spring tide (Figure 4.11c).

4 Conclusions

In summary, this paper used observed hydrodynamics, SSC, and floc properties to constrain the structure of a one-dimensional (vertical) numerical model that coupled hydrodynamics with sediment transport for the York River estuary. Unlike most other recent model studies that have been applied to muddy estuaries, the model used here included formulations that accounted for both sediment bed consolidation and flocculation. A set of 150 individual model runs that varied flocculation model parameters were used to test the sensitivity of the model results and determine a set of parameters that best represented the sediment characteristics for the York. Model parameters were chosen by comparing the modeled and observed values of SSC and the flocs’ distribution mode and spread. This combination of parameters was then used in a
model simulation for a spring-neap cycle that compared the effect vertical transport terms (resuspension, settling, vertical diffusion) and flocculation on sediment concentrations. The results of this study for each component are summarized below.

4.1 Sensitivity

The sensitivity of SSC and floc size distribution to variability in the fractal dimension ($n_f$), collision efficiency ($\alpha$), and breakup efficiency ($\beta$) were as expected. A reduction in $n_f$ reduced the density and settling velocity of individual floc sizes. The lower settling velocities increased the retention of sediment in the water column, which then enhanced the role of aggregation. As a result, the SSC, $D_{50}$, and the spread of the floc size distribution all increased with a decrease in $n_f$. As $\alpha$ increased, aggregation was enhanced, which led to a larger $D_{50}$; therefore flocs with faster settling velocities were formed. The larger settling velocity led to flocs settling to the bed and reducing the SSC. An increase in $\beta$ enhanced the breakup of flocs, which led to a higher SSC and a smaller $D_{50}$. For example, a disaggregation efficiency of $\beta=0.05$ often produced a $D_{50}$ that was two times smaller than $D_{50}$ for a case that used $\beta$ of 0.01.

4.2 Parameterization

This study demonstrated the challenges of choosing parameters for FLOCMOD. The literature from field and laboratory studies reports values for fractal dimension, aggregation, and breakup parameters that vary over large ranges. Also, the effect of changing parameters were not independent, in that similar results could be obtained using different sets of fractal dimensions and collision/breakup efficiencies. Different
sets of parameter choices could yield similar model skills for the various suspended sediment characteristics such as $D_{50}$, distribution mode and spread, and SSC. For example, the combination of $n_f=2.1$, $\alpha=0.3$, and $\beta=0.2$ had the lowest relative error for the distribution spread, but overestimated the distribution mode and SSC. For parameterization, this study applied observation-based estimates by Fall (2020) of fractal dimension and primary particle size and density for the York River estuary. A range of fractal dimensions, and various $\alpha$ and $\beta$ were further tested to determine the combination that would best reproduce a time-series of SSC and floc distributions in the York River estuary that had been measured during a flood tide. The set of parameters that were selected to best represent sediment characteristics over the full water column in the York produced low relative error for SSC and the lowest relative errors for the distribution mode and spread; these values were: $n_f=2.4$, $\alpha=0.35$, $\beta=0.2$ (Figure 4.4a-c).

The relative errors for individual observed samples taken near the seafloor were evaluated in addition to the depth-averaged values to eliminate other model runs that produced similar model skill. While other fractal dimensions were explored, the best-fit $n_f$ of 2.4, equaled the average value determined using the observations from 1-3 m below the surface along the entire York (from the mouth to 20 km downstream of the turbidity maximum; Fall 2020). However, comparisons of model calculations to samples taken in the surface waters showed that the model parameters that worked well in the bottom boundary layer did not provide the strongest model skill for the surface waters. Specifically, the combination of parameters that best represented the sediment distribution in the surface waters had a slightly smaller fractal dimension (2.3) and a
much smaller $\alpha$ (0.1) and $\beta$ (0.05) (Figure 4.4d-f) compared to the values that worked well for bottom waters. This may indicate that the flocs in the surface waters were more compact and less likely to aggregate and breakup than those in the bottom boundary layer. When using flocculation dynamics in a modeling study with limited observational information on the SSC and/or floc distribution, a modeler must decide which metrics to fit (i.e. near-surface SSC, median diameter, and/or average SSC) to parameterize FLOCMOD, and the choice may depend on their specific research questions.

