weftec 2017 CHICAGO
the water quality event™

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

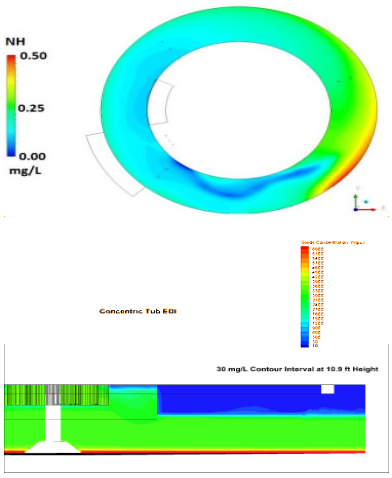
Welcome

Randal W. Samstag, MS, PE, BCEE
Civil and Sanitary Engineer
Bainbridge Island, WA US

WORKSHOPS 90 YEARS

CFD for WRRF: 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

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

Plan for the Workshop: Day 2

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

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WORKSHOPS

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."

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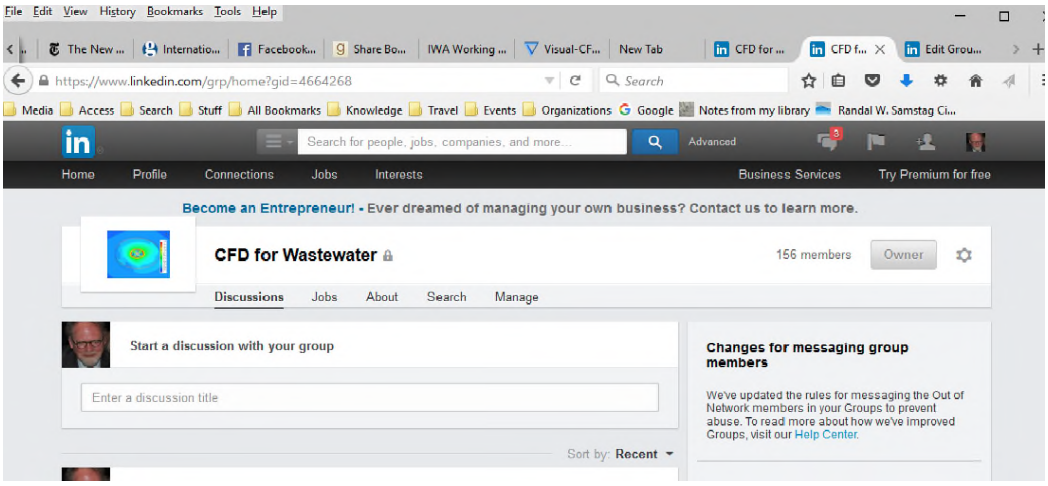
WORKSHOPS

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

Randal W. Samstag, MS, PE, BCEE
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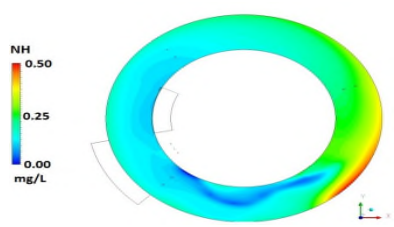
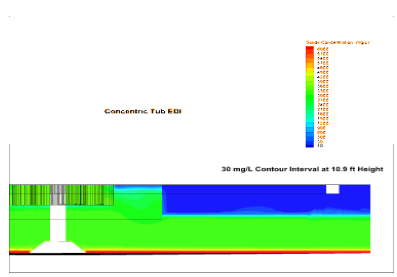
CFD for WRRF: What can it do?

