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

Byung Joon Lee, Fred J. Molz,
Mark A. Schlautman, Abdul A. Khan

2008 South Carolina Water Resources Conference

Clemson University
Environmental Engineering & Earth Sciences
Civil Engineering

Colloidal Contamination !!!

Urban Development

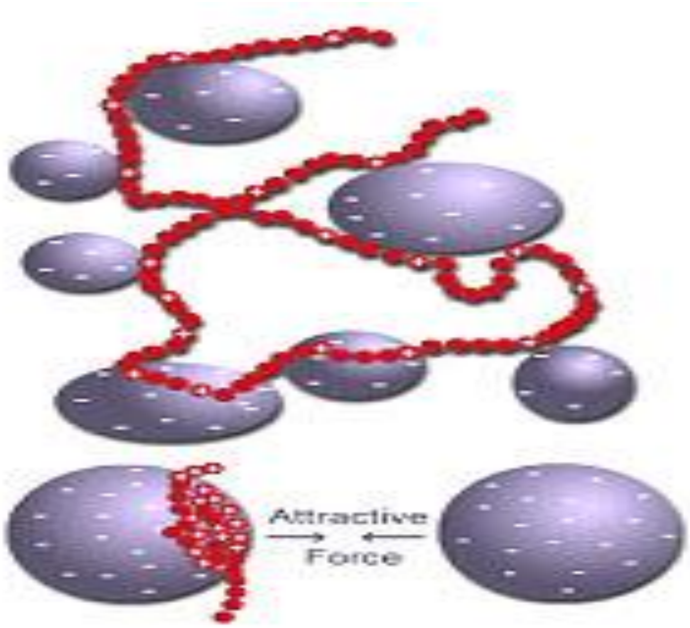
Agriculture Tillage

As a Result

Flocculant-Aided Sediment Retention Pond

Polymer-Induced Flocculation

1. **Bridging Flocculation**
2. **Electrostatic Patch Mechanisms**

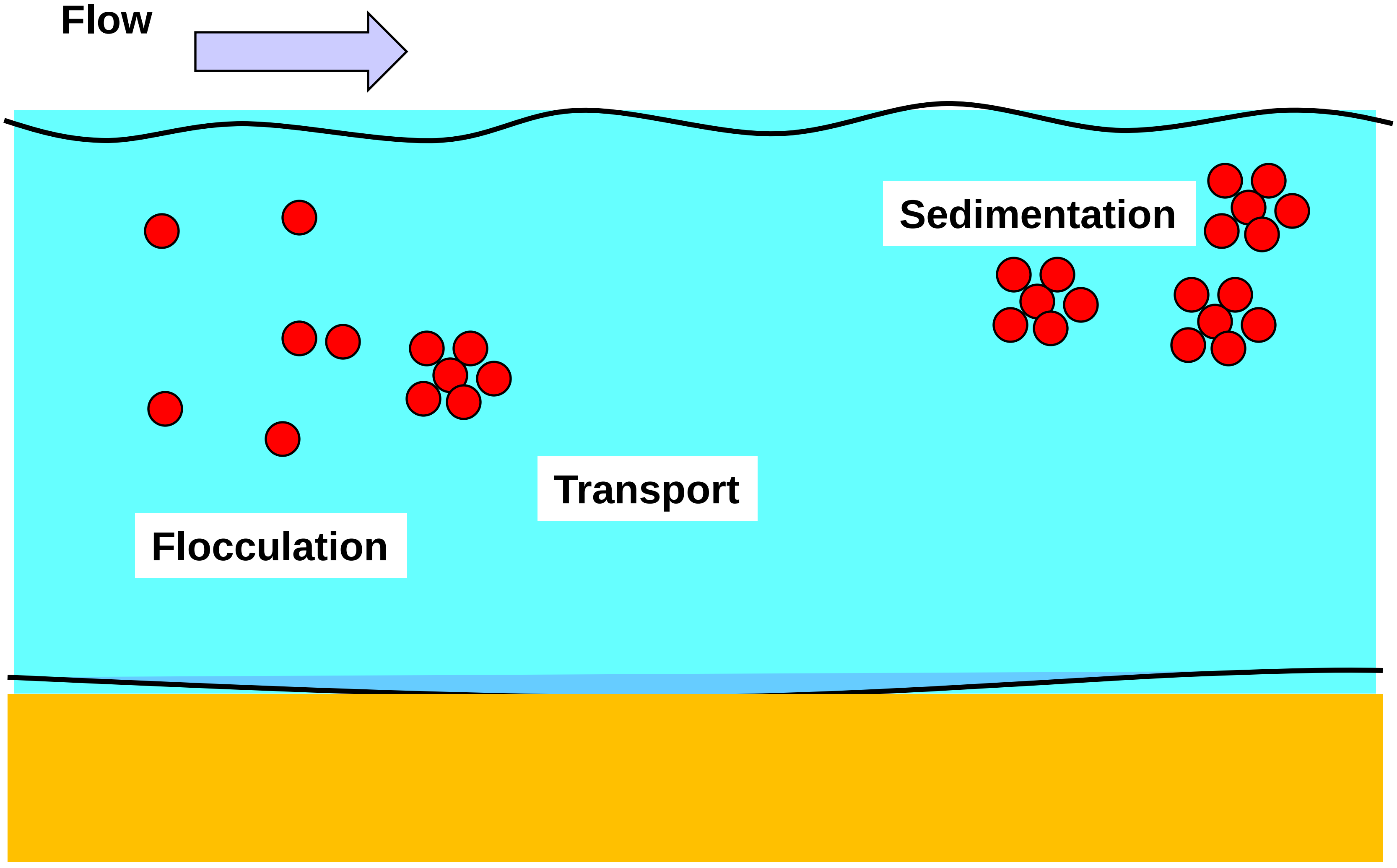


http://rpitt.eng.ua.edu/Class/Erosioncontrol/Module6/Module6.htm
http://hceglobal.com/faqs.asp

