W116: Combining the Power of Whole-Plant Simulators and CFD for the Dynamic Modeling of WWTPs

Presentation: Available Clarifier Models - Setting up a CFD model - Calibration Procedures - Data needed
Alonso Griborio, Hazen and Sawyer
Randal Samstag, Carollo Engineers

Outline

- Background
  - 1-D models
  - 2-D models
  - 3-D models
- Effective use of all levels of models
- Model calibration and validation
  - Data needed
  - Calibration procedures
  - Output validation test
- Case study, 1-D vs. 2-D vs. 3-D

Conservation Equations

1. Continuity (Conservation of Liquid)
   - All levels
2. Conservation of Momentum (F = ma)
   - 2D and 3D
3. Conservation of Mass for all solids and dissolved substances
   - 1D, 2D and 3D
4. Conservation of Energy (including Heat)
   - 2D and 3D

Modeling of Clarifiers - Background
Background in Clarifier Modeling

Secondary settling tank functions

- Clarification
- Thickening
- Storage
- Flocculation

Processes on Secondary Settling Tanks

- Hydrodynamics
- Settling
- Turbulence
- Sludge Rheology
- Flocculation
- Heat Exchange and Temperature

Secondary Settling Tank Models

- Surface overflow rate (early approaches)
- Box Model: 1-D Idealized Solids Flux
- 1-D Models: Drift Flux Model
- 2-D and 3-D Hydrodynamic Models

Early Approaches

- Hazen (1904)
  – Discrete settling in a plug flow in the horizontal plane
- Camp-Dobbins model (1944, 1946)
  – Modification of Hazen model to include vertical mixing
- State Point Analysis
  – Box type model that assumes the limiting flux can be estimated based on a Vesilind type setting equation.
**Hazen**

Removal = $R/H = V_sL/(UH) = V_s/SOR$

**State Point Analysis**

$$SOR 	imes (MLSS)^*(1+\alpha)$$

**1-D models**

- Vertical flow in layers
  - Vitasovic et al (Vesilind Equation)
  - Kinnear (2 phase flow)

**2-D Models**

- Larsen developed the first CFD type of secondary clarifier model (1977)
- LaRock; McCorquodale et al; Rodi et al presented 2D primary and secondary clarifier models from 1980-2000
- Griborio and McCorquodale (2004) developed a general public domain SST model (2Dc) that couples solids and hydrodynamics, five types of settling, flocculation, non-Newtonian flow, and compression rate.
City of Windsor – physical-chemical CSO treatment.

2-D

3-D Models

- Use of commercial CFD package such as FLOW3D and FLUENT
  - Richardson (2000) used FLOW3D with uncoupled solids and hydrodynamics
  - CCNY have developed a comprehensive 3D model (FLUENT) that couples solids and hydrodynamics, five types of settling, flocculation, non-Newtonian flow, and compression rate. Their model has been developed with an extensive field testing program.

Remarks

- All of the four levels of modelling are still in use;
- When used within their limitations these model are still providing useful information for the designers and/or operators of clarifiers.
Roles of Models

<table>
<thead>
<tr>
<th>Level</th>
<th>Strength</th>
<th>Application</th>
<th>Weakness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hazen</td>
<td>Simple</td>
<td>Discrete settling (Grit)</td>
<td>Ignores hydrodynamics</td>
</tr>
<tr>
<td>Limit State</td>
<td>Simple</td>
<td>Zone settling (SST preliminary design and operational)</td>
<td>Ignores hydrodynamics</td>
</tr>
<tr>
<td>1D</td>
<td>Computation speed</td>
<td>All types of settling including 2 phase flows</td>
<td>Ignores hydrodynamics</td>
</tr>
<tr>
<td>2D</td>
<td>Computation speed compared to 3D; runs on laptop.</td>
<td>All clarifiers where there is a dominant flow direction; dynamic simulations.</td>
<td>Ignores lateral non-uniformity in solids and momentum.</td>
</tr>
<tr>
<td>3D</td>
<td>Completeness of governing equations; high spatial resolution.</td>
<td>All clarifiers. Steady state simulations where a dominant flow direction cannot be assumed.</td>
<td>Long execution times; high level of expertise required.</td>
</tr>
</tbody>
</table>