- 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)

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \upsilon\left(\frac{\partial^2 U_i}{\partial x_j^2}\right) + F_i$$

Breakdown of the Momentum Equations (for laminar flow)

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho_r}\frac{\partial P}{\partial x_i} + \upsilon\left(\frac{\partial^2 U_i}{\partial x_j \partial x_i}\right) + g_i \frac{(\rho - \rho_r)}{\rho_r}$$

Unsteady Term

Advective Term

Pressure Term

Diffusion Term

Source Term
(gravity force)

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

$$\frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\delta x_i} = \lambda \frac{\partial^2 \phi}{\partial x_i \partial x_i} + S_\phi$$

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.

$$U_i = \overline{U_i} + u_i \qquad \overline{U_i} = {}^{1}/_{T} \int_0^T U(t+\tau)d\tau$$

$$P = \bar{P} + p \qquad \bar{P} = {}^{1}/_{T} \int_0^T P(t+\tau)d\tau$$

$$\phi = \bar{\phi} + \varphi \qquad \bar{\phi} = {}^{1}/_{T} \int_0^T \phi(t+\tau)d\tau$$

See Henze, J. O. (1975) Turbulence, 2nd Ed, McGraw-Hill.

The Reynolds Averaged Momentum and Scalar Transport Equations

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}\right) + g_i \frac{\rho - \rho_r}{\rho_r}$$

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

Rodi (1980) *Turbulence Models and Their Application in Hydraulics: A state-of-the art review, IAHR / AIRH*.

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

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

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

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

Rodi (1980) *Turbulence Models and Their Application in Hydraulics: A state-of-the art review, IAHR / AIRH*.

RANS Modelling: Eddy Viscosity and Diffusivity

- Simplest model: Prandtl's Mixing Length Hypothesis (Plane mixing layer, width δ)

$$\upsilon_t = l_m^2 \left[\frac{\partial u}{\partial y}\right] \qquad l_m / \delta = 0.07$$

- Two Equation Models: k – epsilon

$$\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_i}\right) + \underbrace{\nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_i}{\partial x_j}}_{P} + \underbrace{\beta g_i \frac{\nu_t}{\sigma_t}\frac{\partial \phi}{\partial x_i}}_{G} - \varepsilon$$

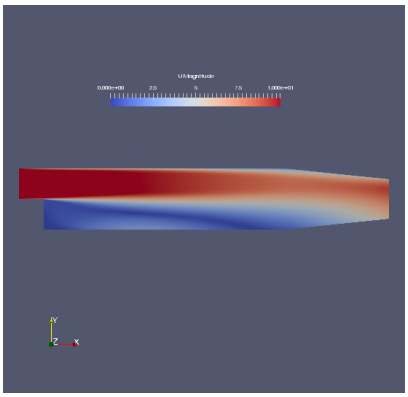
$$\frac{\partial \varepsilon}{\partial t} + U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right) + C_{1\varepsilon}\frac{\varepsilon}{k}(P+G)\left(1 + c_3 R_f\right) - C_{2\varepsilon}\frac{\varepsilon^2}{k} + S_\varepsilon$$

$$\upsilon_t = C_\mu \frac{k^2}{\varepsilon} \qquad \Gamma = \frac{\nu_t}{\sigma_t}$$

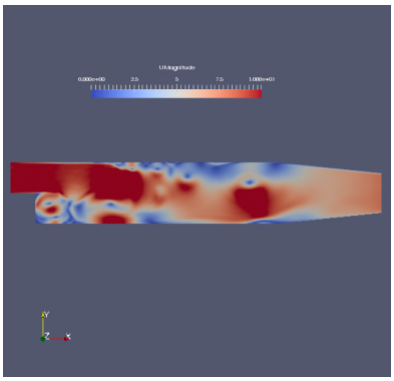
Rodi (1980) *Turbulence Models and Their Application in Hydraulics: A state-of-the art review, IAHR / AIRH*.

