CFD for Wastewater: What Can it Do?

Presentation to the Department of Civil and Environmental Engineering
University of Washington
7 April 2016

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CFD for Wastewater: What Can it Do?

- What is it?
- How is it done?
- What is it good for?
- Who is doing it?
“If we know what is happening within the vessel, then we are able to predict the behavior of the vessel as a reactor. Though fine in principle, the attendant complexities make it impractical to use this approach.” – Octave Levenspiel (1972)

Computational fluid dynamics (CFD) changes this picture. Using CFD, we can compute three-dimensional velocity fields and follow interactions of reactants and products through a tank. We can use this information to optimize tank geometry.
CFD: What is it?
CFD Solves the Reynolds Averaged Navier-Stokes (RANS) Equations by Numerical Schemes

- Continuity Equation: Law of Mass Conservation

\[ \frac{\delta \rho}{\delta t} + \frac{\delta (\rho u_i)}{\delta x_i} = 0 \]

- Momentum Equations: Newton’s Second Law (Incompressible Flow)

\[ \frac{\delta u_i}{\delta t} + u_j \frac{\delta u_i}{\delta x_j} = - \frac{1}{\rho} \frac{\delta P}{\delta x_i} + \nu \left( \frac{\delta^2 u_i}{\delta x_j^2} \right) + F_i \]
Breakdown of the Momentum Equations

\[
\frac{\delta u_i}{\delta t} + u_j \frac{\delta u_i}{\delta x_j} = \frac{1}{\rho} \frac{\delta P}{\delta x_j} - \nu \left( \frac{\delta^2 u_i}{\delta x_j^2} \right) + F_i
\]
The Momentum Equations are a Special Case of the Generalized Transport Equation

\[ \frac{\delta}{\delta t} (\rho \phi) + \frac{\delta}{\delta x_j} (\rho u_j \phi) = \frac{\delta}{\delta x_j} \Gamma \left( \frac{\partial \phi}{\partial x_j} \right) + S \]

- Unsteady
- Advection
- Diffusion
- Source
Discretization Techniques

- Finite difference
- Method of weighted residuals (finite element)
- Finite volume formulation
- Grid-less methods

All of these have been used in CFD for wastewater. Finite difference was the first technique used. Finite element has been used for clarifier modeling. Finite volume formulation is the most common commercial CFD software approach. Grid-less methods have not been much used, but may be promising.
How to eliminate pressure?

• Transform the governing equations:
  – Vorticity / stream function method
• Use iteration and convergence
  – SIMPLE

Both of these methods have been used in CFD for wastewater.
Turbulence Modeling

- Simplest model: Prandtl’s Mixing Length Hypothesis (Plane mixing layer, width $\delta$)

$$ \nu_t = l^2_m \left[ \frac{\partial u}{\partial y} \right] $$

$$ \frac{l_m}{\delta} = 0.07 $$

- Two Equation Models: $k - \varepsilon$

$$ \frac{\delta}{\delta t} (\rho k) + \frac{\delta}{\delta X_i} (\rho k U_i) = \frac{\delta}{\delta X_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\delta k}{\delta X_j} \right] + P_k + P_b - \rho \varepsilon - Y_m + S_k $$

$$ \frac{\delta}{\delta t} (\rho \varepsilon) + \frac{\delta}{\delta X_i} (\rho \varepsilon U_i) = \frac{\delta}{\delta X_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\delta \varepsilon}{\delta X_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (P_k + C_{3\varepsilon} P_b) - C_{2\varepsilon} \rho \frac{k^2}{\varepsilon} + S_\varepsilon $$

$$ \nu_t = C_{\mu} \frac{k^2}{\varepsilon} $$

3D transport models can be coupled to the velocity calculations to simulate sedimentation and mixing.

- **Solids Transport**

\[
\frac{\partial C}{\partial t} = -u_i \frac{\partial C}{\partial x_i} + \frac{\partial}{\partial x_i} \left( v_i \frac{\partial C}{\partial x_i} \right) + V_s \frac{\partial C}{\partial x_k}
\]

- **Vesilind settling**

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

- **Density couple**

\[ \rho = \rho_w + c \left( 1 - \frac{\rho_w}{\rho_s} \right) \]

Samstag, et al. (1992)
3D transport models can be implemented for wastewater quality parameters as well.

