Part 1: Introduction to Open Source CFD for Water Resource and Recovery Facilities

Welcome

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CFD for WRWF: Goal of the Workshop

To gain some understanding of how computational fluid dynamics (CFD) can help us to better understand water resource recovery facilities using an open source tool.
“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 and to improve designs and operation.

Plan for the Workshop: Part 1

<table>
<thead>
<tr>
<th>TIME</th>
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<th>INSTRUCTOR AND AFFILIATION</th>
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</thead>
<tbody>
<tr>
<td>8:30 to 9:15</td>
<td>Welcome and Introduction to CFD for WRRF</td>
<td>Randal Samstag, Civil and Sanitary Engineer</td>
</tr>
<tr>
<td>9:15 to 10:00</td>
<td>Good Modeling Practice for CFD</td>
<td>Edward Wicklein, Carollo Engineers</td>
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<tr>
<td>10:00 to 10:30</td>
<td>Break</td>
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<tr>
<td>10:30 to 12:00</td>
<td>Introduction to CFD using Open FOAM</td>
<td>Nelson Marques, blueCAPE</td>
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<tr>
<td>12:00 to 1:30</td>
<td>Lunch</td>
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<tr>
<td>1:30 to 3:00</td>
<td>Getting Started with OpenFOAM: Example Case (Parshall flume) - Setup, Meshing, Pre Processing, Simulation and Post Processing</td>
<td>Nelson Marques, blueCAPE</td>
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<tr>
<td>3:00 to 3:30</td>
<td>Break</td>
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<tr>
<td>3:30 to 4:00</td>
<td>CFD for flow splitting</td>
<td>Edward Wicklein, Carollo Engineers</td>
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<tr>
<td>4:00 to 5:00</td>
<td>OpenFOAM case: Flow Splitting</td>
<td>Nelson Marques, blueCAPE</td>
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## Plan for the Workshop: Day 2

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<th>TIME</th>
<th>TOPIC</th>
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</thead>
<tbody>
<tr>
<td>8:30 to 9:00</td>
<td>Welcome and Brief Introduction to CFD for WRRF and installation of software for participants who could not attend Day One</td>
<td>Randal Samstag, Civil and Sanitary Engineer Nelson Marques, blueCAPE</td>
</tr>
<tr>
<td>9:00 to 9:30</td>
<td>CFD for mixing</td>
<td>Edward Wicklein, Carollo Engineers</td>
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<tr>
<td></td>
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<td>Stephen Saunders, IBIS Group CFD</td>
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<tr>
<td>9:30 to 10:00</td>
<td>OpenFOAM case study: Mixing</td>
<td>Nelson Marques, blueCAPE</td>
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<td>10:00 to 10:30</td>
<td>Break</td>
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<tr>
<td>10:30 to 11:00</td>
<td>CFD for Sedimentation: Calibration Modeling and Verification</td>
<td>Alonso Griborio, Hazen and Sawyer</td>
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<tr>
<td>11:00 to 12:00</td>
<td>OpenFOAM case study: Sedimentation</td>
<td>Nelson Marques, blueCAPE</td>
</tr>
<tr>
<td>12:00 to 1:30</td>
<td>Lunch</td>
<td></td>
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<tr>
<td>1:30 to 2:00</td>
<td>CFD of Disinfection Facilities</td>
<td>Edward Wicklein and Stephen Saunders</td>
</tr>
<tr>
<td>2:00 to 3:00</td>
<td>OpenFOAM case study: Ultraviolet Disinfection</td>
<td>Nelson Marques, blueCAPE</td>
</tr>
<tr>
<td>3:00 to 3:30</td>
<td>Break</td>
<td></td>
</tr>
<tr>
<td>3:30 to 4:45</td>
<td>OpenFOAM advanced topics: Making your own cases</td>
<td>Nelson Marques, blueCAPE</td>
</tr>
<tr>
<td>4:45 to 5:00</td>
<td>Wrap-up and Adjourn</td>
<td>Randal Samstag, Civil and Sanitary Engineer</td>
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## Sponsors of the Workshop

