Numerical Simulation of Turbulence-Induced Flocculation and Sedimentation in a Flocculant-Aided Sediment Retention Pond

Byung Joon Lee¹†, Fred Molz²

¹Constructional and Environmental Engineering, Kyungpook National University Sangju 742-711, Korea
²Environmental Engineering & Earth Sciences, Clemson University, Clemson, SC 29634, USA

Abstract

A model combining multi-dimensional discretized population balance equations with a computational fluid dynamics simulation (CFD-DPBE model) was developed and applied to simulate turbulent flocculation and sedimentation processes in sediment retention basins. Computation fluid dynamics and the discretized population balance equations were solved to generate steady state flow field data and simulate flocculation and sedimentation processes in a sequential manner. Up-to-date numerical algorithms, such as operator splitting and LeVeque flux-corrected upwind schemes, were applied to cope with the computational demands caused by complexity and nonlinearity of the population balance equations and the instability caused by advection-dominated transport. In a modeling and simulation study with a two-dimensional simplified pond system, applicability of the CFD-DPBE model was demonstrated by tracking mass balances and floc size evolutions and by examining particle/floc size and solid concentration distributions. Thus, the CFD-DPBE model may be used as a valuable simulation tool for natural and engineered flocculation and sedimentation systems as well as for flocculant-aided sediment retention ponds.

Keywords: Computational fluid dynamics, Flocculation, Modeling, Population balance equation, Sedimentation

1. Introduction

In recent years, various best management practices (BMPs) related to the control of sediments during storm events have been developed. Among these BMPs, several suggest that the 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 sediment inflow, which can greatly improve the retention properties of ponds in some cases. Contemporary literature and sediment pond operators support the conclusion that flocculant-aided sediment retention ponds are going to be increasingly important in future as a means of minimizing the detrimental effects of erosion and nonpoint-source water pollution [1-3]. To date, use has been driven more by practicing engineers than by academics. However, the operation of such ponds is complex, 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 flocculant 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 [4]. Hence, the entire field would benefit from a better understanding of flocculation and sedimentation processes and the availability of a realistic, physically based model for designing and optimizing the automated operation of sediment retention ponds. Therefore, there is a need for a realistic theory describing flocculation and non-homogeneous turbulent sedimentation in retention ponds, a practical method for solving the rather complex governing equations, and performance of the required small- and large-scale experiments necessary to characterize the parameters and functions that the theory contains. This paper primarily discusses the mathematical formulation and computation underlying flocculation and sedimentation processes in flocculant-aided sediment retention ponds.

One of the most realistic ways to simulate flocculation and non-homogeneous turbulent sedimentation in retention ponds is by applying population balance equations (PBEs) within a computational fluid dynamics (CFD) framework for solving the Navier–Stokes equations (mass and momentum conservation equations). PBEs have been used to simulate particle/floc ag-

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†Corresponding Author
E-mail: blee@knu.ac.kr
Tel: +82-54-530-1444   Fax: +82-54-530-1449

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gregation phenomena for many scientific and engineering applications. Most PBES derive from the Smoluchowski equation describing a simple particle/floc aggregation process. They are now generalized by incorporating various additional processes, such as particle/floc breakage models, shaping and growth strategies, chemical interaction models, etc. [5-16]. Application of PBES, ranging from fundamental scientific research to advanced engineering applications, has become more practical as computational speed and capacity have increased. However, such applications are still at the forefront of engineering research.

In multi-dimensional simulation, such as simulation of retention pond dynamics, conventional PBES continue to be computationally demanding even with modern computer technologies. For example, in conventional PBES, particles/flocs aggregate in a sequential manner from singlet, to doublet, then to triplet, and so on. Thus, conventional PBES require thousands to millions of particle/floc size classes and associated differential transport-reaction equations to simulate particle/floc growth from nano- or micro-sized constituent monomers to milli-sized aggregates that settle due to gravity. To overcome this computational difficulty in multi-dimensional simulations, the discretized PBE (DPBE) and quadrature method of moments (QMOM) have been proposed.