**Biokinetic Models**
- ASM Models
- Advanced oxidation Models
- Disinfection models

*Figure 5c. Nitrate*

Sobremisana, Ducoste and de los Reyes III (2011)
Multi-phase models can simulate motion of water and air.

\[
\frac{\partial \rho_d}{\partial t} + \frac{\partial}{\partial t} (\rho_d v_i) = 0
\]

\[
\frac{\partial \rho_c}{\partial t} + \frac{\partial}{\partial t} (\rho_c v_i) = 0
\]

\[
\frac{\partial}{\partial t} (\bar{\rho}_d v_i) = - \frac{\partial}{\partial x_j} (\bar{\rho}_d v_i v_j) - \alpha_d \frac{\partial p}{\partial x_i} + \beta_v (u_i - v_i) + T_{d,i}
\]

\[
\frac{\partial}{\partial t} (\bar{\rho}_c v_i) = - \frac{\partial}{\partial x_j} (\bar{\rho}_c v_i v_j) - \alpha_c \frac{\partial p}{\partial x_i} + \beta_v (u_i - v_i) + T_{c,i}
\]

Crowe, Sommerfield and Tusji (1998)
How to Do CFD?
Good Modelling Practice

Wicklein et al. (2016)
How to do CFD?

Software

• Hand Coded
  – Fortran
  – C++

• Commercial platforms (Examples)
  – ANSYS (Fluent and CFX)
  – CD-adapco (STAR-CCM+)
  – Flow Science (FLOW-3D)
  – COMSOL AB (COMSOL Multiphysics)
  – CHAM (PHOENICS)

• Open source platforms
  – OpenFOAM
Hand Coded Interface
TANKXZ
Fluent Interface
Standard OpenFOAM Interface
Visual CFD Interface for OpenFOAM
2015 OpenFOAM Workshop
Surfers Paradise

• Presentations by IWA WG members
• Teaching by Nelson Marques on OpenFOAM
  – Modeling
  – Meshing
  – Simulation
  – Post-Processing
• Example cases
  – Parshall Flume
  – Flow Splitter
  – Clarifier
  – UV Channel
OpenFOAM Workshop
Case Study: Splitter Box
OpenFOAM Workshop
Case Study: Activated Sludge Clarifier

Time: 0 s

alpha.sludge

0 0.001 0.002 0.003 0.00352
What can be done with CFD?

Wastewater Treatment Examples
Case Study: WWT Hydraulics

- Adverse Hydraulics
  - Vortices
  - Pre-rotation
  - Turbulence
  - Velocity Distribution

- Leading to
  - Decreased capacity
  - Poor flow distribution
  - Cavitation
  - Excessive wear

Provided by Jim Wicks, PhD
The Fluid Group
Case Study: WWT Hydraulics

Drop Shafts

➢ To transfer flood water and sewage rapidly down into a main sewer without blockage
➢ Multiphase flow
➢ Velocity dependent grit deposition

Provided by Jim Wicks, PhD
Case Study: WWT Hydraulics

Flow Splits

- Equal transfer of wastewater to multiple downstream units (ensuring solids component accounted for correctly)
- Velocity dependent grit deposition
- Multiphase flow

Provided by Jim Wicks, PhD
Case Study: Biokinetics
Eindhoven WWTP Facility
(The Netherlands)

From Rehman et al. (2014)
Configuration of the Bioreactor

Winter Aeration Package

Outer ring

Recycle Pumps

Summer Aeration package
Geometry

Diffusers simplification

Propellers

Aerators

Recycle pumps

\frac{x}{y} = \frac{X}{Y}
Velocity Vector Plots

- Bad mixing zones due to recirculation
- Averaged out in systemic modeling
- Change in aeration leads to different flow patterns
Dissolved oxygen and ammonia conc. (mg/L)

Oxygen concentration at 3.45m depth

Ammonia concentration at 3.45m depth
Case Study: Jet Mixing in a sequencing batch reactor (SBR)
Case Study: Mixing
CFD of Jet Mixing and Aeration

- 415,350 mixed tetrahedral cells
- 2,108,308 nodes
- Inlet flow into jet nozzles
- Outlet flow to pump suction
- Air added as second phase
- Solids transport, settling, and density impact modeled by UDF

Samstag et al. (2012)
Case Study: Mixing
Velocity Profiles for Pumped Mixing and Aeration

Simulated Pumped Mixing Profile

Simulated Aeration Profile
Case Study: Mixing
Comparison of Pumped Mix Velocity Profiles for Increasing Jet Velocities

Existing (2.5 m/sec Jet)

