Development of a flocculation sub-model for a 3-D CFD model based on rectangular settling tanks

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ABSTRACT

To assess performance and evaluate alternatives to improve the efficiency of rectangular Gould II type final settling tanks (FSTs), New York City Department of Environmental Protection and City College of NY developed a 3D computer model depicting the actual structural configuration of the tanks and the current and proposed hydraulic and solids loading rates. Fluent 6.3.26 was the base platform for the computational fluid dynamics (CFD) model, for which sub-models of the SS settling characteristics, turbulence, flocculation and rheology were incorporated. This was supplemented by field and bench scale experiments to quantify the coefficients integral to the sub-models. The 3D model developed can be used to consider different baffle arrangements, sludge withdrawal mechanisms and loading alternatives to the FSTs. Flocculation in the front half of the rectangular tank especially in the region before and after the inlet baffle is one of the vital parameters that influences the capture efficiency of SS. Flocculation could be further improved by capturing medium and small size particles by creating an additional zone with an in-tank baffle. This was one of the methods that was adopted in optimizing the performance of the tank where the CCNY 3D CFD model was used to locate the in-tank baffle position. This paper describes the development of the flocculation sub-model and the relationship of the flocculation coefficients in the known Parker equation to the initial mixed liquor suspended solids (MLSS) concentration $X_0$. A new modified equation is proposed removing the dependency of the breakup coefficient to the initial value of $X_0$ based on preliminary data using normal and low concentration mixed liquor suspended solids values in flocculation experiments performed.

Key words | CFD modeling, Final Settling Tanks (FSTs), flocculation

INTRODUCTION

New York City Department of Environmental Protection (DEP) is engaged in a comprehensive update of its Waste Water Treatment Plants (WWTPs) for nitrogen removal to alleviate the problem of hypoxia encountered in the receiving waters of the Long Island Sound (LIS). Specific WWTPs, especially those that discharge into the Upper East River (UER) region are being retrofitted for biological nitrogen removal (BNR). As a consequence of the higher mixed liquor suspended solids (MLSS) loading in the aeration tank effluent, the final settling tanks (FSTs) have been the focus of study to ascertain their capabilities to withstand the higher solids and peak flow loadings and still produce an effluent SS that meets the discharge permit limits. The Wards Island WPCP was designed to provide secondary treatment for an average dry weather flow of 12 m$^3$/s, using the step feed activated sludge process. Recognizing the critical nature of FSTs in upgrading plant performance, a three dimensional computer model was developed to assess proposed enhancement alternatives. The model was specifically developed for the Gould II type rectangular tanks for which a detailed description is given by Ramalingam et al. (2007, 2009) and Xanthos et al. (2010). Griborio (2004) and McCorquodale (2005) presented the development and application of a CFD model for performance prediction of circular FSTs under a

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different geometric configuration while McCorquodale (2006) demonstrated how such a model can be used to improve the performance of rectangular FSTs based on a 2D CFD model. Optimum FST performance requires consideration of several design/operating parameters which include tank geometry, solids settling characteristics, solids loading rate and surface overflow rate. The resulting internal tank hydraulics influence energy dissipation, flocculation, density currents, effluent flow uniformity, short circuiting and sometimes re-suspension of settled sludge which are critical in FST performance. This paper addresses initially the development of the flocculation sub-model that was incorporated with the 3D CFD model since flocculation was identified as one of the vital parameters that influences the capture efficiency of SS in the FSTs. The impact of improved flocculation is typically observed by measuring lower dispersed suspended solids (DSS) values along the path of flow (McCorquodale 2006). In-situ DSS measurements performed in the FSTs of Battery “E” at the Wards Island WWTPs indicated that there is a substantial reduction of DSS as flow passes through the confined region between the inlet port and the influent baffle as shown in Figure 1. Thus the modeling of the flocculation potential within this region was selected as a crucial factor for predicting the concentration of SS in the FST effluent.