In the QMOM approach, moments of the particle/floc size distribution, instead of number concentrations of particles/flocs, are used as dependent variables in differential transport-reaction equations to reduce the computational loads that occur in multi-dimensional applications. The lower-order moments then yield key monitoring indices, such as particle/floc sizes and solid concentrations, indirectly through the use of product-difference algorithms [10, 12, 14, 17, 18]. Thus, QMOM provides computational advantages but imposes difficulties for scientists or engineers attempting to understand results because of the more abstract formulation and resulting algorithms.

In the DPBE methodology, particle/floc number concentrations can be tracked as dependent variables in differential transport-reaction equations, similar to the method of conventional PBES. However, the DPBE formulation differs from that of conventional PBES because particles/flocs of DBPE are assumed to double their size from singlet to doublet and then to quadruplet, etc., in the flocculation process. Thus, with only dozens of defined particle/floc size classes, particles/flocs can grow to sizes susceptible to gravity-induced settling, which are thousands to millions of times larger than the size of monomers [7, 12, 19, 20]. In contrast to QMOM, DPBE directly tracks key indices, such as particle/floc sizes and solid concentrations, by simply integrating differential equations without additional data processing steps. Thus, with respect to clearness of results, the DPBE approach may be more intuitive and advantageous than QMOM. Therefore, in this research, the discretized particle transport-reaction model combined with a fluid dynamics model (CFD-DPBE model) was set up, and its applicability was tested in a model pond system. The mathematical formulation and application strategy of the CFD-DPBE model were studied in a two-dimensional computational domain representing the vertical and flow-parallel cross section of a flocculent-aided sediment retention pond.

### 2. Material and Methods

#### 2.1. 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 transport, flocculation, and sedimentation within the pre-obtained flow field.

##### 2.1.1. Computational fluid dynamics

The Reynolds-averaged continuity and Navier–Stokes (RANS) equations, containing a two-equation \( k - \varepsilon \) turbulence model, were solved using FLOW-3D software (Flow Science Inc., Santa Fe, NM, USA) 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 [14, 17, 21].

The RANS equations consist of mass and momentum conservation equations in the differential form given by Eqs. (1) and (2), respectively (we now use the summation convention in writing the 3D equations, wherein sums over the three spatial coordinates are understood when an index is repeated).

\[
\frac{\partial \bar{U}_i}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial \bar{U}_i}{\partial t} + (\bar{U}_j \cdot \nabla) \bar{U}_i = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \bar{U}_i \tag{2}
\]

where:
- \( \bar{U}_i \) is the time-averaged velocity component (m/s), \( t \) represents time (s), \( \rho \) is the fluid density (kg/m$^3$), \( p \) is the piezometric pressure (kg/m$^3$s$^2$), and \( \nu \) is the kinematic viscosity of the fluid (m$^2$/s).

A symmetric second-order tensor \( \bar{\epsilon}_{ij} \) representing Reynolds normal or shear stresses (m$^2$/s$^2$) is modeled with Eq. (3), and \( \bar{v}_p \), the turbulent viscosity (Ns/m$^2$), is specified by Eq. (4).

\[
\bar{\epsilon}_{ij} = 2\frac{k}{3} \delta_{ij} \nu_t \tag{3}
\]

\[
\nu_t = C_\tau \frac{k^2}{\epsilon} \tag{4}
\]

In Eqs. (1) and (2), \( i \) and \( j \) are indices, \( x \) represents coordinate directions (\( i = 1, 2, 3 \) for \( x, y, z \) directions, respectively). \( \bar{U}_i \) is the time-averaged velocity component (m/s), \( t \) represents time (s), \( \rho \) is the fluid density (kg/m$^3$), \( p \) is the piezometric pressure (kg/m$^3$s$^2$), and \( \nu \) is the kinematic viscosity of the fluid (m$^2$/s).