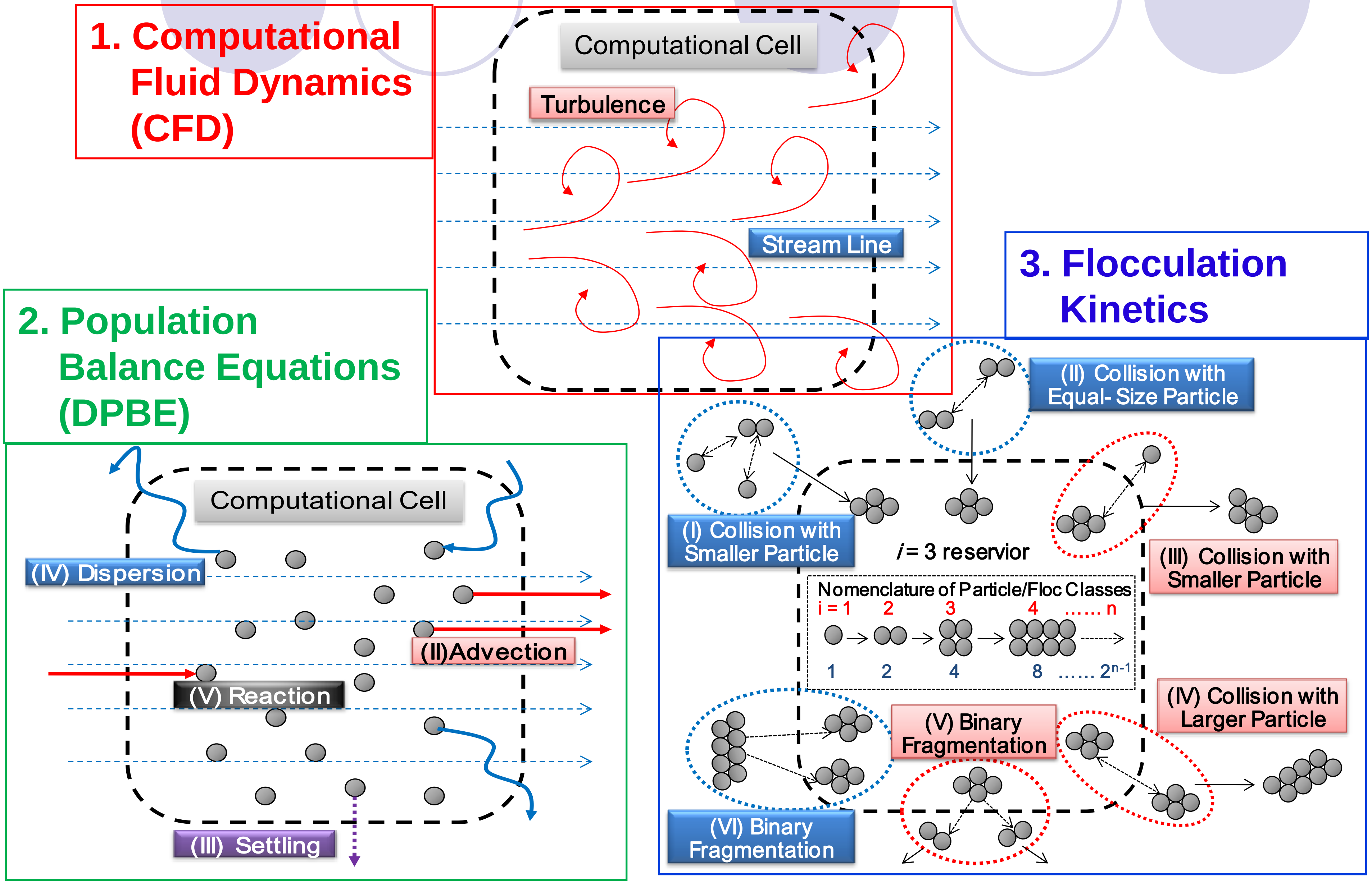
Outline

1. Conceptual Model
    - Flocculation/Sedimentation Model
2. Mathematical Models
    - CFD-DPBE Combined Model
3. Simulation
    - Model Sediment Pond Systems
    - Numerical Strategy
4. Results and Conclusion
    - Steady State Flow Field Simulation
    - Particle/Floc Size and Mass Distribution
5. Future Studies
    - Experiments – Flume Test
    - Other Applications

Conceptual Model : Flocculation and Sedimentation



Mathematical Models : CFD-DPBE model



Mathematical Models : 1. Computational Fluid Dynamics

Mass Conservation Equation : $\dfrac{\partial \langle U_i \rangle}{\partial x_i} = 0$

Momentum Conservation Equation :

$$\frac{\partial \langle U_i \rangle}{\partial t} + \langle U_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\partial \langle u_j u_i \rangle}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i} + \nu \nabla^2 \langle U_i \rangle$$

Turbulence Model : Two-equation κ-ε turbulence model (Fox, 2003)

Model Parameters:

- ***<Ui>*** : Time averaged velocity component
- ***i, j*** : Indices for directional coordinates
- ***t*** : Time
- ***ρ*** : Fluid density
- ***P*** : Piezometric pressure
- ***ν*** : Kinematic viscosity of the fluid.
- ***κ*** : Turbulent kinematic energy
- ***ε*** : Turbulent energy dissipation rate

➢ **FLOW3D®** software was used to simulate turbulent flow within a retention pond.