- **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
  • Good Modelling Practice in Applying Computational Fluid Dynamics for WWTP Modelling, WEFTEC 2012
  • A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling, WST
  • Computational Fluid Dynamics: an important modelling tool for the water sector, IWC Conference
  • Good Modelling Practice in Applying Computational Fluid Dynamics for WWTP Modelling, WST (2016)
  • CFD for Wastewater: An Overview, WST (2016)

• Workshops
  • WEFTEC 2012 (Fluent)
  • WWTMod 2012
  • Watermatex 2015 (OpenFOAM)
  • WEFTEC 2016 (Flow-3D)
  • WEFTEC 2017 (OpenFOAM)

• Book Projects
  • IWA Scientific and Technical Report
  • CFD for Water Book for Students and Practitioners
There is also a LinkedIn Group CFD for Wastewater

Thank you! On with the show.

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Introduction to CFD for Water Resource and Recovery Facilities

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CFD for WRRF: What can it do?

• What is CFD?
• How is it done?
• What is it good for?
• Conclusions
What is CFD (computational fluid dynamics)?

“. . . flows and related phenomena can be described by partial differential equations, which cannot be solved analytically except in special cases. To obtain an approximate solution numerically, we have to use a discretization method which approximates the differential equations by a system of algebraic equations, which can then be solved on the computer.” - Ferziger and Peric (2002) Computational Techniques for Fluid Dynamics, 3rd Edition, Springer.

“Computational fluid dynamics, then, is a separate discipline, distinct from and supplementing both experimental and theoretical fluid dynamics, with its own techniques, its own difficulties, and its own realm of utility, offering new perspectives in the study of physical processes.” - Roach, P.J. (1982) Computational Fluid Dynamics, Hermosa Publishers.

CFD solves the Navier-Stokes Equations by numerical schemes.

- Continuity Equation: Law of Mass Conservation
  \[
  \frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i)}{\partial x_i} = 0
  \]

- Momentum Equations: Newton’s Second Law (incompressible laminar flow)
  \[
  \frac{\partial U_j}{\partial t} + U_j \frac{\partial U_j}{\partial x_j} = - \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \left( \frac{\partial^2 U_i}{\partial x_i^2} \right) + F_i
  \]
Breakdown of the Momentum Equations (for laminar flow)

\[
\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho_r} \frac{\partial P}{\partial x_i} + \nu \left( \frac{\partial^2 U_i}{\partial x_j \partial x_j} \right) + \frac{1}{\rho} \left( \rho - \rho_r \right)
\]

Unsteady Term
Adective Term
Pressure Term
Diffusion Term
Source Term (gravity force)

The momentum equations are a special case of the generalized transport equation (laminar).

\[
\frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_j} = \lambda \frac{\partial^2 \phi}{\partial x_i \partial x_j} + S_\phi
\]

Unsteady
Advection
Diffusion
Source
What about turbulence? One way to model it is to use the Reynolds averaged Navier-Stokes equations (RANS).

- All flow in WRRF is turbulent.
- Turbulent flow is variable in space and time.
- Osborne Reynolds suggested that turbulent flow could be considered as a composite of an average part and a fluctuating part.

\[
U_i = \overline{U}_i + u_i \\
\overline{U}_i = \frac{1}{T} \int_0^T U(t + \tau) d\tau
\]

\[
P = \overline{P} + p \\
\overline{P} = \frac{1}{T} \int_0^T P(t + \tau) d\tau
\]

\[
\phi = \overline{\phi} + \varphi \\
\overline{\phi} = \frac{1}{T} \int_0^T \phi(t + \tau) d\tau
\]


---

The Reynolds Averaged Momentum and Scalar Transport Equations

\[
\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}\right) + g_i \frac{p - \rho \gamma}{\rho},
\]

\[
\frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial \phi}{\partial x_j} - \overline{u_i \phi}\right) + S_\phi
\]

The velocity correlation terms can be modelled in terms of “eddy viscosity” and the transport terms as “eddy diffusivity”.