The 2Dc Clarifier Model - Overview

- A quasi three-dimensional clarifier model
- Developed at the University of New Orleans (UNO)
- Based upon more than 30 years of experience on CFD modeling of clarifiers and published research
- State-of-the-Art tool that has been successfully applied to projects in:
  - Canada
  - USA
  - Japan
  - Korea
  - Australia

Previous 2D hydrodynamic models limitations

- Settling Velocities
- Flocculation
- Compression Rate
- Temperature Simulation and Heat Exchange

Model Calibration
Calibration or Validation? Definitions

- **Calibration**: Initial trials to adjust model parameters to reproduce field conditions (either long term data or field testing data).
- **Validation**: Tests to confirm that a model is representing field conditions. For example by independent stress tests with different flow or settling conditions or operating data.

### Input and Output Parameters for Model Calibration and Validation

#### Input parameters:
- Settling velocity test parameters
- Flow measurements
- MLSS tests
- Flocculation parameters
- Fractionation
- Simulation parameters
- Others like temperature, dry floc density, atmospheric parameters, etc.

#### Output parameters:
- ESS
- Solids profile
- Velocity profile
- Dye behavior
- RAS SS
- Blanket depth
- Solids fraction distribution

### Different Levels of Calibration

- **Four Levels of Calibration**:
  - Level 1
  - Level 2
  - Level 3
  - Level 4

  - Level 1 to Level 4 → decreasing uncertainty

### Different Levels of Calibration

#### Level 1
- Calibrate the model to historical plant data
- Minimum data needed: flows (influent and RAS), MLSS, effluent TSS and SVIs
- Settling coefficients defined based on the SVI
- Calibration normally consists in adjusting basic settling parameters to match historical effluent TSS
Different Levels of Calibration

Level 2
- Similar to CRTC protocol (Dye testing is optional)
- Full-scale testing
- Basic settling parameters, e.g., Vo, K, SVI, are measured
- Data collected include: flows (influent and RAS), MLSS, effluent TSS, RAS TSS, sludge blanket depth, FSS and DSS
- Calibration normally consists in adjusting Takacs equation K2 or the wastewater fractionation and discrete settling velocities

Level 3
- Full-scale testing: average flow and stress testing
- Zone settling and compression rate parameters are measured
- Flocculation kinetics is determined
- Particle size distribution and discrete settling are estimated
- All data collected on Level 2 plus solids profiling. Time series of all parameters are gathered
- Calibration normally consists in adjusting particle size distribution and/or turbulence model parameters

Level 4
- All parameters measured during Level 3 Calibration
- Accurate measurement of particle size distribution (e.g., image analysis, laser reflection, laser diffraction, acoustic spectroscopy, etc.)
- Dye test
- Measurement of Velocity (e.g., drogue test, acoustic doppler)
- Measurement of the floc's dry specific gravity
- Calibration normally consists on adjusting discrete settling velocities or turbulence model parameters

Input Parameter Tests
- Settling velocity testing
- Flow measurement
- MLSS measurement
- Density measurement: lock exchange
- Dispersed solids / flocculation tests
- Particle size distributions
Sludge Settling Velocity Tests

- **Goal:**
  - Establish settling velocity at the time of field tests
- **Sensitive to:**
  - Column shape (Dick 1975)
  - Mixing intensity
  - Temperature

Settling velocity models used in clarifier modeling

\[ V_s = V_o e^{-CK} \]

Settling Velocity Data Fits

\[ V_s = V_o e^{-CK} \]

Takacs versus Flocculation Submodel

\[ V_s = V_o \left\{ e^{-K_1(C-C_{\text{min}})} - e^{-K_2(C-C_{\text{min}})} \right\} \]

- **Takacs Equations:**
  - Calibration of K2
  - K2 is geometry specific
  - Cannot predict effect on ESS of changes in geometry
  - Does not explicitly include discrete settling
  - Less physically based
  - Simpler formulation and shorter computation time

- **Flocculation Model:**
  - Measured KA & KB
  - Measured particle fractionation
  - Can predict effect on ESS of changes in geometry
  - Includes discrete settling
  - More physically based
  - More complex formulation and longer computation time
Thickening/Compression

• Two phase phenomenon
• Similar to soil consolidation
• Weight of overburden results in a piezometric gradient that causes liquid phase to migrate.
• As the solids consolidate, the water being displaced impedes the solids movement. Kinnear used the Karman-Kozeny equation to describe this; the problem is the number of calibration parameters needed to use this approach.