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\[
\frac{\partial k}{\partial t} + (\bar{U}_i \cdot \nabla) k = \nabla \cdot \left( \frac{\nu_t}{\sigma_k} \nabla k \right) + P - \varepsilon \tag{5}
\]
\[
\frac{\partial \bar{c}_i}{\partial t} + \nabla \cdot (\bar{U}_i \bar{c}_i) = \nabla \cdot \left( \frac{\bar{c}_i k_i}{\sigma} \nabla \bar{P}_i \right) + \frac{1}{k_i} \left( C_{ci} \bar{P}_i - C_{ci} \bar{c}_i \right) \\
\bar{P} = -\left( \left( \frac{\partial \bar{U}_i}{\partial x_j} \right) \right) \frac{\partial \bar{U}_i}{\partial x_j}
\]

(6)

\[
2.1.2 \text{ Multi-dimensional discretized population balance equations}
\]

With a given flow field obtained from CFD software, the multi-dimensional DPBE is used to simulate particle/floc transport and flocculation in the ponds. Following Prat and Ducoste [14], a generic mathematical model for the DPBE may be written as

\[
\left[ \frac{\partial n_i}{\partial t} \right] = \left( \frac{\partial}{\partial x} \right) \left( \frac{\partial (U_{ix} n_i)}{\partial x} \right) + \left( \frac{\partial}{\partial y} \right) \left( \frac{\partial (U_{iy} n_i)}{\partial y} \right) + \left( \frac{\partial}{\partial z} \right) \left( \frac{\partial (U_{iz} n_i)}{\partial z} \right) - \left( \frac{\partial C_{ix} \frac{k_i^2}{k} \frac{\partial n_i}{\partial x}}{\partial x} \right) - \left( \frac{\partial C_{iy} \frac{k_i^2}{k} \frac{\partial n_i}{\partial y}}{\partial y} \right) - \left( \frac{\partial C_{iz} \frac{k_i^2}{k} \frac{\partial n_i}{\partial z}}{\partial z} \right)
\]

(II)

\[
\left( \frac{\partial}{\partial x} \left( \frac{C_{ix} \frac{k_i^2}{k} \frac{\partial n_i}{\partial x} \right) + \left( \frac{\partial}{\partial y} \left( \frac{C_{iy} \frac{k_i^2}{k} \frac{\partial n_i}{\partial y} \right) + \left( \frac{\partial}{\partial z} \left( \frac{C_{iz} \frac{k_i^2}{k} \frac{\partial n_i}{\partial z} \right) \right) \right)
\]

(III)

\[
= (agg/break), -u_{x} \frac{\partial n_i}{\partial x}
\]

(IV)

In Eq. (8), \( n_i = n(x, y, z, D, t) \) is number concentration of flocs (/m³) of linear class size \( Di \) (m) \( (i=1, 2, ..., i_{max}) \). \( i = 1 \) is the smallest class size; \( i = i_{max} \) is the largest class size. \( \bar{U}_{ix}, \bar{U}_{iy}, \bar{U}_{iz} \) are mean fluid velocity components in the \( x, y, z \) directions (m/s); \( \rho \) is fluid density (kg/m³); \( \mu \) is fluid viscosity (kg/m/s); \( \varepsilon \) is turbulent energy dissipation rate (m²/s); \( C_{ij} \) is turbulent kinetic energy (m²/s²); \( \xi \) is position and time; \( \bar{U}_{ix}, \bar{U}_{iy}, \bar{U}_{iz} \) mean fluid velocity components in the \( x, y, z \) directions (m/s); \( \rho \) is fluid density (kg/m³); \( k = k(x, y, z, t) \) is turbulent kinetic energy (m²/s²); \( \varepsilon \) is turbulent energy dissipation rate (m²/s); \( C_{ij} \) is standard value of a CFD model constant (see Eq. (4)); and \( u_{x} \) is settlement velocity (m/s) of the \( i \)th floc class due to gravity. On the left-hand side of Eq. (8), the respective terms in brackets represent the storage change (II), particle/floc mean advection (II), and the turbulent dispersion of the particle/floc (III), while on the right-hand side, the source/sink terms (IV) represent the net effects of aggregation, break-up, and settling due to gravity [14]. The coefficients or functions in these later terms are largely empirical and must be determined by experiment. The quantities depending on the turbulent fluid variables \( \bar{U}_{ix}, \bar{U}_{iy}, \bar{U}_{iz}, k, \) and \( \varepsilon \) couple the DPBE equations (Eq. (8)) to the CFD equations (Eqs. (1)–(7)). However, as currently formulated, the CDF equations are solved independent of the DPBE.