4.3 Application of FLOCMOD for the York River Estuary

The model implementation represented conditions in the York River estuary over a spring-neap cycle. Model results showed that the SSC and size distribution quickly adjusted to the reduced flow velocity and increased stratification for neap tide in the surface water and the very near-bed; but the response was slower in the lower-water column ($z/h=0.804$), which took more than four tidal cycles to completely reduce to neap conditions. For the surface waters, the sediment supplied through vertical diffusion was greatly reduced and sediment continued to settle out of the surface during neap leading to a reduction in the SSC to nearly zero, and $D_{16}$, $D_{50}$, and $D_{84}$ dropped below 50 μm. The minor tidal fluctuations in $G$ in the surface waters ceased, and this transition in the SSC and $G$ occurred over a single tidal cycle. For very near the bed, the major source of suspended sediment was erosion from the bed, and the reduction in flow velocity at neap tide changed the near-bed region from being supply-limited to flow-limited (Sanford and Maa, 2001). The applied bed stress and amount of sediment eroded from the bed was reduced during neap, which caused the SSC and floc
sizes to decrease. Additionally, $G$ reduced in magnitude as shown for neap conditions, and this transition in $G$ and SSC occurred over about two tidal cycles. In the lower-water column ($z/h=-0.804$), the reduction of $G$ to neap conditions took more than four tidal cycles. The sediment supply for this location was sediment that was diffused upward from the very near-bed region and sediment settling from above, but the SSC adjusted in a similar time frame as the very near-bed. However, floc sizes adjusted more slowly, similar to $G$.

The model representation of the York River estuary site was analyzed with respect to the relative roles of flocculation and transport processes (vertical diffusion, advection, settling, erosion) contributing to each floc size. As expected, the contribution of vertical advection was minimal. The local rate of change of sediment mass concentration across size classes due to flocculation was often much smaller than those due to erosion, vertical diffusion, and settling. In the very near-bed region, the vertical mass balance was between erosion, which supplied suspended sediment; and vertical diffusion which exported it to overlying water. In the lower water column and surface waters, the vertical transport balance was usually between the settling and vertical diffusion terms. However, the effect of flocculation on the SSC and floc size distribution was evident in the increase in the median floc size in the surface waters toward the end of ebb flow and very near the bed during slack flow. Additionally, the breakup of flocs in the very near-bed at peak flow enhanced the vertical diffusion of sediment by lowering the setting velocity when mixing was elevated.
Table 4.1: The sample start time (Eastern Standard Time) and z/h (depth of the sample / total depth) for each profile sampled on the morning of June 7, 2016 with the CHSD profiling system.

<table>
<thead>
<tr>
<th>Profile</th>
<th>Profile 1 Time; z/h</th>
<th>Profile 2 Time; z/h</th>
<th>Profile 3 Time; z/h</th>
<th>Profile 4 Time; z/h</th>
<th>Profile 5 Time; z/h</th>
<th>Profile 6 Time; z/h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface</td>
<td>7:15 0.30</td>
<td>8:19 0.32</td>
<td>9:18 0.28</td>
<td>10:20 0.21</td>
<td>11:20 0.27</td>
<td>12:17 0.21</td>
</tr>
<tr>
<td>Middle</td>
<td>7:12 0.76</td>
<td>8:17 0.45</td>
<td>9:15 0.40</td>
<td>10:18 0.47</td>
<td>11:18 0.52</td>
<td>12:15 0.82</td>
</tr>
<tr>
<td>Bottom</td>
<td>7:09 0.92</td>
<td>8:15 0.93</td>
<td>9:13 0.62</td>
<td>10:16 0.67</td>
<td>11:15 0.78</td>
<td>12:12 0.95</td>
</tr>
</tbody>
</table>

Table 4.2: The settling velocity ($w_s$; mm s$^{-1}$) of the 11 floc classes ($D_{f,i}$; 1-1024 μm) for all fractal dimensions ($n_f$; 2.0-2.5) used in the sensitivity runs. In all cases, $D_p = 1$ μm and $\rho_p = 2000$ kg m$^{-3}$.