Settling Velocity Models Based on a Two-Phase Approach

\[ V_s = k \frac{(1 - n_1 X)^4}{X} e^{-n_2 X} \]

Cho et al. (1993)

\[ V_s = k \frac{e^{-nX}}{X} \]

Cho et al. (1993) – Simplified Model

These models predict zone and compression settling but fail drastically in the discrete zone.

Sludge Compression Model

\[
V_s = \frac{(1 - E)(\rho_l - \rho_f) g + P_o \left[ \frac{(1 - E)}{(1 - E_g)} \right]^m \frac{\partial E}{\partial z}}{55S_0^2(1 - E)^2 \mu} E^3
\]

\( \rho_l \) and \( \rho_f \) are the liquid and floc densities, \( E \) is the porosity, \( E_g \) is the porosity at the gel point
\( S_0 = 6/dp \) is the specific surface area,
\( dp \) is the particle diameter,
\( \mu \) is the fluid dynamic viscosity,
\( P_o \) is an empirical coefficient,
\( \phi \) and \( \phi_g \) are the solids and gel solid fraction respectively.

Settling Velocity Research (McCorquodale et al. 2004)
Six Months of Settling Velocities

![Graph showing settling velocities](image)

Zone settling and compression rate

![Graph showing settling and compression rates](image)

2Dc settling velocity sub-model – Discrete settling

- Three types of flocs:
  - Big Flocs ($V_s \geq 6 \text{ m/h}$)
  - Medium Flocs ($1.5 \text{ m/h} \leq V_s < 6 \text{ m/h}$)
  - Small Flocs ($V_s < 1.5 \text{ m/h}$)

  - Threshold for hindered settling: 1000 to 1400 mg/L
  - Threshold for discrete settling: 500 to 650 mg/L
  - Non-settleable particles: Flocculated Suspended Solids (FSS)

<table>
<thead>
<tr>
<th>Settling Region</th>
<th>Settling Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X \leq \text{FSS}^*$</td>
<td>Non-settleable</td>
</tr>
<tr>
<td>$\text{FSS}^* &lt; X \leq \text{Discrete Threshold}$</td>
<td>Discrete settling</td>
</tr>
<tr>
<td>$\text{Discrete Threshold} &lt; X \leq \text{Hindered Threshold}$</td>
<td>Flocculent settling</td>
</tr>
<tr>
<td>$\text{Hindered Threshold} &lt; X \leq \text{Compression Threshold}$</td>
<td>Hindered settling</td>
</tr>
<tr>
<td>$X &gt; \text{Compression Threshold}$</td>
<td>Compression settling</td>
</tr>
</tbody>
</table>
The flocculation sub-model includes:

- Aggregation of primary-dispersed particles due to shear induced flocculation including flock breakup model
- Aggregation of primary-dispersed particles due to differential settling flocculation
- Implicitly models the filtration of particles in the sludge blanket

Shear induced flocculation (Parker et al., 1970)

\[
\frac{dn}{dt} = K_B \cdot X \cdot G^n - K_A \cdot X \cdot n \cdot G
\]

Where: 
- \( X \) is the MLSS concentration (g/L),
- \( G \) the root-mean-square velocity gradient (s\(^{-1}\)),
- \( K_A \) a floc aggregation coefficient (L/g),
- \( K_B \) a floc breakup rate coefficient (s\(^{-1}\)),
- \( m \) the floc breakup rate exponent (dimensionless), and
- \( n \) is the primary particle number concentration (g/L).

Calibration consists in determining \( K_A \) and \( K_B \)

Differential settling flocculation

\[
\frac{dC_i}{dt} = -\frac{3}{2} k_{di} \frac{C_i C_2}{\rho_i \rho_2} \left( 1 + 2 \frac{d_i}{d_2} \right) \frac{C_1}{d_2} (V_{s2} - V_{s1})
\]

Subscript \( i \) is for unflocculated–primary particles and subscript \( 2 \) is for flocculated–flocs particles
- \( C \) is concentration
- \( d \) is cross sectional diameter
- \( \rho \) is density
- \( K_{di} \) is a kinetic constant between 1 & 2
- \( V_s \) is the settling velocities

UNO 2Dc Clarifier Model: Calibration and Validation of the Model
Model calibration