$$-u_i u_j = \nu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} k \sigma_{ij}$$

$$k = \frac{1}{2} \left( u_1^2 + u_2^2 + u_3^2 \right)$$

$$-u_i \phi = \Gamma \left( \frac{\partial \phi}{\partial x_i} \right)$$


---

RANS Modelling: Eddy Viscosity and Diffusivity

- Simplest model: Prandtl’s Mixing Length Hypothesis (Plane mixing layer, width $\delta$)
  
  $$\nu_t = I_m \left[ \frac{\partial u}{\partial y} \right] \quad I_m = 0.07$$

- Two Equation Models: $k – \text{epsilon}$

  $$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \nu_t \frac{\partial k}{\partial x_j} \right) + C_{1k} \frac{\epsilon}{k} \left( P + G \right) \left( 1 + c_1 R_e \right) - C_{2k} \frac{\epsilon^2}{k} + S_k$$

  $$\nu_t = C_1 \frac{k^2}{\epsilon} \quad \Gamma = \frac{\nu_t}{\sigma_x}$$

Another Turbulence Modelling Approach: Large Eddy Simulation

- **RANS Simulation (Steady State)**
- **LES Simulation (Transient)**

Discretization

- 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.
Finite Difference Method (2D MAC)

Horizontal Momentum Eqn.

\[
\frac{\partial u}{\partial t} + \frac{\partial (u^2)}{\partial x} + \frac{\partial (uv)}{\partial y} + \frac{\partial p}{\partial x} = \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g_x
\]

Finite Difference Equivalent

\[
\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \frac{u_{i+1,j}^n - u_{i-1,j}^n}{2\Delta x} + \frac{(u_{i+1/2,j+1/2}^n)(v_{i+1/2,j+1/2}^n) - (u_{i-1/2,j+1/2}^n)(v_{i-1/2,j+1/2}^n)}{\Delta y}
\]

\[
+ \frac{p_{i,j} - p_{i+1,j}}{\Delta x} + v \left( \frac{u_{i+1/2,j+1/2}^n + u_{i+1/2,j-1/2}^n - 2u_{i+1/2,j}^n}{\Delta x^2} \right) + \frac{(u_{i+1/2,j+1}^n + u_{i+1/2,j-1}^n - 2u_{i+1/2,j}^n)}{\Delta y^2}
\]  


Finite Element Method (2D)

- Interpolate the velocity and pressure fields
  \[
  u = \sum_t u_t \phi_t^u (\xi, n) \quad v = \sum_t v_t \phi_t^v (\xi, n) \quad p = \sum_t p_t \phi_t^p (\xi, n)
  \]
- Substitute interpolations into the governing equations.
  - Continuity
  - X/Y momentum
- Solve the system of equations iteratively

Finite Volume Method (2D)

Continuity Eqn.

\( p_{j,k} \)
\( u_{j-1,k} \)
\( v_{j,k} \)
\( v_{j,k+1} \)
\( x \) Momentum Eqn.

\( p_{j+1,k} \)
\( u_{j+1,k} \)
\( v_{j,k} \)
\( v_{j,k+1} \)
\( y \) Momentum Eqn.

\( p_{j,k+1} \)
\( u_{j-1,k} \)
\( v_{j,k+1} \)
\( v_{j+1,k} \)


Grid-less Methods

- Vortex Methods
  - Developed by Chorin
  - Random walk of “vortex blobs”

- SPH
  - “Lagrangian” method developed from astrophysics

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.

The Vorticity / Stream Function Method

\[ \zeta = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \quad \text{Definition of Vorticity} \]

\[ \frac{\partial \zeta}{\partial t} + \frac{\partial (v \zeta)}{\partial x} + \frac{\partial (u \zeta)}{\partial y} - \frac{1}{Re} \left( \frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 \zeta}{\partial y^2} \right) = 0 \quad \text{Vorticity Transport Eqn.} \]

\[ u = \frac{\partial \psi}{\partial y} \quad v = -\frac{\partial \psi}{\partial x} \quad \text{Definition of Stream Function} \]

\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \zeta \quad \text{Poisson Eqn. for Stream Function} \]