To track particle/floc fates with the DPBE, both Eulerian and Lagrangian tracking methods are applicable. However, in this research, the Eulerian method rather than the Lagrangian method, which tracks individual particles or flocs, was applied to observe the distribution of scalars within the entire computational domain (Eulerian [12, 14, 18, 22, 23] and Lagrangian [24]).

To obtain the particle/floc settling velocity in Eq. (8), Stokes equation was used in the context of fractal theory, which represents the structural characteristics of aggregating particles/flocs. Even though many complex and elaborate particle/floc settling equations have been developed, including those involving interaction or drag coefficients with ambient flow, the standard Stokes equation was applied as a prototype in this research [25, 26]. Fractal theory describes particle/floc packing or growth structure with constituent monomers in which particle/floc size follows a power-law function with respect to the number of monomers in a given floc size (Eq. (10)) [27–32]. Stokes equation combined with fractal theory is given by Eq. (9) [16, 33–35]. In Eqs. (9) and (10), \( D_i \) represents floc diameter of size class \( i \) (m), \( D_{i-1} \) is monomer diameter (m), \( k \) is fractal dimension, \( \gamma \) is lacunarity (generally set as 1, which implies no lacunarity), \( \rho \) is particle density (kg/m³), \( \rho_w \) is fluid density (kg/m³), \( g \) is gravitational acceleration (9.81 m/s²), and \( q \) is fluid viscosity (kg/m/s). In Eq. (10), \( 2^\gamma \) represents the number of monomers forming an \( i \)th particle/floc by following the discretized size classification strategy of the DPBE, which will be described in the following section.

\[
u_{x} = \frac{g}{16\eta} \left( \rho - \rho_w \right) D_{i-1}^{2\gamma} D_{i-1}^{2\gamma-1}
\]

(9)

\[
D_{i-1} = D_{i-1} \left( \frac{1}{k} \right)^{1/2\gamma}
\]

(10)

2.1.3 Kinetics of particle/floc aggregation and breakage

The core part of a multi-dimensional DPBE (Eq. (8)) is the sink and source terms, which characterize the aggregation and break-up kinetics ((agg/break)). These terms are written as a series of differential equations in Eq. (11). The particle/floc number concentration in a certain discrete size range \( (n_i) \) is used as a dependent variable of a partial differential equation. Following the discretization scheme of the DPBE, each mean particle size class contains two times the number of constituent monomers in the previous smaller class. Thus if \( i \) is the beginning (irreducible) particle size, class 1 will contain particles of size \( \delta \), class 2 will contain particles of size \( 2\delta \), class 3 will contain sizes \( 2\delta, 3\delta \), class 4 will contain sizes \( 3\delta, 4\delta \), class 5 will contain sizes \( 4\delta \), and so on. Because the maximum particle size in class \( i \) increases as \( 2^{\delta/\gamma} \), 30 classes will contain particle sizes varying from \( \delta \) to \( 2^{30} \delta \), which represents a growth factor of more than 288 million. Ignoring transport and settling for notational convenience, the partial differential equations with discrete particle/floc size sets may be written as

\[
\frac{\partial n_i}{\partial t} = (agg/break) = n_i \sum_{j=1}^{\infty} 2^{i-j} a(i-1,j) b(i-1,j) n_j + \sum_{j=1}^{\infty} 2^{i-j} a(i-1,j) b(i-1,j) n_j \]

(11)