FIELD EVIDENCE AND LABORATORY TESTS

DSS tests indicate that in a good performing FST there is a progressive decrease in DSS from the inlet region through the ‘flocculation’ zone as well as in the settling zone. It appears that this decrease is at least in part due to inlet zone flocculation. The unresolved question is: *what are the mechanisms for this flocculation?* There is also a question of the required residence time for flocculation to occur. The jar test is currently the most common way to relate hydrodynamics to flocculation rates. In this test the G value is estimated by the power input, P and the liquid viscosity, ν,

\[ G_{\text{jar}} = \left( \frac{P}{\nu V_{\text{ol}}} \right)^{1/2} \]

where \( V_{\text{ol}} \) is the jar volume. It is noted the \( G_{\text{jar}} \) has units of a velocity gradient (1/s) as in shear strain; however, in a jar test there are two types of stress: shear and normal. Recent literature (Graber 1998, Mei & Hu 1999) shows that both of these stresses and the associated strain tensors are important in flocculation. Since both of these types of stresses are present in the jar test, this G does represent some of this effect on flocculation. However, \( G_{\text{jar}} \) is a volumetric mean which may include zones of floc formation and floc break-up; e.g. there may be floc break-up in the highest shear zones (near the stirrer) and floc formation in the interior zones with low shear but high turbulence intensities. Thus it is likely that the G value that actually should be associated with flocculation is lower than \( G_{\text{jar}} \). The flocculation zone of an FST typically has very low macroscopic shear stresses since the loss of kinetic energy (KE) is not dominantly due to shear but internal instability in which KE is converted to turbulent

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![Figure 1](https://iwaponline.com/wst/article-pdf/63/2/213/445183/213.pdf) | Reduction in DSS value along the length of the final tank.
KE as the influent jet expands. Thus, data from such a test inherently should not be directly used in full scale systems such as FSTs.

There are many anecdotal observations that support the effectiveness of inlet flocculation features in an FST. Most of these involve a skirt that helps to define the flocculation zone and retain the high SS. There is evidence that opposing jets provide better flocculation than uni-directional jets, Shaw et al. (2005). In all cases, the flocculation devices alter the tank hydraulics making it difficult to separate the benefits of the improved flocculation from the improved hydraulics (Griborio et al. 2006).

**FLOCCULATION IN CFD MODELS**

Flocculation is the growth of smaller particles into larger aggregates and the net flocculation in a settling tank is the total sum of floc aggregation and breakup. The mechanism of flocculation has been studied extensively and the current understanding of this aggregation phenomena has been discussed in Maximova & Dahl (2006). The modeling of flocculation is reviewed in Thomas (1999). The mechanisms of flocculation can be subdivided into:

- perikinetic coagulation, which is brought about by molecular diffusion and Brownian motion;
- orthokinetic coagulation, where the spatial and temporal velocity gradients in the liquid cause particles in a region of higher velocity to overtake those moving at slower velocity;
- differences in the settling velocities (differential settling) of the particles whereby faster settling particles overtake those which settle more slowly and coalesce with them.

The mechanism of floc breakup has been identified by Parker et al. (1971) as:

- floc erosion caused by surface shearing forces exceeding the shear strength of the bonds joining the primary particles to the floc, releasing primary particles in the suspension
- floc breakup as a result of filament fracture that occurs when excessive tensile stresses are applied on the floc.

Figure 2 below shows the flow process in a typical Gould II type clarifier. A major reduction of DSS is observed around the inlet zone, which is dominated by turbulence mixing. Laboratory jar tests have also shown that the flocculation rate is directly related to the hydrodynamic shear in the range that is typically achieved in the inlet region of the FST. This suggests that shear related orthokinetic coagulation is the major mechanism for flocculation.

Parker et al. (1970, 1971) developed a differential equation that has been used to model flocculation in a turbulent environment

\[
\frac{dX_i}{dt} = K_B \cdot X \cdot G^2 - K_A \cdot X \cdot X_i \cdot G
\]

where, \(X_i\) is the concentration of primary (large) particles (number/L), \(X\) is the MLSS initial concentration (g/L), \(G\) is the mean velocity gradient (s\(^{-1}\)), \(K_A\) (L/g) and \(K_B\) (s) are experimentally determined coefficients for floc aggregation and break up, respectively.

This equation sums the potential floc formation due to turbulent mixing and floc breakup due to the stresses applied on the floc and has been widely used in FST modeling, such as the model developed by Griborio (2004). This is the equation that has been incorporated into the CCNY CFD model for flocculation.

