Simulation of Turbulent Flocculation and Sedimentation in Flocculent-Aided Sediment Retention Basins

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Abstract. We have developed a model which combines Computational Fluid Dynamics (CFD) with multi-dimensional Discretized Population Balance Equations (DPBEs) to simulate turbulent flocculation and sedimentation processes in flocculant-aided sediment retention basins. Our CFD-DPBE model generates steady state flow field data and simulates flocculation and sedimentation processes in a sequential manner. Up-to-date numerical algorithms such as operator splitting and Leveque’s flux-corrected upwind schemes were applied to cope with computational problems caused by complexity and nonlinearity of the population balance equations with advection dominated flow conditions. In a simulation study using a 2-dimensional simplified pond geometry, the applicability of our CFD-DPBE model was demonstrated by tracking mass balances and floc size evolutions and by examining particle/floc size and solid concentration distributions. Our CFD-DPBE model will be a valuable simulation and analysis tool for natural and engineered flocculation and sedimentation systems.

INTRODUCTION

In recent years, various Best Management Practices (BMPs) have been developed that relate to the control of sediments during storm events (USDOT, 2002). Among these BMPs, several suggest that removal of clay and other colloidal-sized particles by retention or detention ponds may be enhanced by the addition of flocculating agents. A few operators are now experimenting with the addition of such agents to the inflows of sediment retention ponds and often have observed greatly improved retention properties of the ponds. Reading contemporary literature and also talking to sediment pond operators both support the reasoning that flocculent-aided sediment retention ponds are going to become increasingly important in future years as a means to minimize the detrimental effects of erosion and non-point-source water pollution (Gowdy and Iwinski, 2007; Harper, 2007). To date, use of flocculating agents has been driven more by practicing engineers than by researchers. However, the operation of sediment retention ponds is complicated, involving turbulent flow of variable intensity, different pond geometries, particle growth due to flocculation, sedimentation of particle size classes at different rates, and various schemes for time-dependent flocculent additions. Most existing pond systems are not designed in a consistent manner based on fundamental principles. For example, many designs are based simply on an ad hoc rule such as a set pond volume per hectare of drained area (Akan and Houghtalen, 2003). Therefore, the entire field would benefit from a better understanding of the flocculation and sedimentation processes and the availability of a realistic, physically-based model for designing and optimizing the automated operation of sediment retention ponds. This paper deals primarily with the mathematical formulation and computational aspects underlying flocculation and sedimentation processes in flocculent-aided sediment retention ponds. In this study, a discretized particle transport-reaction model combined with a fluid dynamics model (CFD-DPBE model) was developed and its applicability was tested for a model pond system.

BACKGROUND AND MATHEMATICAL MODELS

The CFD-DPBE model consists of (1) CFD software to obtain the Reynolds-averaged turbulent flow field, and (2) multi-dimensional DPBE software containing particle/floc aggregation and break-up kinetics to simulate flocculation and sedimentation within the previously-obtained flow field.

Computational Fluid Dynamics (CFD)

The Reynolds-Averaged continuity and Navier-Stokes (RANS) equations, containing a two-equation $k - \varepsilon$ turbulence model, were solved using FLOW-3D® software to simulate turbulent fluid motion within a retention pond. In the CFD-DPBE model, particles/flocs are assumed to travel via fluid motion and to aggregate or disintegrate due to impact and shear forces or effects (Fox, 2003; Prat and Ducoste, 2006). The velocity gradient ($G = \sqrt{\nu/\varepsilon}$), which is obtained from the two-equation $k - \varepsilon$ turbulence model, controls the rate of particle/floc aggregation and break-up in the DPBEs and thus serves as a coupling term between the turbulent flow field (CDF problem) and the DPBEs (Prat and Ducoste, 2006).
Discretized Population Balance Equations (DPBES)