<table>
<thead>
<tr>
<th>$n_f$</th>
<th>$D_{f,i}$ = 1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>32</th>
<th>64</th>
<th>128</th>
<th>256</th>
<th>512</th>
<th>1024</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>0.00054</td>
<td>0.0011</td>
<td>0.0022</td>
<td>0.0043</td>
<td>0.0086</td>
<td>0.017</td>
<td>0.035</td>
<td>0.069</td>
<td>0.14</td>
<td>0.28</td>
<td>0.55</td>
</tr>
<tr>
<td>2.1</td>
<td>0.00054</td>
<td>0.0011</td>
<td>0.0012</td>
<td>0.0025</td>
<td>0.0053</td>
<td>0.0110</td>
<td>0.024</td>
<td>0.052</td>
<td>0.110</td>
<td>0.24</td>
<td>0.52</td>
</tr>
<tr>
<td>2.2</td>
<td>0.00054</td>
<td>0.0011</td>
<td>0.0012</td>
<td>0.0028</td>
<td>0.0065</td>
<td>0.0150</td>
<td>0.035</td>
<td>0.079</td>
<td>0.180</td>
<td>0.42</td>
<td>0.96</td>
</tr>
<tr>
<td>2.3</td>
<td>0.00054</td>
<td>0.0013</td>
<td>0.0033</td>
<td>0.0081</td>
<td>0.0200</td>
<td>0.049</td>
<td>0.120</td>
<td>0.300</td>
<td>0.73</td>
<td>1.80</td>
<td>4.40</td>
</tr>
<tr>
<td>2.4</td>
<td>0.00054</td>
<td>0.0013</td>
<td>0.0014</td>
<td>0.0038</td>
<td>0.0099</td>
<td>0.0260</td>
<td>0.069</td>
<td>0.180</td>
<td>0.480</td>
<td>1.30</td>
<td>3.30</td>
</tr>
<tr>
<td>2.5</td>
<td>0.00054</td>
<td>0.0015</td>
<td>0.0043</td>
<td>0.0120</td>
<td>0.0350</td>
<td>0.098</td>
<td>0.280</td>
<td>0.780</td>
<td>2.20</td>
<td>6.30</td>
<td>18.0</td>
</tr>
</tbody>
</table>

Table 4.3: Model runs that had the lowest relative error on average for a designated metric, the surface samples, or the full water column. $n_f =$ fractal dimension, $\alpha =$ collision efficiency, and $\beta =$ breakup efficiency.