![Figure 2](https://iwaponline.com/wst/article-pdf/63/2/213/445183/213.pdf) | Illustration of typical Gould II type clarifier.
DEFINITION OF G

The velocity gradient G in the equation above has not yet been defined rigorously. The most frequently cited study was by Camp & Stein (1943),
\[
\Phi = \mu G^2 = \mu \left[ \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial v}{\partial x} \right)^2 \right] (2)
\]
where they introduced the root-mean-square velocity gradient as an approximation to the fluid shear velocity G, \( \Phi \) is the dissipation function or viscous energy dissipation rate per unit volume, and \( \mu \) is the dynamic viscosity. Several researchers (Timothy & Mark 1997; Graber 1998; Francisco & Ismael 2005) have shown that the traditional definition of G should be modified to:
\[
\mu G^2 = \mu \left[ 2 \left( \frac{\partial u}{\partial y} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + 2 \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right] (3)
\]
This includes the particle collisions due to the relative motion caused both by shear strain and normal strain. Assuming locally Gaussian and isotropic turbulence, the G can be also calculated based on the local turbulence kinetic energy dissipation rate \( \epsilon \) (Mei & Hu 1999), represented as:
\[
G = \sqrt{\frac{\epsilon}{\nu}} (4)
\]
Where \( \nu \) is the kinematic viscosity. This method of calculating G includes all the shear and normal components of the flow and can be easily implemented with the k-\( \varepsilon \) turbulence model. The result is also intrinsically the same as given by equation 5 from the definition of energy dissipation term in the k-\( \varepsilon \) model. The flocculation coefficients \( K_A \) and \( K_B \) in equation (1) are typically determined using jar test experiments. In this test the G value is estimated by the power input, \( P \) and the viscosity \( \nu \);
\[
G = \sqrt{\frac{P}{\nu V}} (5)
\]
where \( V \) is the total volume of the jar. This averaged G value for a jar test is usually provided by the manufacturer in the form of a chart that plots G vs. the RPM of the stirrer. Experiments (Ducoste 1997) have shown that while a constant power input has been applied to a stirrer in a jar, turbulence intensity and local turbulent energy dissipation rate varies and is dependent on the impeller type and jar size. Additionally, the calculation of G by the traditional jar test method assumes total transfer of power and by dividing the entire volume it gives an average value for the reactor. However, flocculation is a local phenomenon and average values are not appropriate when modeling FSTs. Thus, applying flocculation coefficients determined by the jar test to the full-scale FST is questionable (Graber 1998). In fact, Equation 5 is derived from the case of an one-dimensional, laminar flow, where the G-value is homogeneous. In FSTs, the total dissipation of turbulent flow is caused by the large scale mean velocity gradient and the turbulent dissipation at a much smaller scale, the Kolmogorov micro scale (\( \eta \)). Hence, G is not a conservative variable and cannot be simply averaged without accounting for the distribution mentioned above.

Therefore, the value of G in the jar test was calculated using the CFD model by simulating the test in the model and the resultant G value was used to perform nonlinear data regression on multiple jar test flocculation data to obtain the flocculation coefficients \( K_A \) and \( K_B \), namely \( 8.5 \times 10^{-4} \) (L/g) and \( 7.8 \times 10^{-8} \) (s), respectively. The volume weighted average of G provided by the manufacturer was plotted in Figure 3 along with the values calculated from equation 5. Numerical simulations have shown that the value of mass weighted G calculated from the CFD simulations result in smaller values than that obtained from the manufacturer’s chart.

MODEL CALIBRATION

The calibration of floc aggregation and break-up coefficient, \( K_A \) and \( K_B \), can be performed in a flocculation jar test.

**Figure 3** | Plots of flocculation coefficient \( K_A \) vs. G obtained from.
The integrated form of Parker’s equation (1) for the calculation of flocculation in a batch flocculator is given by equation (6) (Wahlberg et al. 1994):

\[ X(t) = \frac{K_B \cdot G}{K_A} + \left( X_0 - \frac{K_B \cdot G}{K_A} \right) \cdot e^{-\frac{K_A \cdot X_0}{K_B}} G t \]  

(6)

where \( X_0 \) is the initial particle concentration and \( X(t) \) is the particle concentration in the jar at time \( t \). The particle concentration \( X_0 \) can be determined from the SS concentration of the supernatant after settling the sample for 30 minutes, and \( X(t) \) is determined from the supernatant SS concentration after settling the flocculated sample at a certain \( G \) value at different jar flocculation intervals. Subsequently the calibration factor \( K_A \) and \( K_B \) can be obtained through data fitting. Traditionally aeration tank effluent was used in the flocculation jar test, thus \( K_A \) and \( K_B \) was calibrated for the MLSS range from 1500–3000 mg/L.

