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

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Abstract. We have developed a model which combines **C**omputational **F**luid **D**ynamics (CFD) with multi-dimensional **D**iscretized **P**opulation **B**alance **E**quations (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 **B**est **M**anagement **P**ractices (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 **R**eynolds-**A**veraged continuity and **N**avier-**S**tokes (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 ($G=\sqrt{\varepsilon/v}$), 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:

$$\left[\frac{\partial n_i}{\partial t}\right] + \left[\frac{\partial}{\partial x}(\langle U_x\rangle n_i) + \frac{\partial}{\partial y}(\langle U_y\rangle n_i) + \frac{\partial}{\partial z}(\langle U_z\rangle n_i)\right]$$
$$-\left[\frac{\partial}{\partial x}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial z}\right)\right]$$
$$= (agg/break)_i - u_{gi}\frac{\partial n_i}{\partial z} \qquad (1)$$

In Equation (1), $n_i = n(x, y, z, D_i, t)$ = number concentration of flocs of linear class size D_i ($i=1, 2, \dots i_{max}$; $D_1 \leq D_i \leq D_{max}$; for all D_i, n_i is called the population density function), x, y, z, t = position and time, $<U_x>$, $<U_y>$, and $<U_z>$ = mean fluid velocity components in the x, y and z directions, ρ = fluid density, $k = k(x,y,z,t)$ = turbulent kinetic energy, $\varepsilon = \varepsilon(x,y,z,t)$ = turbulent energy dissipation rate, $C_\mu = 0.09$ = standard value of a CFD model constant, and u_{gi} = settlement velocity of the i-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 ($(agg/break)_i$). These terms are written as a series of differential equations in Equation (2) (Hounslow *et al.*, 1988; Spicer and Pratsinis, 1996).

$$\frac{\partial n_i}{\partial t} = n_{i-1}\sum_{j=1}^{i-2}2^{j-i+1}\alpha(i-1,j)\beta(i-1,j)n_j + \frac{1}{2}\alpha(i-1,i-1)\beta(i-1,i-1)n_{i-1}^2$$
$$-n_i\sum_{j=1}^{i-1}2^{j-i}\alpha(i,j)\beta(i,j)n_j - n_i\sum_{j=i}^{(max\,i)}\alpha(i,j)\beta(i,j)n_j - a(i)n_i + \sum_{j=i+1}^{(max\,i)+2}b(i,j)a(j)n_j \qquad (2)$$

In Equation (2), several empirical or theoretical factors or functions ($\alpha, \beta, a,$ and b) are incorporated into the aggregation and break-up kinetics. In particle/floc aggregation kinetics, the collision efficiency factor (α) represents the physicochemical properties of solid and liquid which cause inter-particle attachments (aggregation), while the collision frequency factor (β) represents the mechanical properties of fluids which induce inter-particle collisions. The particle/floc breakage constant (a) and the break-up distribution function (b) represent the kinetics of the breakage process and the fate of the broken fragments, respectively.

NUMERICAL METHODS

As the first step of the CFD-DPBE simulation procedure, the commercial CFD code (FLOW-3D®) was used to generate steady state flow field data in the influent,

turbulent mixing zone of the model pond. Among various built-in models of FLOW-3D®, RANS and the two equation k-ε turbulence models were applied to simulate flow velocities and turbulence. This resulted in nodal values for ($\langle Ux\rangle, \langle Uy\rangle, \langle Uz\rangle, k$, and ε) (Equations (1)).

After the CFD simulation, the multi-dimensional DPBEs were solved with an in-house program based on the finite-difference method and codified with MATLAB®. In these simulations, two significant numerical obstacles were identified and overcome in our preliminary research. Firstly, the complexity and nonlinearity of a large number of coupled DBPEs in an advection-dominated application resulted in computational overload. To increase computational efficiency, we applied an operator splitting algorithm in which particle/floc advection was split from particle/floc dispersion-reaction (Langseth *et al.*, 1996). Secondly, a standard central-differencing **F**inite **D**ifference **M**ethod (FDM) was not optimal for simulating advection-dominated flow conditions with high Peclet numbers. Therefore, Leveque's flux-corrected upwind algorithm was applied to solve scalar transport equations in advection dominant conditions (Leveque, 1996).