Mathematical Models : 2. Multi-dimensional DPBE

Multi-Dimensional DPBEs (30 Differential Equations) :

$$\underbrace{\left[\frac{\partial n_i}{\partial t}\right]}_{(I)} + \underbrace{\left[\frac{\partial}{\partial x}(\langle U_x\rangle n_i) + \frac{\partial}{\partial y}(\langle U_y\rangle n_i) + \frac{\partial}{\partial z}(\langle U_z\rangle n_i)\right]}_{(II)} + \underbrace{u_{gi}\frac{\partial n_i}{\partial z}}_{(III)}$$

$$\underbrace{-\left[\frac{\partial}{\partial x}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(C_\mu \frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial z}\right)\right]}_{(IV)} = \underbrace{(agg\,/\,break)_i}_{(V)}$$

Fractal Theory: $D_i = D_0\left(2^{i-1}\right)^{1/D_f}$ **Stokes' Law :** $u_{gi} = \frac{g}{18\eta}\left(\rho_s - \rho_w\right) D_0^{3-D_f} D_i^{D_f - 1}$

Model Parameters:

- n_i : Number concentration of class size *Di*
- $<U>$: Time averaged velocity component
- C_μ : CFD model constant = 0.09
- D_0 : Particle diameter of monomer
- D_i : Average particle diameter of ***i***-th class
- D_f : Fractal dimension
- ρ_s : Particle density
- ρ_w : Fluid density
- g : Gravitational acceleration
- η : Fluid viscosity

➢ **The multi-dimensional DPBE** is used to simulate particle/floc transport and flocculation in the ponds.

Mathematical Models : 3. Aggregation/Break-up Kinetics

Aggregation and Breakage Kinetics (Ding *et al*, 2006):

$$\frac{\partial n_i}{\partial t} = (agg/break)_i = \underbrace{n_{i-1}\sum_{j=1}^{i-2} 2^{j-i+1}\alpha(i-1,j)\beta(i-1,j)n_j}_{(I)} + \underbrace{\frac{1}{2}\alpha(i-1,i-1)\beta(i-1,i-1)n_{i-1}^2}_{(II)}$$

$$\underbrace{-n_i\sum_{j=1}^{i-1} 2^{j-i}\alpha(i,j)\beta(i,j)n_j}_{(III)} \underbrace{-n_i\sum_{j=i}^{(max\ i)}\alpha(i,j)\beta(i,j)n_j}_{(IV)} \underbrace{-a(i)n_i}_{(V)} + \underbrace{\sum_{j=i+1}^{(max\ i)+2} b(i,j)a(j)n_j}_{(VI)}$$

Collision Efficiency

$$\alpha(i,j) = \frac{1}{1+\left(\left(D_i+D_j\right)/\left(2D_c\right)\right)^3}$$

Collision Frequency

$$\beta(i,j) = \frac{1}{6}\left(\frac{\varepsilon}{\nu}\right)^{1/2}\left(D_i+D_j\right)^3 \quad if\ \ D_i, D_j \le D_c$$

$$\beta(i,j) = \frac{1}{6}\left(\frac{\varepsilon}{\nu}\right)^{1/2} 8\left(D_c\right)^3 \quad if\ \ D_i, D_j \ge D_c$$

Breakup Kinetics& Distribution Function

$$a(i) = a_0 V_i^{1/3}$$

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

Model Parameters:

$\alpha(i,j)$: Collision Efficiency Factor Between Particle Size Classes *i* and *j*