In Eq. (11), the processes indicated by the various Roman numerals are (I) \( i \)-sized particle/floc generation by collision with other smaller particle/floc classes, (II) generation by collision within the \( i-1 \) class, (III) disappearance by collision with smaller classes, (IV) disappearance by collision with equal or larger classes, (V) disappearance by fragmentation of the \( i \) class, and (VI) generation by fragmentation of larger classes. These mecha-
With respect to particle/floc breakage kinetics, the size-dependent kinetic function shown in Eq. (14) has been commonly applied in previous studies [9, 30, 36, 37]. To simulate the fate of the broken fragments, the binary break-up distribution function was applied in our pond simulations because of its simplicity and robustness in computation. In the discretized PBE scheme, the binary break-up distribution function becomes 2, because one parent particle/floc is assumed to produce two equally sized daughter fragments in the break-up process (Eq. (15)) [30, 36].

In Eqs. (14) and (15), $a_i$ is the selection rate constant, and $V_i$ is volume of the $i$th class particle/floc size.

$$a_i = a_i V_i^{1/3}$$  \hspace{1cm} (14)

$$b(i, i-1) = \frac{V_i}{V_{i-1}} - 2$$  \hspace{1cm} (15)

### 2.2. Numerical Simulation

In the first step of the CFD-DPBE simulation procedure, the commercial CFD code (FLOW-3D) was used to generate a steady state flow field in the model pond. RANS and the two-equation $k$-$\epsilon$ turbulence models were selected to simulate flow velocities and turbulence. This resulted in nodal values for $\langle U_i \rangle$, $\langle V_i \rangle$, $\langle U_{ij} \rangle$, $k$, and $\epsilon$ (Eqs. (1)–(7)). Three different flow conditions that represent low, moderate, and high turbulence conditions were simulated with FLOW-3D, thus data resulting from three steady state flow fields were obtained and saved for the subsequent multi-dimensional DPBE simulation.

After the CFD simulation, the multi-dimensional DPBE was solved with an in-house program based on the finite-difference method and codified with MATLAB (MathWorks, Naticks, MA, USA). In these simulations, two significant numerical obstacles were identified and overcome in our preliminary research. First,
Numerical Simulation of Flocculation and Sedimentation

the complexity and nonlinearity of a large number of coupled partial differential (DBPE) equations in an advection-dominated application resulted in a computational overload. To increase computational efficiency, we applied an operator-splitting algorithm in which particle/floc advection was split from particle/floc dispersion-reaction [38-40] (Table 1). Thus, the advection terms and the dispersion-reaction terms were applied sequentially at each time step. Second, a standard central-differencing finite difference method was not optimal for simulating advection-dominated flow conditions with high Peclet numbers. Previous studies have shown that upwind differencing methods produce much improved results for a given node separation [41-44]. Leveque’s flux-corrected upwind algorithm was applied to solve scalar transport equations in advection-dominated conditions [41-45]. In this algorithm, particle/floc concentration \( n_i \) of a computational cell was updated at each time step with the inflow and outflow, which are determined by velocities through cell interfaces and concentrations of neighbor computational cells at each time step. Table 1 outlines the numerical scheme used to solve the multi-dimensional DPBE with operator splitting and flux-corrected upwind algorithms. At each time step, particle/floc advection equations were solved with LeVeque flux-corrected upwind scheme and stepwise particle/floc dispersion-reaction equations were calculated implicitly with the Gauss–Seidel iterative method.

Fig. 2 shows schematic diagrams of a flocculant-aided sediment retention pond that consists of a turbulent mixing zone at the inlet and a subsequent sedimentation basin. This turbulent mixing zone may function as an effective flocculation basin with high fluid turbulence. Chemical flocculant is assumed to be injected at the inlet of the pond, so particles/flocs will begin aggregating immediately after entering the basin.

Fig. 3 shows the two-dimensional computational domain representing a simplified turbulent mixing zone in a sediment retention pond.