Another Turbulence Modelling Approach : Large Eddy Simulation

RANS Simulation (Steady State)



LES Simulation (Transient)

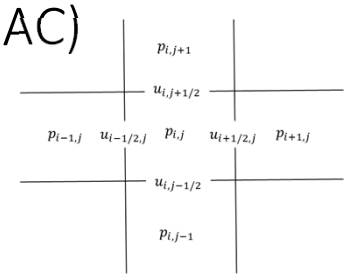


Discretization

- 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

$$\frac{\left(u^{n+1}_{i+1/2,j} - u^{n}_{i-1/2,j}\right)}{\Delta t} = \frac{u^2_{i,j} - u^2_{i-1,j}}{\Delta x} + \frac{(u_{i+1/2,j-1/2})(v_{i+1/2,j-1/2}) - (u_{i-1/2,j+1/2})(v_{i-1/2,j+1/2})}{\Delta y}$$

$$+ \frac{p_{i,j} - p_{i+1,j}}{\Delta x} + \nu \left(\frac{\left(u_{1-3/2,j} + u_{1-1/2,j} - 2u_{i+3/2,j}\right)}{\Delta x^2} + \frac{\left(u_{i+1/2,j+1} + u_{i+1/2,j-1} - 2u_{i+1/2,j}\right)}{\Delta y^2} \right) + g_x$$

Harlow, F.H. and Welch, J. E. (1965) Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surface, *Physics of Fluids*, V. 8 Number 12.

Finite Element Method (2D)

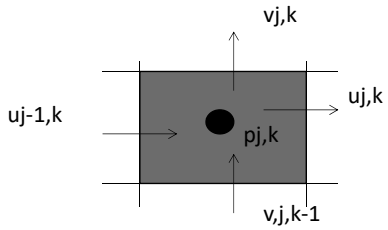
- Interpolate the velocity and pressure fields

$$u = \sum_l u_l \phi_l^u(\xi, n) \qquad v = \sum_l v_l \phi_l^v(\xi, n) \qquad p = \sum_l p_l \phi_l^p(\xi, n)$$

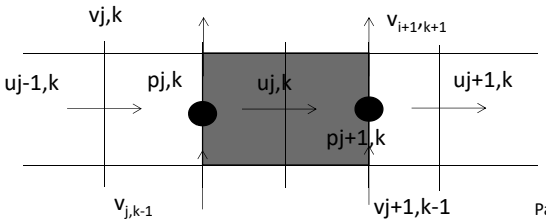
- Substitute interpolations into the governing equations.
  - Continuity
  - X/Y momentum
- Solve the system of equations iteratively

Fletcher, C.A.J (2006) *Computational Techniques for Fluid Dynamics*, *Volume II*, 2nd Ed. Springer-Verlag.

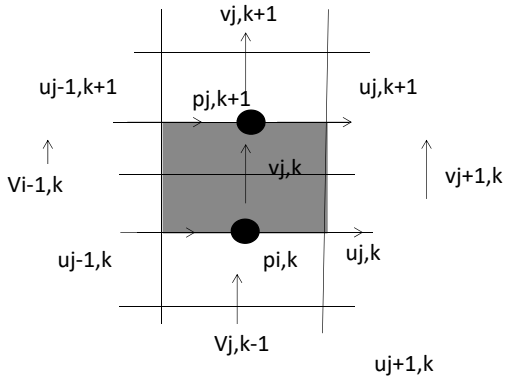
Finite Volume Method (2D)



Continuity Eqn.



x Momentum Eqn.



y Momentum Eqn.

Patankar, S. V. (1980) *Numerical Heat Transfer and Fluid Flow*, Hemisphere Publishing.

Grid-less Methods

- Vortex Methods
  - Developed by Chorin
  - Random walk of "vortex blobs"
- SPH
  - "Lagrangian" method developed from astrophysics

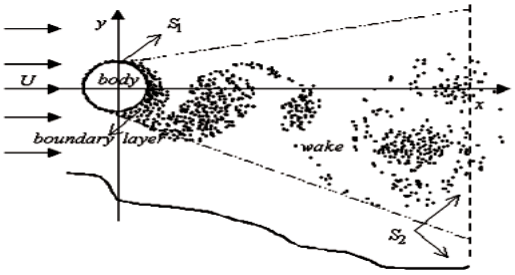


Figure 1. Flow around a bluff body.

PEREIRA, L. A. A.; HIRATA, M. H. and SILVEIRA NETO, A.. Vortex method with turbulence sub-grid scale modelling. *J. Braz. Soc. Mech. Sci. & Eng.* [online]. 2003, vol.25, n.2 [cited 2015-05-01], pp. 140-146 .