<table>
<thead>
<tr>
<th>Designation</th>
<th>$n_f$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>Best-fit Metric</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>2.1</td>
<td>0.30</td>
<td>0.20</td>
<td>Distribution Spread</td>
</tr>
<tr>
<td>Case 2</td>
<td>2.2</td>
<td>0.20</td>
<td>0.15</td>
<td>Distribution Mode</td>
</tr>
<tr>
<td>Case 3</td>
<td>2.3</td>
<td>0.10</td>
<td>0.05</td>
<td>Surface samples</td>
</tr>
<tr>
<td>Reference</td>
<td>2.4</td>
<td>0.35</td>
<td>0.20</td>
<td>Full water column</td>
</tr>
</tbody>
</table>
Figure 4.1: Map of the York River estuary, southeast VA, USA. The locations of the Virginia Institute of Marine Science (VIMS) and the United States Coast Guard (USCG) training center in Yorktown, VA are designated with the black stars. The location of the fixed piling at Claybank (CB) is marked with the black square. The inset in the bottom left shows the observation locations discussed in Sections 2.1-2.2, for the AWAC, ADV tripod, and survey with the profiling system in comparison to the piling.
Figure 4.2: A schematic of the 1D model setup with the vertical grid resolution for the water column, the observations, and instrumentation used to drive the 1D model. Note: the sediment bed has 10 vertical layers.
Figure 4.3: The time- and spatially-averaged SSC for the (a) surface meter and (b) bottom meter of the water column. The time- and spatial-average (c) $D_{50}$ by volume concentration and (d) distribution spread for the bottom meter of the water column. The range in $n_f$ is 2.0-2.5, $\alpha$ is 0.1-0.5, and $\beta$ is 0.01-0.2. Note: The surface meter indicates an average for depths 0-1 m in the model, the Y-axis is larger in panel (b), and the larger light green star represents the model parameters chosen to best represent the York River estuary sediment distribution samples described in Section 2.2.
Figure 4.4: The average relative error of all the samples (top row) and surface samples only (N=3-4; bottom row) for the (a,d) distribution spread, (b,e) distribution mode, and (c,f) SSC. Fractal dimension ranged from 2.0-2.5, collision efficiency (α) ranged from 0.1-0.5, and breakup efficiency (β) ranged from 0.01-0.2. Note: The larger light green star represents the model with the set of parameters chosen to best represent flocculation in the York River estuary. Circled cases in (f) are shown in Figures 4.6 and 4.7.
Figure 4.5: The relative error for observed SSC sample numbers 1-19, from the (a) surface, (b) middle, (c) bottom and (d) the depth-averaged for model runs with \( n = 2.4 \) including the reference run (green stars) and runs with larger values for \( \beta \). Legend shows the values of \( \alpha \) and \( \beta \). Note: SSC sample 2 was an outlier and was removed.
Figure 4.6: The average (N=10) (a) volume fraction size distribution normalized by the maximum value and (b) cumulative volume fraction size distribution for the circled model runs in Figure 4.4f, including the reference run (bold green line), Case 1 (thin orange line), Case 2 (bold yellow line), and Case 3 (thin purple line).
Figure 4.7: The SSC samples (black stars) and model SSC profiles (lines) for the circled model runs in Figure 4.3f, including the reference run (bold green line), Case 1 (thin orange line), Case 2 (bold yellow line), and Case 3 (thin purple line). Note: The X-axis is logarithmic, sample times are from the samples labeled middle in Table 1, and panel (a) is near slack before flood on June 7, 2016.
Figure 4.8: Timeseries of the (a) model density anomaly from the idealized estuary, and (b) the u-velocity from the AWAC for the spring-neap cycle application of the York River estuary. Note: Positive velocity values indicate flood flow and negative values indicate ebb flow.
Figure 4.9: Timeseries of $D_{50}$ by volume for the (a) surface ($z/h=0.006$) and (b) bottom ($z/h=0.994$) for the spring-neap cycle from June 1-15, 2016. The red boxes indicate the time periods for peak spring, the transition between spring to neap and peak neap conditions.
Figure 4.10: Timeseries of (a-c) SSC (μL L⁻¹), (d-f) √G (s⁻¹/₂), (g-i) SSC/√G ratio, and (j-l) $D_{eq}$ (μm) for the peak spring conditions (a,d,g,j), transition from spring to neap (b,e,h,k) and peak neap conditions (c,f,i,l).
Figure 4.11: Timeseries of the magnitude of the fractional difference between $D_{50}$ and $D_{eq}$ ($\frac{(D_{50}-D_{eq})}{D_{50}}$) for (a) peak spring conditions, (b) transition from spring to neap, and (c) peak neap conditions. Blue colors indicate that the modeled $D_{50}$ was smaller than the $D_{eq}$; yellow to green colors indicate that $D_{50}$ was larger than $D_{eq}$.
Figure 4.12: Timeseries of (a-c, g-l, m-o) SSC (black lines) and \( V_G \) (blue lines), and (d-f, j-l, p-r) \( D_{10} \) (blue lines), \( D_{50} \) (black lines), \( D_{84} \) (red lines), and \( D_{eq} \) (green lines) for (a-f) the surface \((z/h=0.006)\), (g-l) the lower water column \((z/h=0.804)\), and (m-r) very near the bed \((z/h=0.994)\) during peak spring \((a,d,g,j,m)\), the transition from spring to neap \((b,e,h,k,n,q)\), and peak neap conditions \((c,f,l,o,r)\). Vertical dashed lines are defined using the local peak in velocity at each height.
Figure 4.13: Timeseries of the (a) applied bed stress (Pa; positive values correspond with flood flow while negative values correspond with ebb flow), (b) the accumulation of sediment in the bed (cm; negative values correspond to net erosion of sediment, and positive values correspond to net deposition compared to the bed at the first time step), and (c) erodibility of the sediment bed, calculated as the amount of sediment mass (kg m$^{-3}$) eroded from the bed at an applied bed stress of 0.2 Pa (Fall et al. 2014). Note: Black lines represent instantaneous values, the red lines show the running means, and the blue boxes bracket peak spring, the transition period, and peak neap conditions, respectively.
Figure 4.14: The transfer of mass concentration for each floc size in the surface water (3 cm below the surface) over a tidal cycle during peak spring conditions from (a) slack before ebb to (b) slack after flood. The label in the bottom right of each figure panel is the $u$-velocity for the near-bed location at that time. Positive values mean that the process added mass to that size; negative values indicate that the process removed mass from that size.
Figure 4.15: The transfer of mass concentration for each floc size in the surface waters (3 cm below the surface) over a tidal cycle during peak neap conditions from (a) slack before ebb to (b) slack after flood. The label in the bottom right of each figure panel is the u-velocity for the near-bed location at that time. Positive values mean that the process added mass to that size; negative values indicate that the process removed mass from that size. Note: The Y-axis is 2 orders of magnitude smaller than during spring tide (Figure 4.14), also the u-velocity at the surface is slightly out of phase with the u-velocity near-bed as shown in Figure 4.12.
Figure 4.16: The transfer of mass concentration for each floc size in the lower water column ($z/h=0.804$; ~100 cmab) over a tidal cycle during peak spring conditions from (a) slack before ebb to (b) slack after flood. The label in the bottom right of each figure panel is the $u$-velocity for the near-bed location at that time. Positive values mean that the process added mass to that size; negative values indicate that the process removed mass from that size.
Figure 4.17: The transfer of mass concentration for each floc size very near the sediment bed during peak spring conditions from (a) slack before ebb to (b) slack after flood. The label in the bottom right of each figure panel is the $u$-velocity for the near-bed location at that time. Positive values mean that the process added mass to that size; negative values indicate that the process removed mass from that size.
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Future Directions in Applying Flocculation Models
Chapter 5: Future Directions in Applying Flocculation Models