Shown in Figure 1 are schematic diagrams of a flocculent-aided storm-water retention pond which consists of a turbulent mixing zone at the inlet and a subsequent sedimentation basin. When applying chemical flocculants, the turbulent mixing zone at the inlet will function as an effective flocculation region with high fluid turbulence. Chemical flocculent is assumed to be injected at the inlet of the pond so that particles/flocs will begin aggregating immediately after entering the basin.

Initial 2-D simulations were applied to a turbulent mixing zone having dimensions of 2 m (height) $\times$ 10 m (length). The size of each computational cell was set as 0.2 m $\times$ 0.2 m. Both inlet and outlet were treated as continuous boundaries ($Flux_{in}= Flux_{out}$), while the water surface was treated as a closed boundary ($Flux_{out} = 0$). The bottom
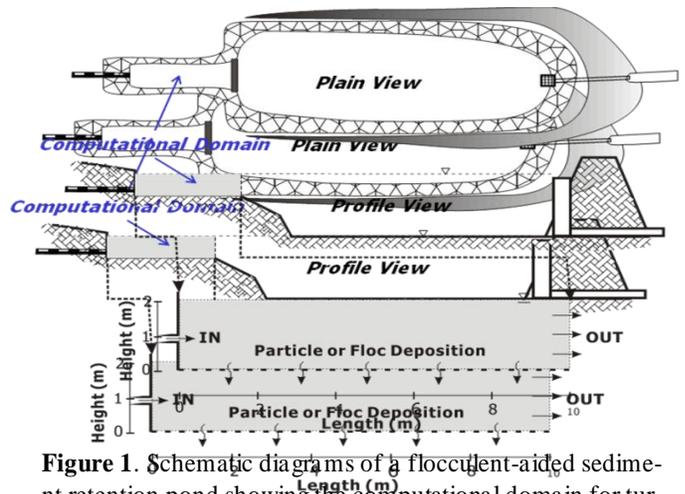

Figure 1. Schematic diagrams of a flocculent-aided sedime-nt retention pond showing the computational domain for tur-bulent mixing zone and flocculation of a flocculent-aided storm-water retention pond with a fore-bay flocculation basin and a discharge drain.

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 m^3/m/min, which is equivalent to 2.5 minutes of mean hydraulic residence time ($t_{mean} = Volume/FlowRate$) 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 1.47×10^{15} /m^3.

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 ($G=(\varepsilon/\nu)^{1/2}$), 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
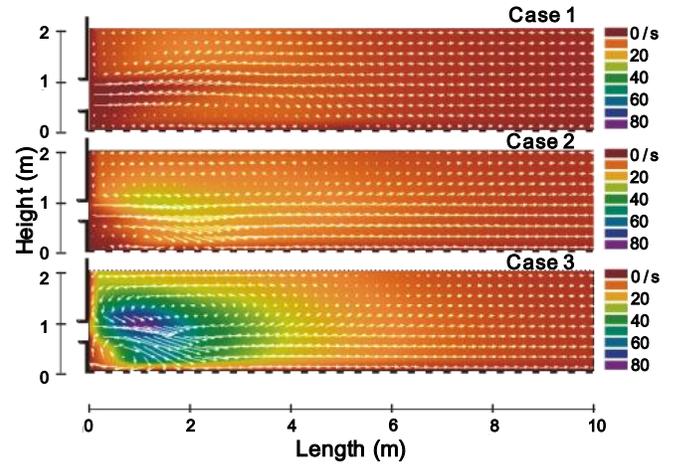

Figure 2. Steady state flow field profiles from CFD simulation for (a) Case 1: low turbulence, (b) Case 2: moderate turbulence, and (c) Case 3: high turbulence. Arrows and colors represent flow velocities and shear rates, respectively.
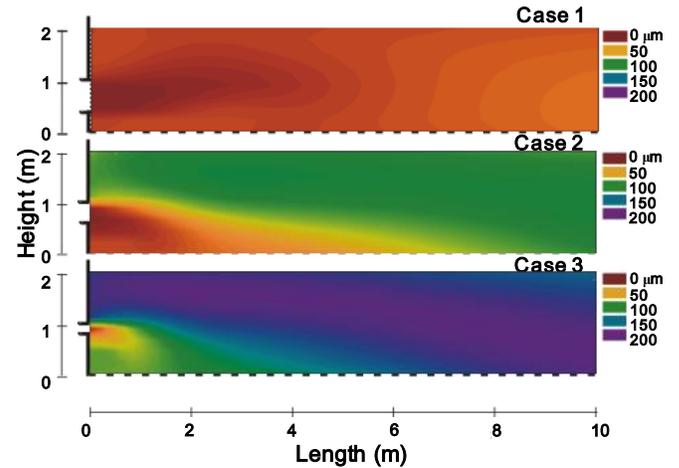