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

$$\zeta = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}$$ Definition of Vorticity

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (v\zeta)}{\partial x} + \frac{\partial (v\zeta)}{\partial y} - \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 \zeta}{\partial y^2}\right) = 0$$ Vorticity Transport Eqn.

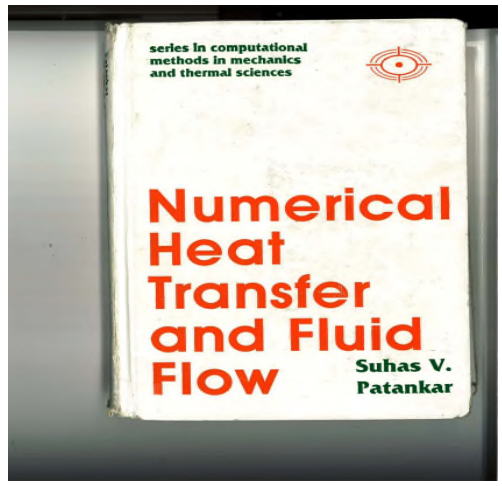
$$u = \frac{\partial \psi}{\partial y} \qquad v = -\frac{\partial \psi}{\partial x}$$ Definition of Stream Function

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \zeta$$ Poisson Eqn. for Stream Function

Roach, P.J. (1982) *Computational Fluid Dynamics*, Hermosa Publishers.

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



Patankar, S. V., (1980) *Numerical Heat Transfer and Fluid Flow*.

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

- Solids Transport

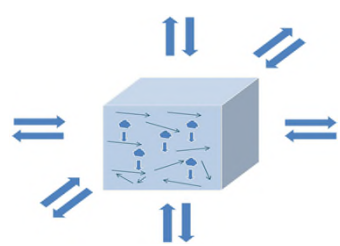
$$\frac{\partial C}{\partial t} = \frac{-u_i \partial C}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_s}\frac{\partial C}{\partial x_i}\right) + V_s \frac{\partial C}{\partial x_k}$$

- 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)

(2D) Volume of Fluid (VOF) Method: Hirt and Nichols (1981)

Continuity Equation:

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$$

Momentum Equations:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{1}{\rho}\frac{\partial p}{\partial x}+\upsilon\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{1}{\rho}\frac{\partial p}{\partial y}+\upsilon\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)$$

Fluid Marker Equation:

$$\frac{\partial F}{\partial t}+u\frac{\partial F}{\partial x}+v\frac{\partial F}{\partial y}=0$$

HIRT AND NICHOLS

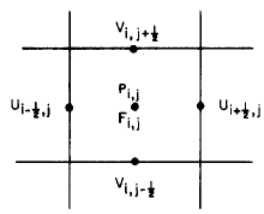


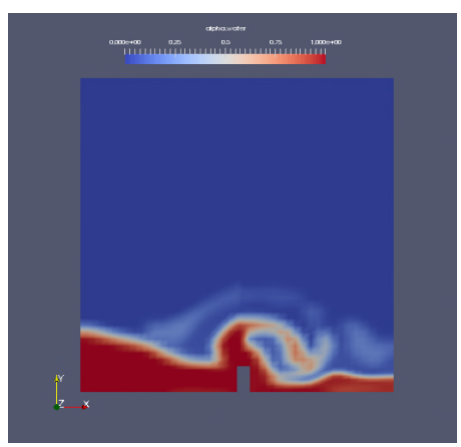
FIG. 2. Location of variables in a typical mesh cell.