With a given flow field obtained from CFD software, the multi-dimensional DPBES are used to simulate particle/floc transport and flocculation in the ponds. Following Prat and Ducoste (2006), a generic mathematical model for the DPBES may be written as:

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x} \left( U_i n_i \right) + \frac{\partial}{\partial y} \left( U_j n_i \right) + \frac{\partial}{\partial z} \left( U_k n_i \right) = \frac{\partial}{\partial x} \left( C^{\mu} \varepsilon \frac{\partial n_i}{\partial x} \right) + \frac{\partial}{\partial y} \left( C^{\mu} \varepsilon \frac{\partial n_i}{\partial y} \right) + \frac{\partial}{\partial z} \left( C^{\mu} \varepsilon \frac{\partial n_i}{\partial z} \right)$$

$$= \text{agg break}, -n_i \frac{\partial n_i}{\partial z}$$

In Equation (1), $n_i = n(x, y, z, D_i, t) = \text{number concentration of flocs of linear class size } D_i(i=1, 2, ..., i_{\text{max}}; D_1 \leq D_i \leq D_{\text{max}}; \text{for all } D_i, n_i \text{ is the population density function}, x, y, z, t = \text{position and time}, <U_i>, <U_j>, \text{and } <U_k> = \text{mean fluid velocity components in the } x, y \text{ and } z \text{ directions}, \rho = \text{fluid density}, k = k(x,y,z,t) = \text{turbulent kinetic energy}, \varepsilon = \varepsilon(x,y,z,t) = \text{turbulent energy dissipation rate}, C^{\mu} = 0.09 = \text{standard value of a CFD model constant}, \text{and } u_{\text{set}} = \text{settlement velocity of the } i\text{-th floc class due to gravity.}$

Kinetics of particle/floc aggregation and breakage

Key components of the multi-dimensional DPBES (Equation (1)) are the sink and source terms which characterize the aggregation and break-up kinetics ($\text{agg break}$). These terms are written as a series of differential equations in Equation (2) (Hounslow et al., 1988; Spicer and Pratsinis, 1996).

$$\frac{\partial n_i}{\partial t} = n_i \sum_{j=1}^{2^{\max}} \beta(\text{i-j})\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-j)\beta(i-
layer of the turbulent mixing zone was set as a closed boundary for fluid but an open boundary for settling particles/flocs. In other words, settling particles/flocs were allowed to move through the bottom layer of the zone, thereby leaving the domain, while fluid remained in the computational domain. The volumetric influent flow rate was set initially at a fixed value of 8 m³/min, which is equivalent to 2.5 minutes of mean hydraulic residence time $(t_{\text{mean}} = \text{Volume/FlowRate})$ within the computational turbulent mixing zone. However, to create different levels of fluid turbulence and to compare the effects of turbulent intensity on flocculation efficiency, influent flow velocities were set at three different values (0.222, 0.334, and 0.667 m/s) by adjusting the inlet width. Influent clay particles (monomers) were modeled as spheres with 1 μm diameter and 2.65 kg/L density. The influent solid concentration was set as 2 g/L, which is equivalent to a particle number concentration as $1.47 \times 10^{15}$/m³.

**RESULTS AND DISCUSSION**

In the CFD simulation with the commercial FLOW-3D© code, three steady state flow fields were obtained for the model inlet zone. These flow fields are shown in Figure 2, with (a) Case 1: low, (b) Case 2: moderate, and (c) Case 3: high turbulent conditions, which were induced by the different influent flow velocities of 0.222, 0.334, and 0.667 m/s. Arrows and colors in Figure 2 represent mean flow velocity vectors ($<U>$) and shear rate distributions ($G=(e/v)^{1/2}$), respectively. In the low turbulent condition (Case 1), velocity vectors were uniformly directed from the inlet to the outlet and shear rates were low, with a maximum shear rate of 13.5 s⁻¹. However, in the high turbulent condition (Case 3), a swirling zone above the inlet was identified, and high shear rates near the inlet were observed with a maximum shear rate of 79.3 s⁻¹. Moderate turbulent flow conditions (Case 2) showed flow characteristics between the two extreme cases. Later in this paper we will illustrate the effects of velocity and shear rate distributions on flocculation efficiencies.

