A shear-limited flocculation model for dynamically predicting average floc size

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Introduction

Scientists and engineers rely on physics-based models to evaluate the transport and deposition of sediment in water systems. The accuracy of such models depends on the selection of an appropriate sediment settling velocity, w_s. w_s of cohesive and non-cohesive sediment is determined by the size, density, and shape of the sediment. For non-cohesive particles, w_s is relatively easy to calculate as the size, density, and shape do not change with the time scale of simulation. However, for cohesive sediment, the settling speed is not as simple to determine. The reason for this is that cohesive particles can create aggregates, called flocs, which are orders of magnitude larger than their constituent grains (Fig. 1). Furthermore, flocs can grow or shrink in size depending on environmental conditions such as sediment mineralogy, water column chemistry and organic content, suspended sediment concentration, turbulent shear stress, and floc shape.

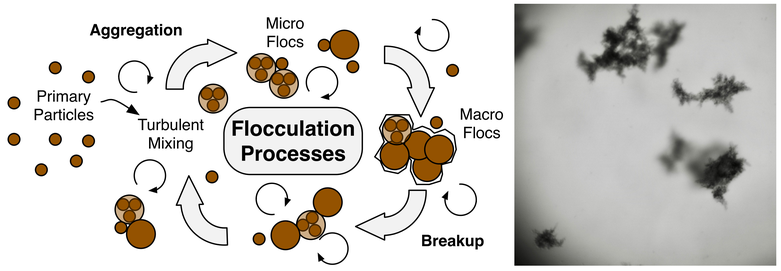

Figure 1: Flocculation process schematic and sample image

Study Aim

The purpose of this study is to present a new model for predicting floc size in a dynamic way as a function of the hydrodynamic conditions and inherited floc sizes. The new model is a simple modification to the existing Winterwerp (1998) floc size model. The modification is significant in that it yields predictions that are more inline with observations and theory regarding the upper limit on ultimate floc size, and allows the model to predict floc sizes across a range of suspended sediment concentration values with out recalibrating the model.

Background: Winterwerp (1998) Flocculation Model

The Winterwerp (1998) model (W98) is a single class size model that predicts the average size of a floc population with time. It is based on a collision-driven aggregation kernel and shear-driven break up kernel. Written in a Lagrangian frame of reference, the W98 model takes the form of,

$$\frac{dD}{dt} = \underbrace{\frac{k_A^{'}}{n_f}\frac{D_p^{n_f-3}}{\rho_s} GCD^{4-n_f}}_{\text{Aggregation Kernel}} - \underbrace{\frac{k_B^{'}}{n_f} DG\left(\frac{D-D_p}{D_p}\right)^p \left(\frac{\mu G}{F_y/D^2}\right)^q}_{\text{Erosion/Breakup Kernel}} \tag{1}$$

where $k_A^{'}$ and $k_B^{'}$ are calibration coefficients for the model, D is the floc size, n_f is the fractal dimension of the floc, D_p is the primary particle size, ρ_s is the density of the sediment. Winterwerp (1998) suggested that $p = 1$ to ensure $D_e \propto G^{-1/2}$ when $n_f = 2$, and that q be set to $q = 0.5$ to ensure that D_e (and hence w_s) is $\propto C$ as found in stagnant column settling tests (e.g., Hwang, 1989).

Experience has shown that the W98 model it tends to **over predict the dependency of floc size on concentration**. This can be seen using data from Tran et al. (2017) in figure 2, where the model is calibrated to data at $C = 50$ mg/L and then used to predict the floc size time series at $C = 400$ mg/L.

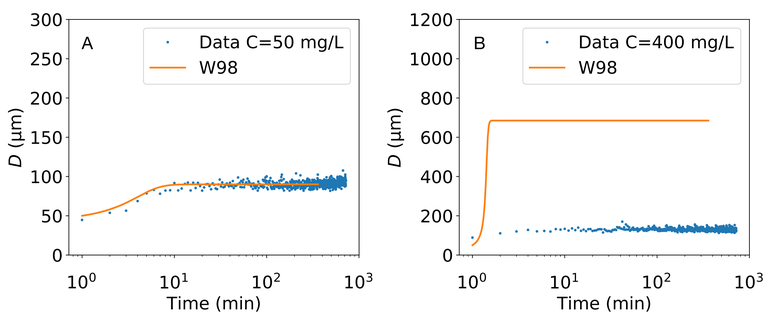

Figure 2: Winterwerp (1998) model compared with Tran et al. (2017). The Winterwerp (1998) is calibrated to 50 mg/L. For these calculations $G = 50$ s^{-1}, $n_f = 2$, $F_y = 10^{-10}$ N, $k_A^{'} = 0.45$, $k_B^{'} = 1.16$E-6, $\rho_s = 2650$ kg/m^3, $\mu = 1 \times 10^{-3}$ N-s/m^2, and $D_p = 5$ μm