A dynamic flocculation model has the ability to represent variability in floc size distribution over a range of conditions; however, applying a dynamic flocculation model to natural floc populations is not without its challenges. The population balance model, FLOCMOD, used in this study was computationally expensive; and because it uses some iterative methods, it was also difficult to predict the runtime required for specific model runs a priori. For these reasons, creativity would be needed to reduce the computational cost to apply FLOCMOD to a regional-scale domain. Limits on the iterative process that requires convergence in FLOCMOD could be placed, which would reduce the computational cost and also make runtime more predictable. This was done to some extent in our model runs, with no discernable impact on model calculations. Another option would be to incorporate the flocculation timescale formulation from Winterwerp (2002) and to activate FLOCMOD only when needed. For example, flocculation was usually important in the bottom grid cell, and the flocculation model might be used when the timescale for flocculation was on the order of minutes. The use of the flocculation timescale would require an additional model parameter or the development of a relationship between the breakup efficiency, $\beta$ (Verney et al. 2011) that is already defined in FLOCMOD, and the breakup coefficient, $k_B$ (Winterwerp 2002) used for the flocculation timescale estimation.

The comparison of the model results to observed SSC and floc distribution showed the characteristics of the floc population vary in both space and time. Flocs in the surface waters appeared to be less likely to aggregate. The current formulation of the
FLOCMOD does not account for variability in the efficiencies of aggregation and disaggregation. Modifications could be made to the collision ($\alpha$) and breakup ($\beta$) efficiencies to allow these parameters to vary with relative depth ($z/h$), flow velocity, SSC, or a combination to account for variability in the strength of the flocs throughout the water column.

The structure of the flocs as represented by the fractal dimension ($n_f$) has also been observed to vary in space and time as flocs grow and break (Dyer and Manning 1999; Guo et al. 2017; Chapalain et al. 2018; Fall 2020). For example, in the York River, recent observations indicated that macroflocs tended to have a larger $n_f$ than microflocs (Fall 2020). Recent studies have developed numerical expressions to represent the change in structure with floc growth and breakup (Maggi et al. 2007; Xu et al. 2010; Son and Hsu 2011). A modification in $n_f$ would be difficult to incorporate into the COAWST modeling system, however, because the floc density and settling velocity both vary with $n_f$. The settling scheme in COAWST requires that the settling velocity of each size class remain constant throughout the water column (Warner et al. 2008). However, a modification in the vertical advection scheme to allow the settling velocity of a size class to vary while maintaining numerical stability could eliminate this limitation.

However, these modifications to $\alpha$, $\beta$, or $n_f$ in FLOCMOD or another flocculation model could further increase the number of user-defined parameters as well as the computational costs. Additional research would be required to constrain new parameters and to develop methods that can be applied to keep computational costs
low. The trade off would be the flexibility and ability to apply the flocculation model to a wider range of conditions and model domains.
References