$\beta(i,j)$: Collision Frequency Factor

$a(i)$: Breakup Kinetic Constant

$b(i,j)$: Breakup Distribution Function

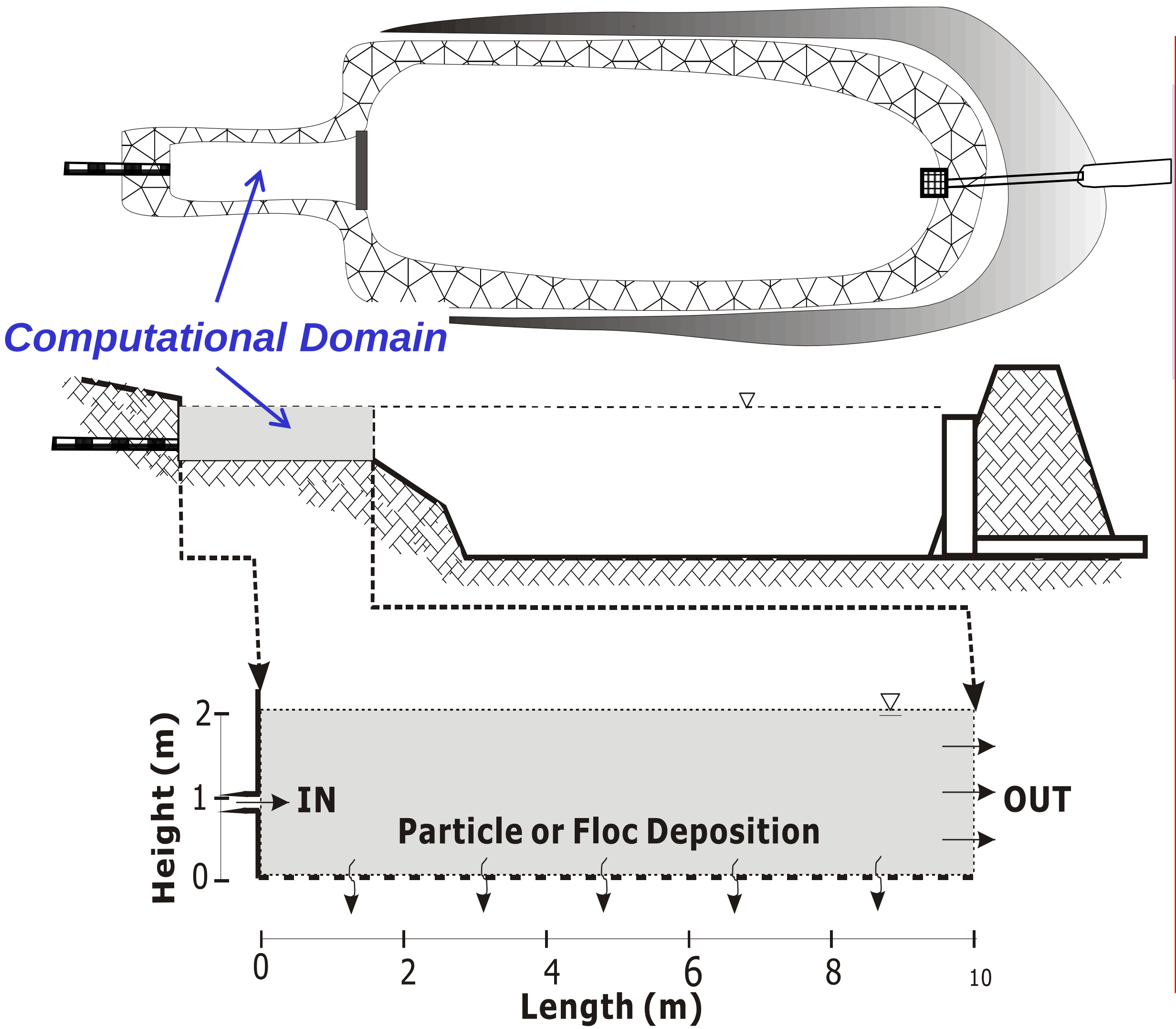
a_0 : Selection Rate Constant

V_i : Mean Particle Volume of *i*-th Class

D_i : Mean Diameter of *i*-th Class

D_c : Critical Diameter

Simulation : 1. Model Pond System



Model Pond

- **The Turbulent Mixing Zone** functions as a flocculation basin with high fluid turbulence

Computational Domain

- 2 Dimensional
- 2 m x 10 m Area
- 10 x 50 Mesh Lines

Simulation : 2. Numerical Strategy

1. Generate Steady State Flow Field Data with FLOW-3D®
2. Solve the DPBE Equation with MATLAB ®

- **INITIALIZATION**
  - Supporting data (flow field data from CFD, solid and liquid properties)
  - Computational system layout (Dimensions, Mesh)
- **DPBE CALCULATION (Operator Splitting Algorithm)**

↓

Leveque's flux-corrected upwind scheme (Advection)

$$\frac{\partial n_i}{\partial t}+\frac{\partial}{\partial x}\left(\langle U_x\rangle n_i\right)+\frac{\partial}{\partial y}\left(\langle U_y\rangle n_i\right)+\frac{\partial}{\partial z}\left(\langle U_z\rangle n_i\right)+u_{gi}\frac{\partial n_i}{\partial z}=0$$