• Adapting the model to reproduce field or experimental data:
  – Identify the geometry and operational parameters to be evaluated
  – Measure the settling properties of the sludge:
    • Discrete
    • Zone
    • Compression settling
  – Measure the flocculation kinetic constants
  – Adjust fractionation and/or compressibility
  – Adjust the diffusion coefficients

Model calibration – Identify and input the clarifier geometry and operational parameters

Marrero WWTP
SOR = 1.0 m/h ~ 590 gpd/ft²
MLSS = 2800 mg/L, RAS SS = 8400 mg/L
RAS= 50%

Discrete settling

The settling velocities of large and medium flocs are found by direct measurement (visual inspection) in a column batch test using a light source, a scale and a stopwatch

Zone and compression settling

\[ V_s = V_o e^{-k_1 X} \quad \text{Hindered Threshold (} X_h < X \leq \text{ Compression Threshold} \]

\[ V_s = V_c e^{-k_c X} \quad X > \text{ Compression Threshold} \]
Determination of Settling Properties

\[ V_s = V_0 e^{-kX} \]

Calibration of the flocculation sub-model

- Collect a MLSS sample (About 15.0 Liters)
- Use a six-paddle stirrer and fill each jar with 2.0 L of mixed liquor (avoiding unnecessary delays)
- Assign a flocculation time to each jar, e.g., 0, 2.5, 5, 10, 20, 30 minutes
- Mix the samples at a G of approximately 40 s\(^{-1}\)
- Allow the sample to settle for 30 minutes
- Take a supernatant sample from each jar
- Measure the TSS

Marrero WWTP SST

- MLSS = 2800 mg/L
- SOR = 1 m/h

Measured Settling Properties

**Discrete Zone**
- \( f_1 = 0.742, \ V_{s1} = 10.8 \text{ m/h} \)
- \( f_2 = 0.255, \ V_{s2} = 3.0 \text{ m/h} \)
- \( f_3 = 0.003, \ V_{s3} = 0.7 \text{ m/h} \)

**Hindered and Compression Zone**
- \( V_0 = 10.54 \text{ m/h}, \ K_1 = 0.40 \text{ L/g} \)
- \( V_c = 3.20 \text{ m/h}, \ K_c = 0.18 \text{ L/g} \)
- \( \text{FSS}^* = 4.3 \text{ mg/L} \)

**Field Data**
- Expon. (Field Data)

- \( X_{k_0} = 30 \times e^{-0.45 \text{X}} \)
- \( R^2 = 0.98 \)

**Equation 2.39**

\[ C = a + (C_0 - a) e^{-kgtX} \]

\[ n_t = \frac{K_A - G}{K_A} \times \left( 1 - \frac{K_B - G}{K_A} \right) e^{-K_A X G t} \]

Wahlberg et al. (1994)

La Motta et al. (2003)
Particle Size Distributions

- McCorquodale et al. developed a semi-empirical simple method to estimate fractionation and discrete settling for 3 particle sizes.
- City College New York Modified the method.
- Accurate methods for measuring PSD include:
  - Image analysis
  - Laser reflection
  - Laser diffraction
  - Acoustic spectroscopy
- In Situ vs. Ex Situ Techniques

Output Validation Tests

- Solids profile testing
- Velocity profile testing
- Dye transport testing
  - RTD
  - Continuous dye snapshot
- Sludge blanket monitoring

Solids Profile Measurement

- Sampling Method
  - Larsen:
    - Kemmerer
  - Crosby:
    - Solids Distribution Test - Sample pumps
  - Esler:
    - Optical device
Solids Profile Visualization

Solids Profile Comparison to Simulation
Field Test (Crosby SD test)  Simulation (2DC)

Velocity Profile Measurement
• Larsen built his own ultrasonic velocity probe
• Commercial probes: ADV
• Drogues
• Concerns:
  • Low velocities
  • Probe sensitivity
  • Difficult to hold still!

Velocity Profile Visualizations
Dye Tests: Residence Time Distribution Tests

Sludge Blanket Monitoring

- Dynamic monitoring of sludge blanket
- Sludge judge
- Difficulties: What is the threshold concentration of the “sludge blanket?”