Table 1. The simplified numerical algorithm for solving the CFD-DPBE model

| Initialization | Supporting data (flow field data from CFD, solid and liquid properties) |
| - Computational system layout (dimensions, mesh) |
| DPBE calculation (operator splitting algorithm) |
| ↓ LeVeque flux-corrected upwind scheme (advection) |
| \[ \frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x} \left( \left( U_+ \right) n_i \right) + \frac{\partial}{\partial y} \left( \left( U_+ \right) n_i \right) + \frac{\partial}{\partial z} \left( \left( U_+ \right) n_i \right) + u_x \frac{\partial n_i}{\partial x} = 0 \] |
| ↑ FDM calculated with Gauss-Seidel iteration (dispersion and reaction) |
| \[ \frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x} \left( \left( C \right) \frac{k_D}{\partial x} \right) + \frac{\partial}{\partial y} \left( \left( C \right) \frac{k_D}{\partial y} \right) + \frac{\partial}{\partial z} \left( \left( C \right) \frac{k_D}{\partial z} \right) \text{ (agg / break)} = 0 \] |

Post-processing
- Mass balance, particle/floc diameters, solid concentrations, etc.

CFD-DPBE: computational fluid dynamics–discretized population balance equation, FDM: finite difference method.
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 initially set to the fixed value of 8 m$^3$/min, which is equivalent to 2.5 min of mean hydraulic residence time ($t_{\text{HRT}} = \text{Volume} / \text{FlowRate}$) within the model 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 inlet width. Influent clay particles (monomers) were assumed to be spheres with a diameter of 1 μm and density of 2.65 g/L. The influent solid concentration was set to 2 g/L, which is equivalent to a particle number concentration of 1.47 × 10$^{10}$/m$^3$.

In the CFD-DPBE simulation, three empirical model constants ($D_f$, $D_c$, and $a_c$) were used for aggregation and break-up kinetics. The fractal dimension ($D_f$) was selected as 2.5, which is an intermediate value in the dataset obtained from previous studies [33, 35, 46, 47]. A critical diameter ($D_c$) and breakage kinetic constant ($a_c$) were chosen rather arbitrarily as 100 μm and 10/s following Ding’s recent flocculation theory [36]. However, these constants are previous site-specific values, so it is ultimately recommended that more applicable constants be measured with settling and kinetic experiments appropriate for retention pond applications.

### 3. Results and Discussion

In the CFD simulation with the commercial FLOW-3D code, three steady state flow fields were obtained for the model-mixing zone. These flow fields are shown in Fig. 4 with case 1, low; case 2, moderate; and case 3, high turbulence conditions, which were induced by the different influent flow velocities of 0.222, 0.334, and 0.667 m/min, respectively. The arrows and contours in Fig. 4 represent mean flow velocity vectors ($\vec{v}$) and shear rate distributions ($G = (\vec{\varepsilon} \cdot \vec{v})^{1/2}$), respectively. In the low turbulence condition (case 1), velocity vectors were uniformly directed from the inlet to the outlet, and shear rates were limited to a low level with a maximum shear rate of 13.5/s (Fig. 4(a)). However, in the high turbulence condition (case 3), a swirling zone was identified above the inlet, and high shear rates, with a maximum of 79.3/s, were observed near the inlet (Fig. 4(c)). The moderate turbulent flow condition (case 2) showed flow characteristics intermediate between the two extreme cases (Fig. 4(b)).

With steady state flow field data obtained from the CFD simulation, solutions to the multi-dimensional DPBE were obtained with an in-house program. At the beginning, the consistency and stability of the developed numerical algorithms were tested by monitoring solid mass balances and particle/floc size evolution.