t+Δt

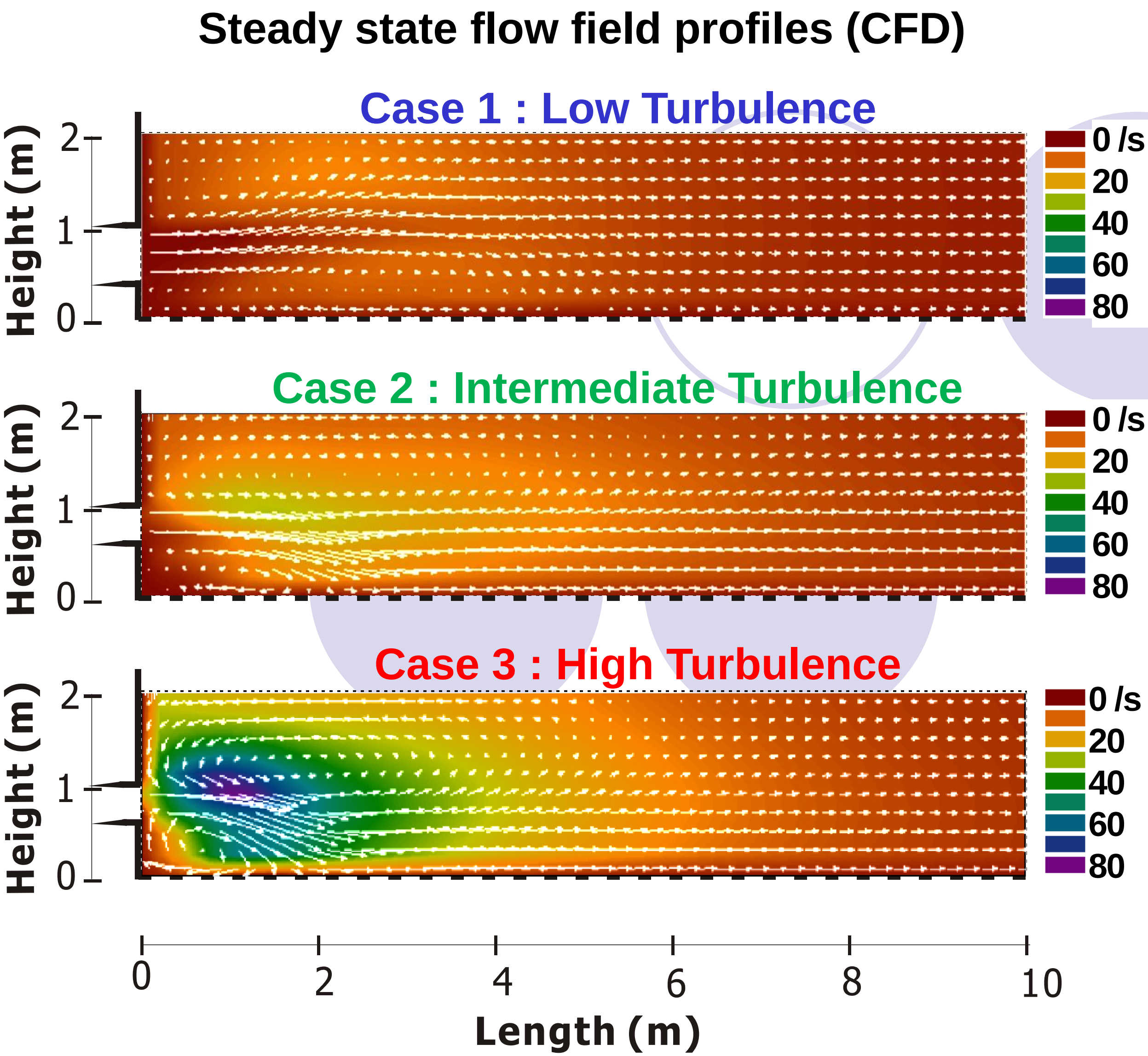
FDM calculated with Gauss-Siedel iteration (Dispersion and Reaction)

$$\frac{\partial n_i}{\partial t}-\frac{\partial}{\partial x}\left(C_\mu\frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(C_\mu\frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(C_\mu\frac{k^2}{\varepsilon}\frac{\partial n_i}{\partial z}\right)-(agg/break)_i=0$$

↑

- **POST PROCESSING**
  - Mass balance, Particle/floc diameters, Solid concentrations, etc.

Results : 1. Steady State Flow Field Simulation



- ➢ Arrows and colors represent flow velocities and shear rates.

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

- ➢ Influent flow velocities were set at three different values (0.222, 0.334, and 0.667 m/s) by adjusting inlet width, to create different levels of fluid turbulence, and to compare the effects of turbulent intensity on flocculation efficiency.

Results : 2. Consistency and Stability Tests

Solid Mass Balance:

$$Mass\ Balance(\%) = \frac{Mass_{out,acc} + Mass_{deposit,acc} + Mass_{retained}}{Mass_{in,acc}}$$