F=1 if fluid is present
F=0 if fluid is not present

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

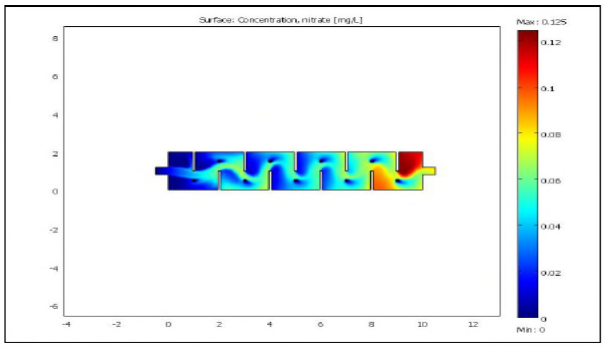
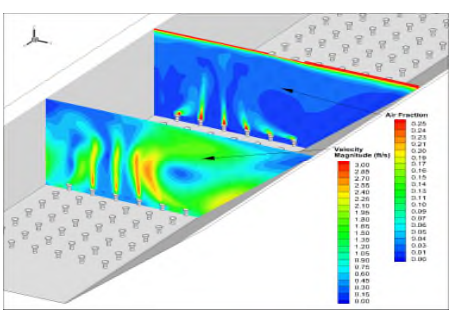


Figure 5c. Nitrate

Sobremisana, Ducoste and de los Reyes III (2011)

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



$$\frac{\partial \overline{\rho}_d}{\partial t} + \frac{\partial}{\partial t}(\overline{\rho}_d v_i) = 0$$

$$\frac{\partial \overline{\rho}_c}{\partial t} + \frac{\partial}{\partial t}(\overline{\rho}_c v_i) = 0$$

$$\frac{\partial}{\partial t}(\overline{\rho}_d v_i) = -\frac{\partial}{\partial x_j}(\overline{\rho}_d v_i v_j) - \alpha_d \frac{\partial p}{\partial x_i} + \beta_V (u_i - v_i) + T_{d,i}$$

$$\frac{\partial}{\partial t}(\overline{\rho}_c v_i) = -\frac{\partial}{\partial x_j}(\overline{\rho}_c v_i v_j) - \alpha_c \frac{\partial p}{\partial x_i} + \beta_V (u_i - v_i) + T_{c,i}$$

Crowe, Sommerfield, and Tusji (1998) *Multiphase Flows with Droplets and Particles*.

Drift Flux Model: Another Way to Simulate Solids

Mixture Continuity Equation

$$\frac{\partial \rho_m}{\partial t} + \nabla.(\rho_m v_m) = 0$$

Drift Equation

$$\frac{\partial \alpha_d}{\partial t} + \nabla.(\alpha_d\ v_m) = -\nabla.\left(\frac{\alpha_d \rho_c}{\rho_m} v_{dj}\right) + \nabla.\Gamma\nabla\alpha_d$$

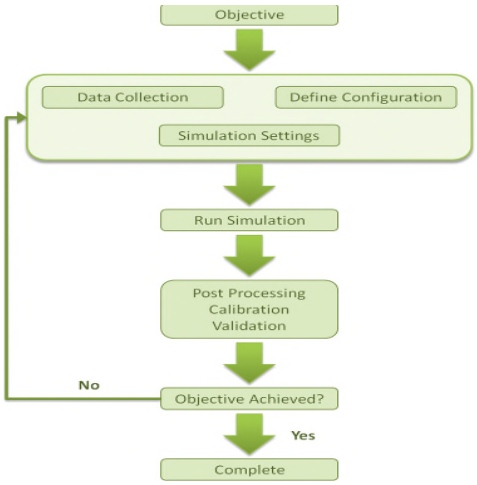
Mixture Momentum Equation

$$\frac{\partial \rho_m v_m}{\partial t} + \nabla.(\rho_m v_m v_m) = -\nabla.P_m + \nabla.[\tau + \tau^t] - \nabla.\left(\frac{\alpha_d}{1-\alpha_d}\frac{\rho_c \rho_d}{\rho_m} v_{dj} v_{dj}\right) + \rho_m g + M_m$$

Brennan, D. (2001) *The Numerical Simulation of Two-Phase Flows in Settling Tanks,* PhD Dissertation, University of London.