SIMPLE: Semi-Implicit Pressure Linked Equations

• Guess the pressure field
• Solve the momentum equations
• Solve pressure correction
• Calculate velocities
• Solve for other properties (temperature, solids)
• Update the pressure field and iterate to convergence


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

• Solids Transport

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

• 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)

Continuity Equation:
\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = 0 \]

Momentum Equations:
\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \]
\[ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \]

Fluid Marker Equation:
\[ \frac{\partial F}{\partial t} + u \frac{\partial F}{\partial x} + v \frac{\partial F}{\partial y} = 0 \]

Hirt and Nichols (1981), Volume of Fluid Method, Los Alamos Scientific Laboratory, Los Alamos, NM.

VOF can be used for open water surface problems.

- An elementary tutorial in OpenFOAM is based on VOF method using the interFoam solver.
- The famous dam break problem was simulated first using the MAC method by Harlow and Welsh.
- This simulation using a RANS turbulence approach.
3D transport models can be implemented for wastewater quality parameters as well.

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

Sobremisana, Ducoste and de los Reyes III (2011)

Multi-phase models can simulate motion of water and air.

\[
\frac{\partial \bar{\rho}_v}{\partial t} + \frac{\partial \bar{\rho}_v v}{\partial t} (\bar{\rho}_d v_i) = 0 \\
\frac{\partial \bar{\rho}_d}{\partial t} + \frac{\partial \bar{\rho}_d v_i}{\partial t} (\bar{\rho}_d v_i) = 0 \\
\frac{\partial}{\partial t} (\bar{\rho}_d v_i) = - \frac{\partial}{\partial x_j} (\bar{\rho}_d v_i v_j) - \alpha_d \frac{\partial \bar{p}}{\partial x_i} + \beta_v (u_i - v_i) + T_{d,i} \\
\frac{\partial}{\partial t} (\bar{\rho}_v v_i) = - \frac{\partial}{\partial x_j} (\bar{\rho}_v v_i v_j) - \alpha_v \frac{\partial \bar{p}}{\partial x_i} + \beta_v (u_i - v_i) + T_{v,i}
\]

Drift Flux Model: Another Way to Simulate Solids

Mixture Continuity Equation

\[ \frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m v_m) = 0 \]

Drift Equation

\[ \frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d v_d) = -\nabla \cdot \left( \frac{\alpha_d \rho_d v_d}{\rho_m} \right) + \nabla \cdot \mathbf{I} \nabla \alpha_d \]

Mixture Momentum Equation

\[ \frac{\partial \rho_m v_m}{\partial t} + \nabla \cdot (\rho_m v_m v_m) = -\nabla P_m + \nabla \cdot [\tau + \tau] - \nabla \left( \frac{\alpha_d \rho_d v_d}{1-\alpha_d \rho_m} \right) + \rho_m g + M_m \]


How to Do CFD? Good Modelling Practice

How to do CFD?
Software

• Hand Coded
  • Fortran
  • C++

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

• Open source platforms
  • OpenFOAM

Hand Coded Interface:
TANKXZ
Fluent Interface

blueCFD-Core Windows OpenFOAM Interface
Visual-CFD Interface for OpenFOAM

What can be done with CFD? Wastewater Treatment Examples

Examples you will learn to simulate in these workshops:

- Parshall Flume (Day 1)
- Splitter Box (Day 1)
- Mixing Tank (Day 2)
- Clarifier (Day 2)
- UV Disinfection (Day 2)

OpenFOAM Simulation
Case Study: Splitter Box
OpenFOAM Simulation
Case Study: Activated Sludge Clarifier

What’s CFD Good For? Conclusions

- Improve flow and solids splitting in distribution channels
- Optimize tank geometry
  - Evaluation of the impacts of reactor geometry on performance
  - Evaluation of location for control sensors
- Evaluate the impacts of mixing on performance
- Verify simpler models
- Improve basic understanding of process behavior
Further Reading

- Hirt and Nichols (1981), Volume of Fluid Method, Los Alamos Scientific Laboratory, Los Alamos, NM.
- 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.

Thank you!

Questions?

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