in/out : In or out of the pond

deposit : Deposit on the bottom

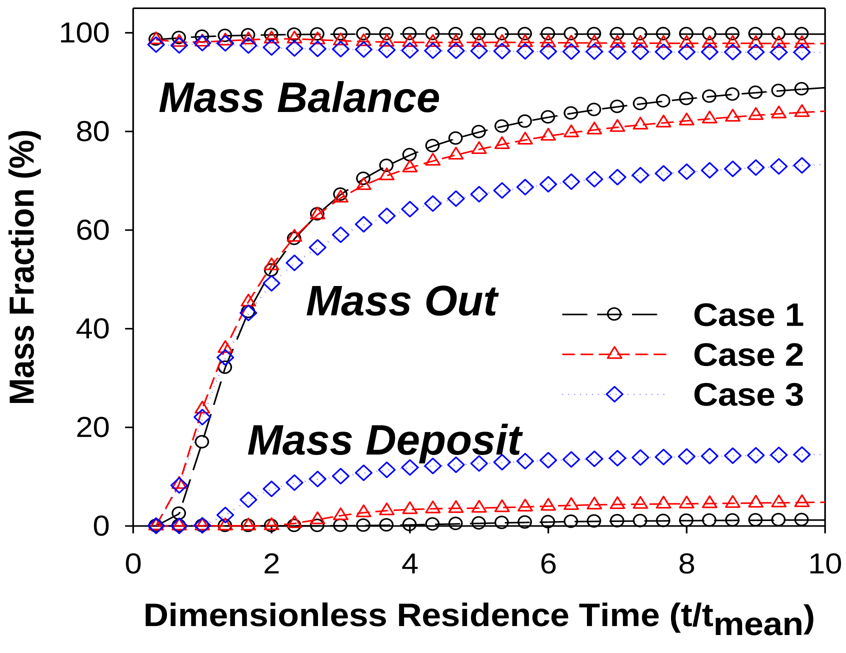
retained : Retained in the pond

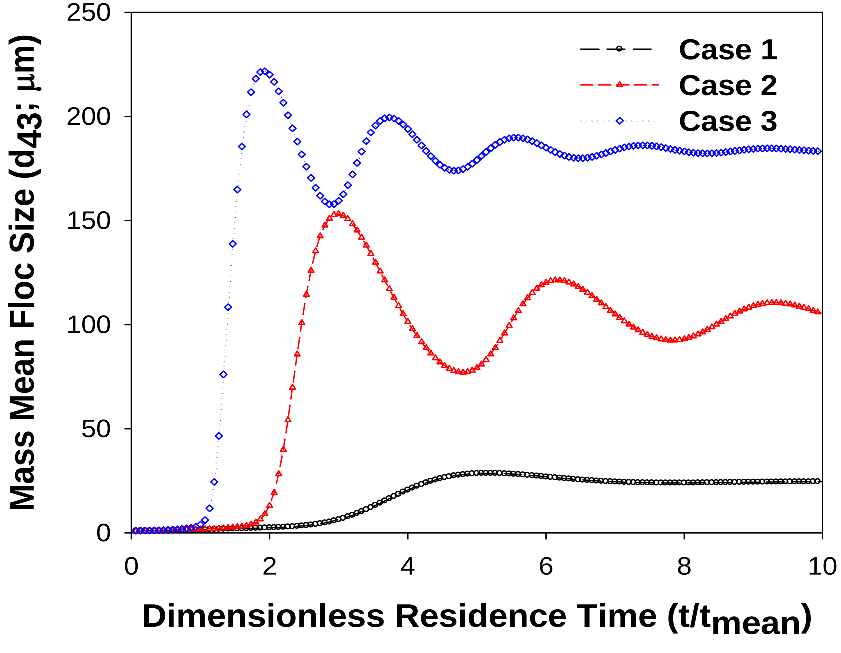
Mass Mean Diameter:

$$D_{43} = \frac{\sum m_i D_i}{M} = \left(\frac{m_1}{M} D_1 + \frac{m_2}{M} D_2 + \cdots + \frac{m_I}{M} D_I \right)$$