Mass balances were calculated with Eq. (16) and monitored as shown in Fig. 5(a). In Eq. (16), Mass$_{\text{in,acc}}$, Mass$_{\text{deposit,acc}}$, Mass$_{\text{settle,acc}}$, and Mass$_{\text{manual}}$ represent time-integrated masses caused by inflow at the inlet, outflow at the outlet, deposition on the bottom, and retention in the pond, respectively, with time progression. Theoretically, Mass$_{\text{in,acc}}$ should equal to the sum of Mass$_{\text{deposit,acc}}$, Mass$_{\text{settle,acc}}$, and Mass$_{\text{manual}}$ that is, the mass balance calculated from Eq. (16) should be 100%. Contrary to our expectation, mass balances for low, moderate, and high turbulence conditions were all below, or slightly below, 100% at steady state conditions (99.7%, 97.8%, and 96.1%, respectively). However, these balances were in an acceptable error range, considering the approximating nature and complexity of the numerical methods. In Fig. 5(a), the mass fractions by particle/floc deposition on the bottom (Mass$_{\text{deposit,acc}}$ / Mass$_{\text{in,acc}}$) are shown for the three different turbulence conditions. The mass fraction by deposition in the high turbulence condition (case 3) was found to be much higher than that in the low turbulence condition (case 1) because high turbulence enhanced flocculation and the subsequent sedimentation processes. These mass fractions and balances became stabilized as the mixing zone systems approached steady state conditions.

$$\text{Mass Balance(\%)} = \frac{\text{Mass}_{\text{settle,acc}} + \text{Mass}_{\text{deposit,acc}} + \text{Mass}_{\text{retained}}}{\text{Mass}_{\text{in,acc}}} \tag{16}$$

[Fig. 4. Steady state flow field profiles from computational fluid dynamics 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.]
Numerical Simulation of Flocculation and Sedimentation

In Fig. 5(b), after the fastest growing phase, mass mean particle/floc diameter \((D_{\text{mean}})\) oscillated and then appeared to stabilize gradually. As mentioned in the previous section, the CFD-DPBE model consists of highly coupled nonlinear equations, which may produce fluctuating results. Strogatz [49] discussed the tendency of such nonlinear equations to produce oscillatory behavior in numerical simulations. A variety of phenomena can contribute to this behavior, including ‘chaotic’ behavior. Thus, the observed oscillatory behaviors shown in Fig. 5(b) were ascribed to the nonlinear nature of the CFD-DPBE model. Such behavior should be examined closely in future experimental and modeling studies.

After examining the consistency and stability of the CFD-PBE model and the mass-weighted mean particle/floc size \((D_{\text{mean}})\), solid concentration distributions at steady state conditions were investigated in the model-mixing zone. Figs. 6 and 7 show the distributions of mass-weighted mean particle/floc size and solid concentration, respectively, in the three different turbulent flow fields. In case 1, with low turbulence, mass mean particle/floc sizes were less than 27 \(\mu\text{m}\), and solid concentrations were near-homogeneously distributed without particle/floc deposition. However, in case 3 with high turbulence, mass-weighted mean particle/floc sizes grew to 195 \(\mu\text{m}\), which is a sufficient size for the particles/flocs to escape the computational system by settling and being deposited on the bottom. 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. Further, 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 exposed 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 to about 200 \(\mu\text{m}\), while those right next to the swirling zone remained below 50 \(\mu\text{m}\).

Table 2 summarizes results from the CFD-PBE simulations after reaching steady state. Mass-weighted mean particle/floc size \((D_{\text{mean}})\) and deposited mass fraction \((\text{Mass}_{\text{deposit,acc}}/\text{Mass}_{\text{in,acc}})\) 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, respectively. As expected, turbulence in sediment retention ponds enhance flocculation efficiency in the mixing zone, at least to a certain extent. In Fig. 8, the cumulative mass distributions of particles/flocs flowing through the outlet are shown for the three different turbulence conditions studied. As expected, for the low turbulence condi-

\[
D_{\text{new}} = \frac{\sum m_i D_i}{M} = \left( \frac{m_1}{M} D_1 + \frac{m_2}{M} D_2 + \cdots + \frac{m_i}{M} D_i \right)
\]  

(17)

\[
\text{Mass}_{\text{deposit,acc}} / \text{Mass}_{\text{in,acc}} \]

\[
D_{\text{mean}}^* \mu\text{m}
\]

\[
\%
\]