The Primary Issue with the W98 Model

Winterwerp (1998) model was developed under the assumption that the predicted floc size would be less than the Kolmogorov microscale, η; however, the model often predicts floc sizes in great excess of η — an outcome that is physically unrealistic as many authors have noted that the maximum floc size is bounded by η (e.g., Parker et al., 1972; Coufort et al., 2005; Kumar et al., 2010; Cartwright et al., 2011; Braithwaite et al., 2012). For example, equilibrium floc size, D_e, equation derived from letting $dD/dt = 0$ in the W98 model (equation 1) with $n_f = 2$, $p = 1$, and $q = 0.5$ is as follows:

$$D_e = D_p + \left(\frac{k_A^{'}}{k_B^{'}}\frac{1}{\rho_s}\right)\left(\frac{\mu}{F_y}\right)^{-1/2} CG^{-1/2} \tag{2}$$

Note that there is no bound on D_e, and that D_e is linearly related to C.

Model Modifications

To remedy this limitation, we propose a simple modification to the Winterwerp (1998) floc erosion rate model that is a function of D/η. We start with the same breakup kernel as in the W98 model (equation 1), but propose that q should be a function of D/η. Based on trial and error, we propose the following linear model for q,

$$q = c_1 + c_2\frac{D}{\eta} \tag{3}$$

where c_1 and c_2 are constant coefficients. For the case when $D \ll \eta$, Equation 3 reduces to $q = c_1$ similar to the original W98 formulation. However, as D approaches η, q increases from this baseline value of $q = c_1$ and therefore limits flocs size. The c_2 coefficient is used to adjust the equation for the strength of the flocs and therefore ultimate floc size. Equation 3 can be used along with the primary W98 equation (equation 1) to predict floc size, and it is the major outcome of this study.

Model Behavior

As stated above, modifying c_2 can adjust the limit of the size of the flocs. As you can see in figure 3, while varying the value of c_2 only affects the value of $C = 50$ mg/L marginally, the variation of c_2 can dramatically change the difference between $C = 50$ mg/L and $C = 400$ mg/L.

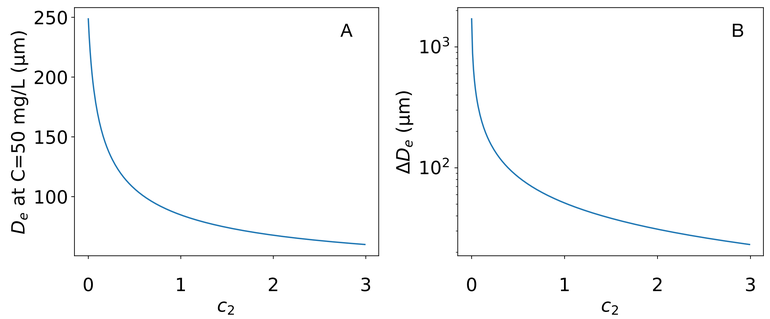

Figure 3: Change in the equilibrium floc size, D_e, and the difference between the predicted equilibrium floc size at $C = 50$ mg/L and $C = 400$ mg/L.

The new model is also bound by the Kolmogorov microscale. Figure 4 shows how the new model and the Winterwerp (1998) model diverge as floc size increases. Additionally it can be see that the new model stays below the Kolmogorov microscale while the Winterwerp (1998) model goes far beyond it.