Conclusions: Output validation tests

- Solids profiles
  - Relatively easy to measure
  - Directly comparable to model results
- Velocity profiles
  - More difficult to measure directly
- Dye tests
  - Useful for flow distribution issues
  - Continuous test not commonly used
- Dynamic blanket monitoring
  - Useful for rough monitoring of test conditions
  - Not as quantitative as solids profiles
Case Study Number 1: Comparison of Models

- One-dimensional (1D) Model (State Point)
- Two-dimensional (2D) Model (UNO CFD)
- Three-dimensional (3D) Model (Zhou CFD)

1D Model (Clariflux)

- Developed by Carollo Engineers
- Solves solids flux equations based on measured settling velocity coefficients (or SVI)
- Calculates state point for steady state operation
  - SOR Line
  - MLSS Line
  - RAS line

State Point Model

Clariflux Model Results

Test Condition (33% RAS)
Clariflux Model Results
Increased RAS

Suspended Solids Conc., mg/l

2D Model – UNO Model

- Developed by Griborio, McCorquodale, and associates at the University of New Orleans
- Two-dimensional model based on
  - Vorticity / stream function model
  - Turbulent hydraulics
  - Radial flow coordinates (axi-symmetric)
  - Discrete Settling
  - Hindered Settling
  - Compression
  - Flocculation

2D Model Results
Model Runs

- All tests run at 3,600 mg/L
- Settling coefficients as measured in the field
- Dynamic model runs
- 350 minutes simulation time (5.8 hours)
2D Model Results
Summary of Model Runs

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>1</td>
<td>Calibration Run</td>
<td>300</td>
<td>3,300</td>
<td>300</td>
<td>3.5</td>
<td>1,550</td>
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<td>Slit Inlet and Standard Baffle</td>
<td>3.5</td>
<td>1,800</td>
<td>100</td>
<td>3.5</td>
<td>2,200</td>
<td>14.4</td>
<td>14.4</td>
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<tr>
<td>3</td>
<td>High Slit</td>
<td>5.5</td>
<td>1,800</td>
<td>100</td>
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<tr>
<td>4</td>
<td>Curved Baffle</td>
<td>3.5</td>
<td>1,800</td>
<td>100</td>
<td>3.5</td>
<td>2,200</td>
<td>14.4</td>
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<td>Curved Baffle, High Slit</td>
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<td>1,800</td>
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<td>3.5</td>
<td>2,200</td>
<td>14.4</td>
<td>14.4</td>
</tr>
</tbody>
</table>

3D Model (Zhou CFD)

- Developed by Siping Zhou and J. A. McCorquodale
- Three-dimensional solution based on
  - Control volume model
  - K-epsilon turbulence model
  - Generalized coordinates
  - Hindered settling
  - Density-coupled solids transport
  - No flocculation or compression modeling

Existing Inlet

- Four openings in vertical feed pipe
- No energy dissipating feed-well

Prototype of Improved Inlet
3D Model Results (SVI 110)

Existing

Optimized

3D Model Results (SVI 190)

Existing

Optimized

3D Model Results

Summary of Model Runs

<table>
<thead>
<tr>
<th>Clarifier Configuration</th>
<th>Operating Conditions</th>
<th>1D Model Results</th>
<th>2D Model Results</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Flow Rate (mgd)</td>
<td>SVI</td>
<td>RAS</td>
</tr>
<tr>
<td>Existing clarifier</td>
<td>3.5</td>
<td>33.3</td>
<td>12,000</td>
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<tr>
<td>Inboard/End Launder</td>
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</table>

Conclusions from Modeling

- 1D model
  - Confirmed clarification capacity at 3.5 mgd
  - Clarifiers can be RAS limited at 33%
- 2D models
  - Reasonable verification of field tests
  - Inboard effluent launders slightly better than end launders and Stamford baffle
- 3D Model
  - Increased RAS rate without optimized inlet caused clarification failure
  - Optimized inlet can result in significant improvement with higher RAS ratio
Case Study 2: Comparison of Tangential Versus Puzzled Inlet

Fluent UDF Model
- Commercial CFD with k-epsilon turbulence model
- User-defined functions (UDF) add settling velocity, flocculation, solids transport, and density coupling
- Two or three-dimensional
- Capable of very refined grids

Overall Solids Profile

Tangential Inlet

Puzzled Inlet

Model Center-well Velocity Profiles

Tangential Inlet

Puzzled Inlet
Fluent UDF Model
Inlet Velocities

Tangential Inlet  Puzzled Inlet