### Table 2. Flow field characteristics and flocculation/sedimentation efficiencies for three different turbulent conditions in the mixing zone

<table>
<thead>
<tr>
<th>Flow turbulence level</th>
<th>Flow field characteristic</th>
<th>Flocculation/sedimentation efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(v_{\text{in}} \text{ (m/s)})</td>
<td>(G^* \text{ (l/s)})</td>
</tr>
<tr>
<td>Case 1</td>
<td>Low</td>
<td>0.222</td>
</tr>
<tr>
<td>Case 2</td>
<td>Moderate</td>
<td>0.334</td>
</tr>
<tr>
<td>Case 3</td>
<td>High</td>
<td>0.667</td>
</tr>
</tbody>
</table>

*Maximum values in the computational domain.

*Averaged values along the outlet.

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tion (case 1), the particle/floc size distribution was more weight-
ed toward the small size range than that for the moderate and high turbulence conditions (cases 2 and 3). Thus, in case 1, raw clay particles coming through the inlet are not aggregated properly in the turbulent mixing zone, so a large fraction of particles/flocs may not settle appropriately in the subsequent sedimentation basin. In conclusion, considering the results in Table 2 and Fig. 8 from the steady state CFD-DPBE simulations, the turbulence conditions in a turbulent mixing zone were found to have important effects on both flocculation and subsequent sedimentation efficiencies. Optimization of this situation is an important topic for both experimental and theoretical future studies.

4. Conclusions

The main purpose of this research was to estimate the applicability of a novel CFD-DPBE combined model in simul-

![Fig. 6. Mass-weighted mean floc diameter (D_{f,mm}) distributions in the computational domain. The distributions of case 1 (a), case 2 (b), and case 3 (c) are listed from the top.](image)

![Fig. 7. Solid concentration distributions in the computational domain. The distributions of case 1 (a), case 2 (b), and case 3 (c) are listed from the top.](image)

![Fig. 8. Cumulative mass distribution of particle/floc sizes at the outlet of the model basin.](image)
ing flocculation and sedimentation processes in the turbulent mixing zone of a sediment retention pond. In this modeling and simulation study, the following important findings were identified and discussed:

1) The employed CFD software (FLOW-3D) was a useful tool for generating steady state flow field data, such as flow velocities and shear rates, which were used in subsequent multi-dimensional DPBE simulations.

2) As an alternative to QMOM, DPBE formulation was applied to simulate a multi-dimensional flocculation/sedimentation process. Solution of the multi-dimensional DPBE provides more readily understandable results for engineers and scientists with slightly more computations than QMOM but well within the capabilities of modern personal computers for two-dimensional flow fields.

3) A standard, central-differencing, finite difference approach was judged inadequate for simulating the flocculation and sedimentation processes in sediment retention ponds due to computational instability caused by nonlinearity, advection dominance, and complexity of the DPBE model. Thus, operator-splitting and LeVeque flux-corrected algorithms were applied to overcome the computational difficulties. The detailed numerical model is available from the authors upon request.

4) In application of the CFD-DPBE model, increased turbulence was found to enhance flocculation and sedimentation efficiencies. However, methodology for optimizing this effect requires further study.

This research was limited to pure simulation work without experimental validation. Thus, in future research, batch kinetic experiments and bench- or full-scale pond tests are required to calibrate, validate, and fully understand the CFD-DPBE model. In addition, the irregular behavior shown in Fig. 5(b) requires further investigation.

In summary, the CFD-DPBE model was successfully applied to generate steady state flow field data and numerically simulate flocculation and sedimentation processes in the turbulent mixing zone of a sediment retention pond. Thus, the CFD-DPBE model was shown to be a promising simulator of flocculant-aided sediment retention ponds. Furthermore, the model may be applied to flocculation and sedimentation occurring in various natural and engineering systems, such as water/wastewater treatment, nano-material synthesis, or sediment-depositing estuarine systems [6, 24, 36, 50-52].

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References