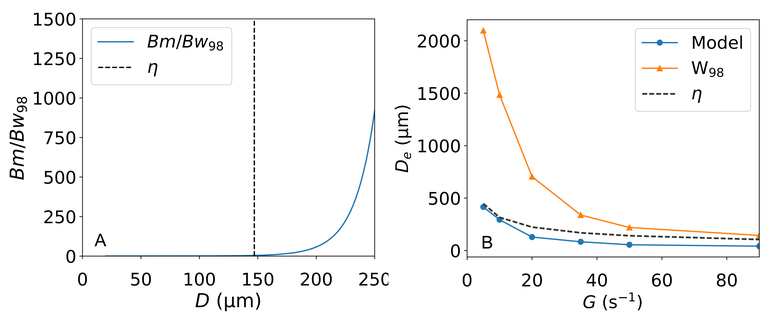

Figure 4: (A) Plot of the ratio of the breakup terms for Winterwerp (1998) model and the new model. (B) Plot of the Winterwerp (1998) and the new model at $C = 400$ mg/L for different shear rates.

Validation with Experimental Data

The new model for q (equation 3, which goes into equation 1) was tested against the floc growth data of Tran et al. (2017) similar to the original test with the baseline W98 model that was shown in figure 2. As in the first test, the floc growth data at $C = 25$ mg/L was used to calibrate the growth and breakup coefficients $k_A^{'}$ and $k_B^{'}$, and these coefficient values where then used to predict the floc growth time series at $C = 400$ mg/L. The result of this analysis shows that the modification does a much better job of capturing the observed trends (figure 5 as opposed to 2).

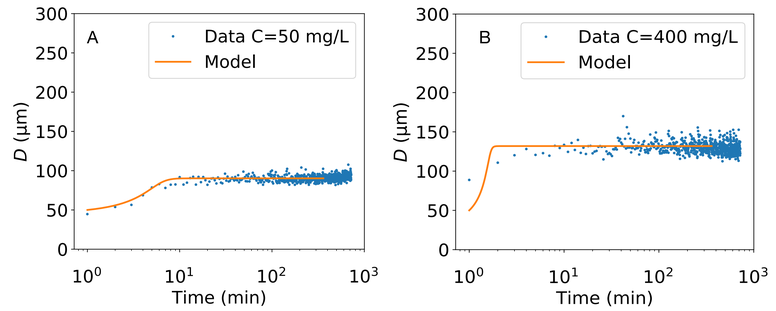

Figure 5: Comparison between the model and data from Tran et al. (2017) for (A) $C = 50$ mg/L and (B) $C = 400$ mg/L. $k_A^{'}$ and $k_B^{'}$ values were calibrated to the data at $C = 50$ mg/L and then used to predict the size $C = 400$ mg/L

In addition to capturing the time dependent change in D, the new model was able to adequately predict the equilibrium floc size measured under a range of concentration values (figure 6A). And it was able to model the change in floc size with time due to a drop in concentration (figure 6A) – all while using the $k_A^{'}$ and $k_B^{'}$ from the initial calibration to the growth data at $C = 50$ mg/L (figure 5A).

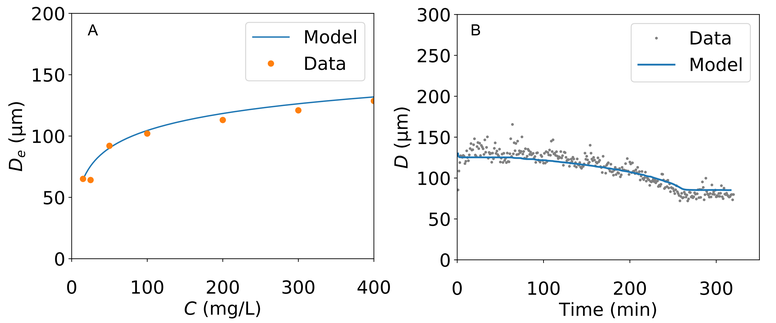

Figure 6: Comparison between the model and data from Tran et al. (2017) for (A) Experiments run at a constant concentration (B) Experiments run with a concentration which drops from $C = 400$ mg/L to $C = 50$ mg/L over 200 minutes

Key Findings

1. A modification to the Winterwerp (1998) model was proposed to address the over dependence of floc size on concentration.
2. This modification was shown to successfully predict time dependent and equilibrium floc size at several concentrations without needing to be recalibrated.
3. The new model limits the size of the flocs to that of the Kolmogorov microscale, η, by drastically increasing the rate of breakup as floc sizes approach η.

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