With steady state flow field data obtained from the CFD simulations, solutions to the multi-dimensional DPBEs were obtained with an in-house program. After verifying consistency and stability of the developed program, mass mean particle/floc size ($D_{43}$) and solid concentration distributions at steady state conditions were investigated in the computational domain. Figures 3 and 4 show the distributions of mass mean particle/floc size and solid concentration, respectively, for the three different turbulent flow fields computed. In Case 1 with low turbulence, mass mean particle/floc sizes were limited to below 27 μm, and solid concentrations were homogeneously distributed without particle/floc deposition. Contrarily, in Case 3 with high turbulence conditions, mass mean particle/floc sizes were expanded to above 50 μm, and the solid concentration became heterogeneous with an intensive concentration area near the outlet.
turbulence, mass mean particle/floc sizes grew up to 195 μm, which are of sufficient size to escape from the computational domain by settling and deposition on the bottom of the inlet zone of the sediment basin. Thus, a longitudinal gradient of solid concentrations was observed in the computational domain due to particle/floc sedimentation. The moderate turbulent flow condition produced results approximately midway between the two extremes. The other interesting finding is that the swirling zones above the inlet in Cases 2 and 3 were found to work as small flocculation compartments. Particles/flocs traveling through these swirling zones are more subject to flocculation and thus tend to grow larger than those passing through the other zones. For example, in Case 3, particles/flocs in the swirling zone grew up to about 200 μm, while those in the region immediately adjacent remained below 50 μm.

**Table 1.** Flow field characteristics and flocculation/sedimentation efficiencies in the computational domain for three different turbulent conditions. *Maximum values in the computational domain. †Mean values at the outlet.

<table>
<thead>
<tr>
<th>Flow Field Characteristics</th>
<th>Flocculation/Sedimentation Efficiencies</th>
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<tr>
<td></td>
<td>Mass particle/floc size ($D_{43}^{*\text{a}}$) (μm)</td>
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<tr>
<td>$V_{in}$ (m/s)</td>
<td>$G^*$ (s⁻¹)</td>
</tr>
<tr>
<td>Case 1</td>
<td>0.222</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.334</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.667</td>
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Summarized in Table 1 are results from CFD-PBE simulations upon reaching steady state. Mass mean particle/floc size ($D_{43}^{*\text{a}}$) and deposited mass fraction (Mass depositing acc/Mass in acc) in Case 3 with the highest influent flow velocity and shear rate were up to 7.5 and 12.1 times higher than those in Case 1 with the lowest influent flow velocity and shear rate. As expected, turbulence enhances flocculation, at least up to a certain point. In Case 1, clay particles traveling through the mixing zone are not aggregating sufficiently and thus a large fraction of particles/flocs may not settle appropriately in the subsequent sedimentation basin. In conclusion, considering the results in Table 1 from the steady state CFD-PBE simulations, conditions in the turbulent mixing zone were observed to have critical effects on both flocculation and subsequent sedimentation efficiencies. How to optimize this situation is an important topic for future study, both experimental and theoretical.

**CONCLUSIONS AND RECOMMENDATIONS**

A CFD-DPBE model was successfully developed to generate steady state flow field data and to numerically simulate flocculation and sedimentation processes in a 2-D representation of the inlet zone for a sediment retention pond. The CFD-DPBE model was demonstrated to be a promising simulator of flocculent-aided storm-water retention ponds. Furthermore, it may be applied to flocculation and sedimentation occurring in various natural and engineered systems such as water/wastewater treatment, nano-material synthesis, or sediment-depositing estuary systems.

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**LITERATURE CITED**