mi : Mass of ***i***-th class particle

M : Total mass of all the classes



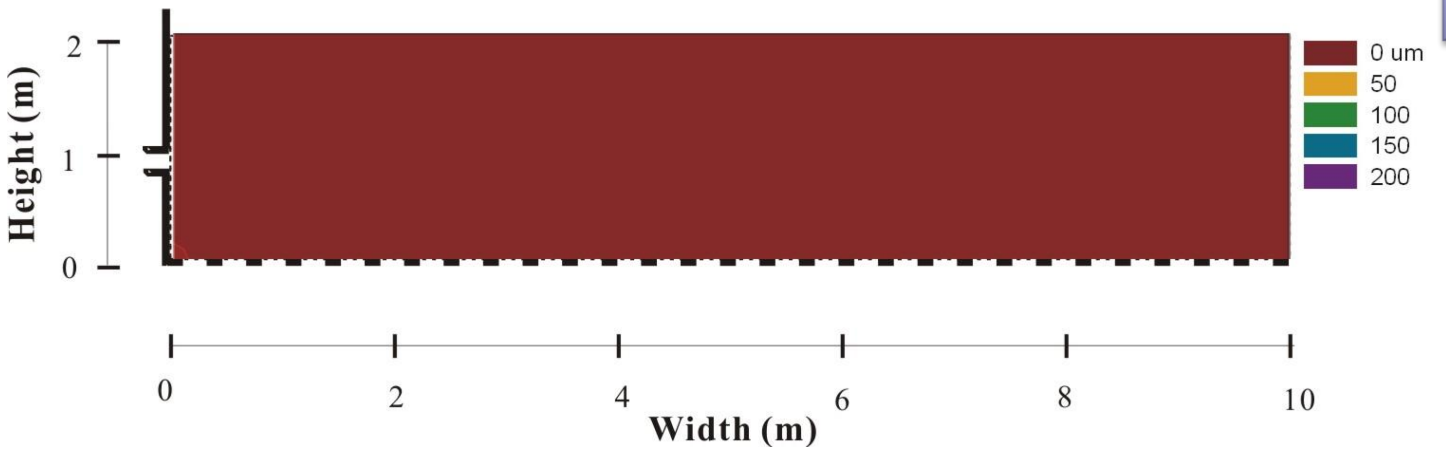


Results : 3. Dynamic Simulation Results

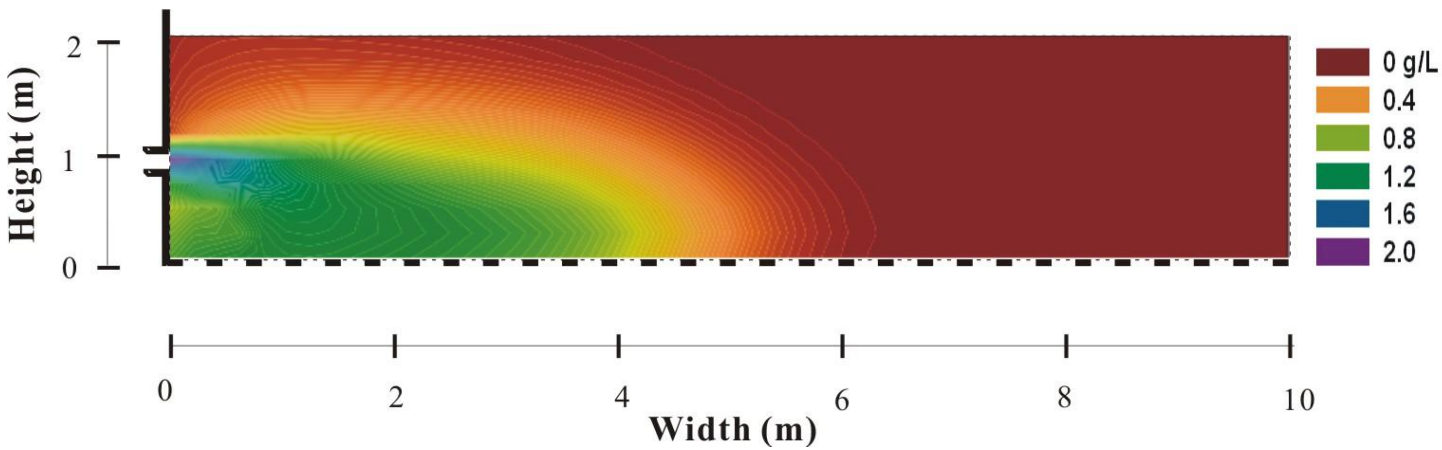
Dynamic Pond Simulation

Movie Clip : 20 sec / 1 frame

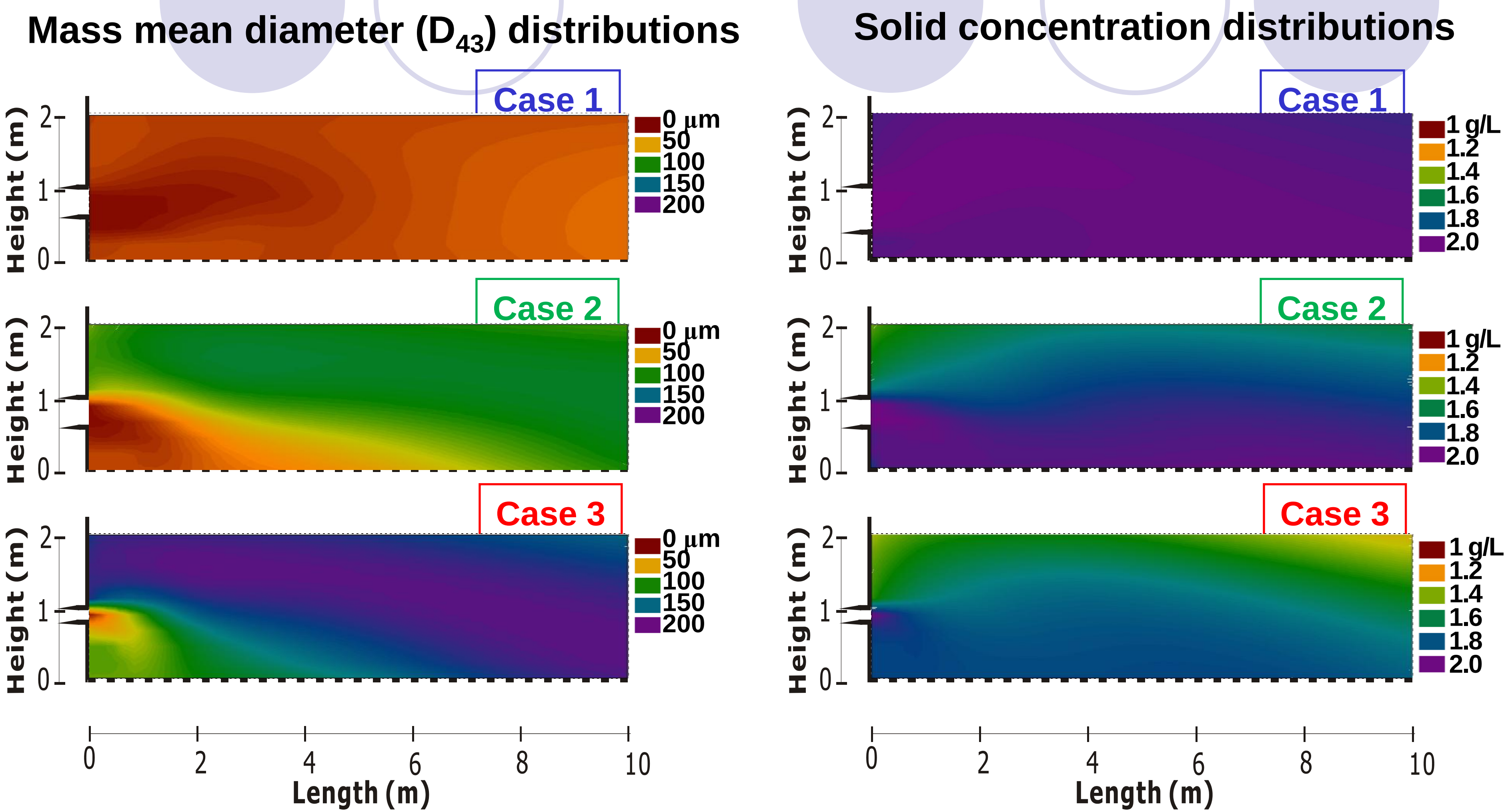
Particle Diameter Evolution



Solid Mass Conc. Evolution



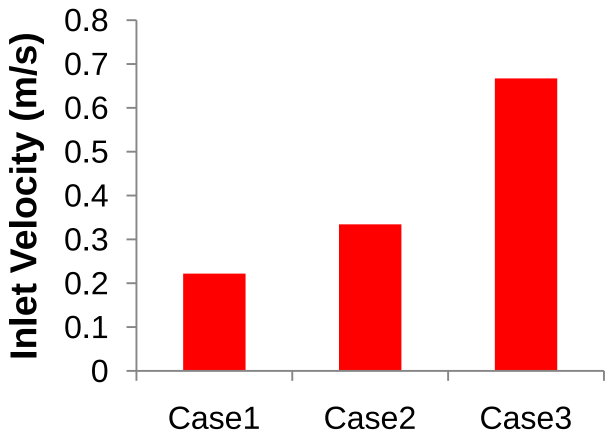
Results : 4. Steady State Simulation Results

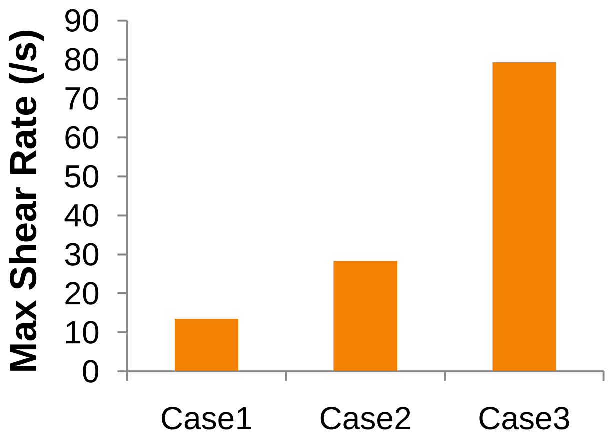


- **Particles/flocs traveling through these swirling zones** are more exposed to flocculation and thus tend to grow larger than those passing through the other zones.

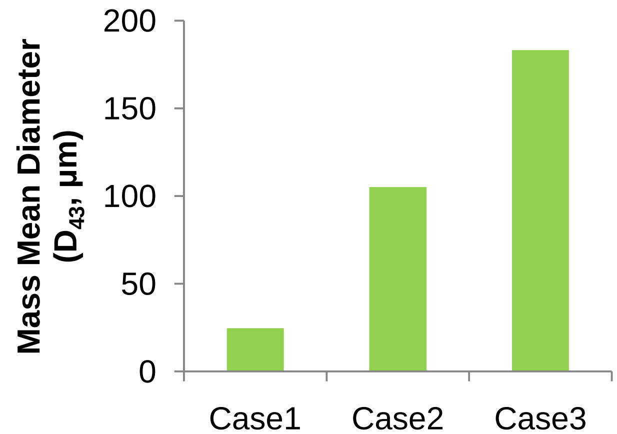
Results : 5. Summary

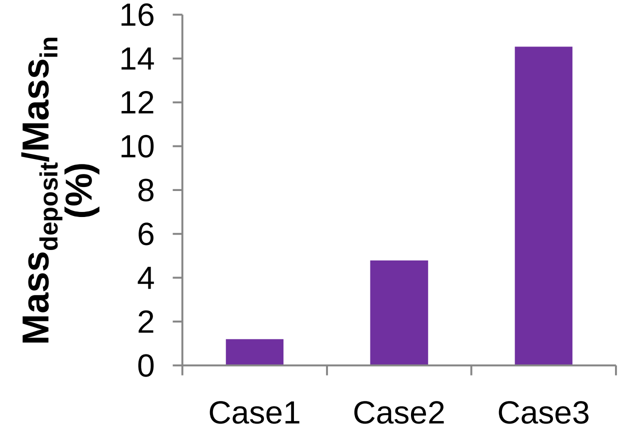
Flow Conditions
Velocity / Turbulence





System Responses
Flocculation / Sedimentation





- **Turbulent conditions** were found to induce critical effects on both flocculation and subsequent sedimentation efficiencies

Conclusion

- **FLOW-3D®** was a useful tool to generate steady state flow field data, such as flow velocities and shear rates, which were used in subsequent multi-dimensional DPBE simulations.
- As an alternative to QMOM, the **DPBE formulation** was applied to simulate a multi-dimensional flocculation/sedimentation process.
- **Operator splitting and Leveque's flux-corrected algorithms** were applied to overcome computational instability caused by nonlinearity, advection dominance and complexity of the DPBE model.
- In applications of the CFD-DPBE model, **increased turbulence** was found to **enhance the flocculation and sedimentation efficiencies**. However, methodology optimizing this effect requires further study.

Ongoing Research : Experimental Validation

Bench-scale 3-Dimensional Flume Test
EEES, Clemson University

Future Research : Various CFD-DPBE Applications

Cohesive Sediment Transport in River, Lake, Estuary

Clarifier in Water/Wastewater Treatment Plants

http://uregina.ca/~sauchyn/geog323/112.jpg
http://www.veoliawaterst.com.au/en/case-studies/7741.htm

Acknowledgments

- Funding
  - USDA-NRCS (NRCS-69-4639-1-0010) for the CLUE Project
  - USDA-CSREES (SC-170027)
  - State of South Carolina