Figure 3. Mass mean floc diameter (D$_{43}$) distributions in the computational domain. The distributions of Case 1, Case 2, and Case 3 are listed from the top.
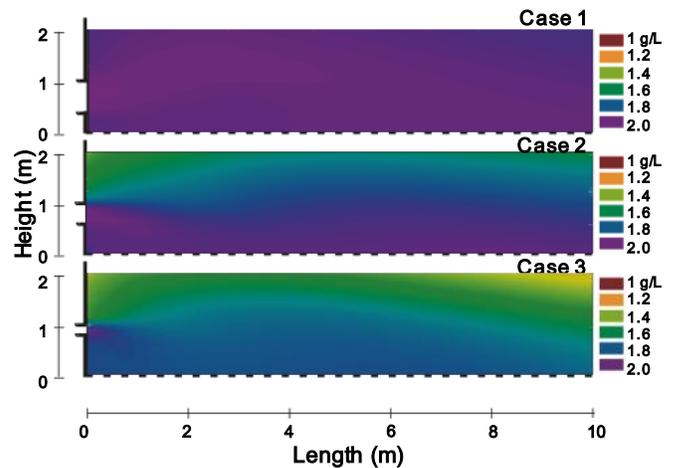

Figure 4. Solid concentration distributions in the computational domain. The distributions of Case 1, Case 2, and Case 3 are listed from the top.

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.

	Flow Field Characteristics		Flocculation/Sedimentation Efficiencies		
	v_{in} (m/s)	G^* (s^{-1})	D_{43}[**] (μm)	$\dfrac{Mass_{deposit,acc}}{Mass_{in,acc}}$	(%)
Case 1	0.222	13.5	24.59	1.204	
Case 2	0.334	28.3	105.2	4.787	
Case 3	0.667	79.3	183.2	14.54	

Summarized in Table 1 are results from CFD-PBE simulations upon reaching steady state. Mass mean particle/floc size (D_{43}) and deposited mass fraction ($Mass_{deposit,acc} / Mass_{in,acc}$) 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-DPBE 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.

LITERATURE CITED

Akan, A. O., and R. J. Houghtalen, 2003, *Urban Hydrology, Hydraulics and Stormwater Quality*, John Wiley & Sons, Hoboken, NJ.

Fox, R. O., 2003, *Computational models for turbulent reacting flows*, Cambridge University Press, UK.

Gowdy, W., and S. R. Iwinski, 2007, Removal Efficiencies of Polymer Enhanced Dewatering Systems. *In Proceedings of the 9th Biennial Conference on Stormwater Research & Watershed Management*, Orlando, FL,May 2 - 3, 2007.

Harper, H. H., 2007, Current research and trends in alum treatment of stormwater runoff. *In Proceedings of the 9th Biennial Conference on Stormwater Research & Watershed Management*, Orlando, FL,May 2 - 3, 2007.

Hounslow, M. J., R. L. Ryall, and V. R. Marshall, 1988, A discretized population balance for nucleation, growth, and aggregation, *AIChE Journal*, 34(1), 1821-1832.

Langseth, J. O., A. Tveito, and R. Winther, 1996, On the convergence of operator splitting applied to conservation laws with source terms, *SIAM J. Numer. Anal.*, 33, 843-863.

Leveque, R. J., 1996, High-resolution conservative algorithms for advection in incompressible flow, *SIAM J. Numer. Anal.*, 33(2), 627-665.

Prat, O. P., and J. J. Ducoste, 2006, Modeling spatial distribution of floc size in turbulent processes using the quadrature method of moment and computational fluid dynamics, *Chemical Engineering Science*, 61, 75-86.

Spicer, P. T., and S. E. Pratsinis, 1996a, Coagulation-fragmentation: universal steady state particle size distribution, *AIChE Journal*, 42, 1612.

USDOT, 2002, *Stormwater Best Management Practices in an Ultra-Urban Setting: Selection and Monitoring*, from *http://www.fhwa.dot.gov/environment/ultraurb/index.htm*