**Modification of Parker’s flocculation model**

Equation 6 represents the main process of growth and decay that are required in a flocculation model. Even though the \( G \) value could be properly defined and correctly calculated through the CFD turbulent model, it does not necessarily represent the actual particle collision frequency in the final settling tank. If the \( G \) value needs to be re-defined to represent the actual collision frequency in a flocculation zone it would appear that the value of \( G \) should represent the collisions due to differential particle acceleration and deceleration in the turbulent eddies as well as collisions due to differential settling and macroscopic velocity gradients. Large floc have different inertia and ‘virtual mass’ compared to primary (unflocculated) particles. This will result in the large particles accelerating and decelerating slower than small particles which under turbulent fluctuations will result in increased relative motion of large and small particles with the consequence of increased probability of collisions. This effect will be similar to the differential settling velocity collision mechanism except that it is dependent on the transfer of coherent kinetic energy into turbulent kinetic energy.

A series of jar tests on flocculation was carried out during November 2009–March 2010 period at the Wards Island WWTP to further test and confirm Parker’s flocculation equation that is currently being used in the model. Samples of the aeration tank effluent were collected for this test and the SS values were in the 1400 to 1600 mg/L range. A portion of this sample was diluted using filtered FST effluent to have the SS in the range of 160 mg/L to 440 mg/L. The range for the diluted sample was typically the range observed when the discrete particle classification tests were carried out during earlier experiments. Both set of samples were then tested using the jar test equipment to compute \( K_A \) and \( K_B \), and the results from this analysis are shown in Figure 4 and Figure 5.

It appears from the results that both \( K_A \) and \( K_B \) are dependent on “\( G \)”, but both have larger values when the sample is diluted. This data shows that the effective collision and breakup frequency is not the same at different SS concentrations. Equation 1 as it stands now, relates the coefficients to both “\( G \)” and the initial SS concentration, \( X_0 \) hence the jar test flocculation experiments suggest that this relationship needs to be further investigated and even modified before using it in the flocculation sub-model.
Several permutations to modify the equation were attempted to fit the collected data to satisfy both the low and high concentration ranges. One hypothesis that is being mulled here is that when the activated sludge has good settling properties (SVI in the 80–120 mL/g range), the primary difference between the low and high concentration sludge is the particle size factor rather than the particle quantity. If particle size is the dominant factor, could the floc break up coefficient be more impacted by the total surface area of the sludge particle rather than the relative numbers present? If the existing equation is re-written without the dependence of X₀ on K_B, the equation will take the following form shown in equation (7):

\[
\frac{dX_l}{dt} = K_B \cdot G^2 - K_A \cdot X_l \cdot G
\] (7)

Figure 6 and Figure 7 have been plotted with the modified equation which reflects the independence of K_B from the initial value of X₀ and the data appears to fit much better than in the previous case using equation 1 as shown in Figure 4 and Figure 5. It appears that the modified result may have resolved the issue of the dependency of flocculation coefficient on the initial SS concentration X₀. This of course is just a single dilution attempt and the authors very well realize that the hypothesis has to be tested for a wide range of dilutions to be proven. This is work that is ongoing and the modified equation will be rigorously tested for different dilution ranges before attempting to come to any definite conclusions.

CONCLUSIONS

Flocculation was identified as a critical parameter in improving final settling tank performance to lower the effluent SS. The flocculation sub-model currently being used in the CCNY 3D CFD model uses the turbulent flocculation equation developed by Denny Parker (1971). The dependence of the floc aggregation and floc break up coefficients on the initial mixed liquor concentration was subjected to tests by conducting jar test experiments at two extreme concentrations. Preliminary conclusions arrived after these experiments suggest that the floc break up coefficient may not be as closely related to the initial concentration as previously thought of. It may be governed by the surface area of the particle more than the quantity of particles as suggested by the better fit obtained using the modified equation (7). The biology of a good settling floc when diluted to the discrete settling range may be more subject to environmental shear forces rather than breakage occurring due to collisions and mixed liquor concentrations. This is part of a series of on-going experiments with more dilution ranges planned for testing prior to arriving at more fundamentally substantiated conclusions.

REFERENCES


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