3.0 m/sec Jet

3.5 m/sec Jet

4.0 m/sec Jet
Case Study: Mixing
Comparison of Solids Profiles for Increasing Jet Velocities

Existing (2.5 m/sec Jet)

3.0 m/sec Jet

3.5 m/sec Jet

4.0 m/sec Jet
Case Study: Mixing
Comparison of Density-coupled and Neutral Density Simulations

Density-coupled

Solids transport model calculates the local solids concentration based on flow regime. The influence of the local solids concentration on the local density is then iteratively calculated. This approach was verified by the field solids profile test data.
Case Study: Mixing
Comparison of Density-coupled and Neutral Density Simulations

Neutral Density

Solids transport model calculates the local solids concentration based on flow regime.
Influence of the local solids concentration on the local density was turned off.
This approach over-predicted measured solids mixing.
Case Study: Activated Sludge Clarification (Calibration)

Samstag et al. (2010)
Case Study: Activated Sludge Clarifier

- Radial flow clarifier
- Questions:
  - Optimum Depth?
  - Optimum Inlet?
  - Optimum Feedwell?
  - Optimum Effluent Zone?
Radial Flow Clarifier CFD Model

- 3D Fluent CFD
- 1,100,000 hexahedral cells
- K-epsilon turbulence model
- User defined functions (UDF) to implement
  - Solids settling and transport
  - Density coupling
Case Study: Activated Sludge Clarifier Calibration CFD
Case Study: Activated Sludge Clarifier
Alternative Inlet Configurations
Case Study: Activated Sludge Clarifier
Alternative Velocity Vector Plans
Case Study: Activated Sludge Clarifier

Alternative Velocity Plans
Case Study: Activated Sludge Clarifier
Alternative Velocity Profiles
Case Study: Activated Sludge Clarifier
Comparison Solids Profiles
Case Studies: Disinfection

- Dye, disinfectant, and microorganism transport in a chemical disinfection system

Provided by Steven Saunders, P.E.
Case Study: Dissolved Air Flotation

DAF

- Seawater DAF – desalination use
- Prediction of absolute maximum capacity (typically 10-20% above design max)
- Comparison of nozzle design and air introduction

Provided by Jim Wicks, PhD
Case Study: Digesters

Digesters

- Non-Newtonian flow above 3% DS
- Rheology for all digestates difficult to measure. Typically we use a library of values for various dry solids contents (and for various sludge types)
- Useful for optimising methane gas production; reducing foaming; limiting solids deposition and avoiding ‘dead’ volumes.

Provided by Jim Wicks, PhD
Who is Doing CFD?

• IWA CFD Working Group
  “The WG intends to solve shortcomings arising from lack of knowledge of CFD in the water and wastewater community in the short term by producing papers and books as well as hands-on training for the IWA MIA members (and beyond). Furthermore, a book dedicated for training new people in the water/wastewater field will be produced.”
IWA CFD Working Group
Management Team
IWA CFD Working Group

Work Products

• **Published Papers**
  – Computational Fluid Dynamics (CFD): What is Good CFD-Modeling Practice and What Can Be the Added Value of CFD Models to WWTP Modeling? 2012 WEFTEC
  – A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling, 2012 WST
  – Computational Fluid Dynamics: an important modelling tool for the water sector 2012 IWC Conference
  – Good Modelling Practice in Applying Computational Fluid Dynamics for WWTP Modelling 2016 WST

• **Submitted Papers**
  – CFD for Wastewater: An Overview (in review) WST

• **Workshops**
  – WEFTEC 2012 (Fluent)
  – WWTMod 2012
  – Watermatex 2015 (OpenFOAM)
  – WEFTEC 2016 (FLOW-3D)
  – IWA Biennium 2016 (Proposed)

• **Book Plans**
  – IWA Scientific and Technical Report
  – CFD for Water Book for Students and Practitioners
There is also a LinkedIn Group CFD for Wastewater
Further Reading

- Levenspiel 1972 *Chemical Reaction Engineering*.
- Sobremisana, Ducoste, and de los Reyes III 2011 Combining CFD, floc dynamics, and biological reaction kinetics to model carbon and nitrogen removal in an activated sludge system. Water Environment Conference, WEFTEC Conference.
- Amato, T. and Wicks, J. 2009 The practical application of computational fluid dynamics to dissolved air flotation, water treatment plant operation, design and development’. *J. Wat. Supply: Research & Technology - AQUA*, 58(1), pp 65-73.
Thank you!
Questions?

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