How to Do CFD? Good Modelling Practice

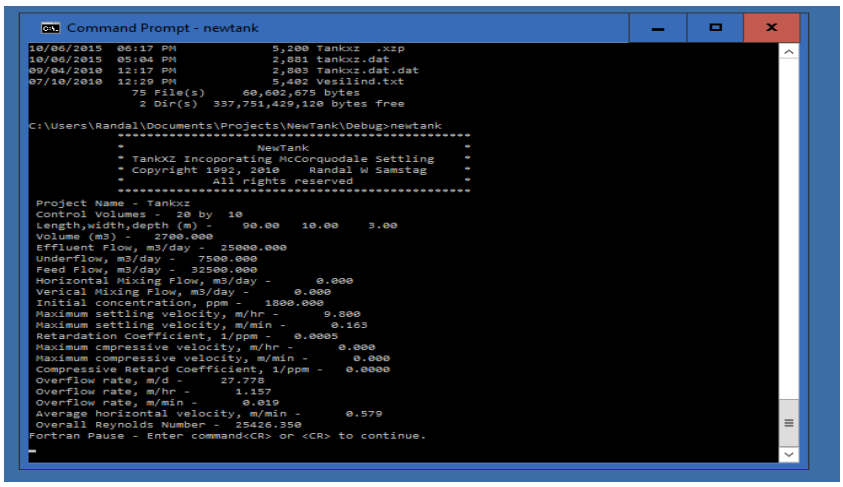
Wicklein et al. (2016) Good modelling practice in applying computational fluid dynamics for WWTP modelling, *WST*, 73 (5) 969-982.



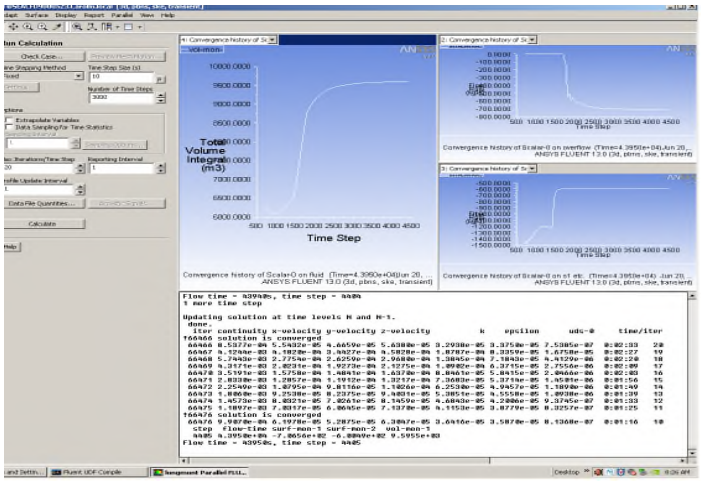
How to do CFD? Software

- 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

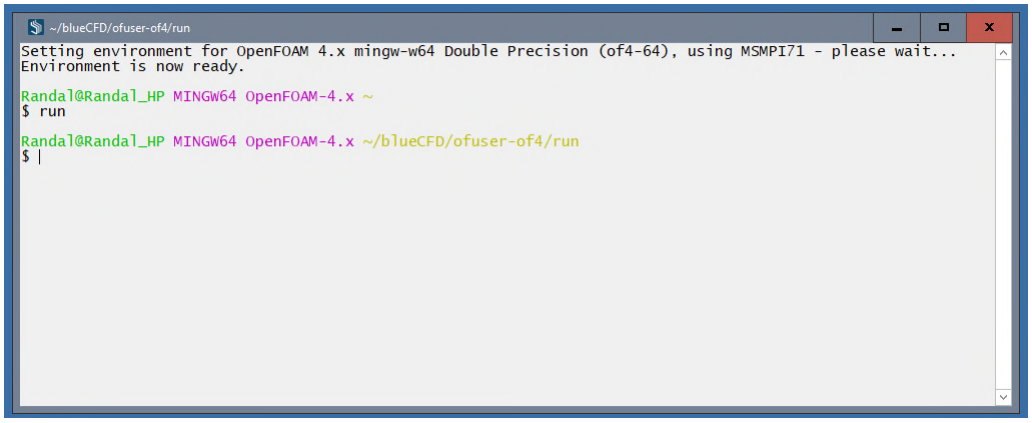
Hand Coded Interface: TANKXZ



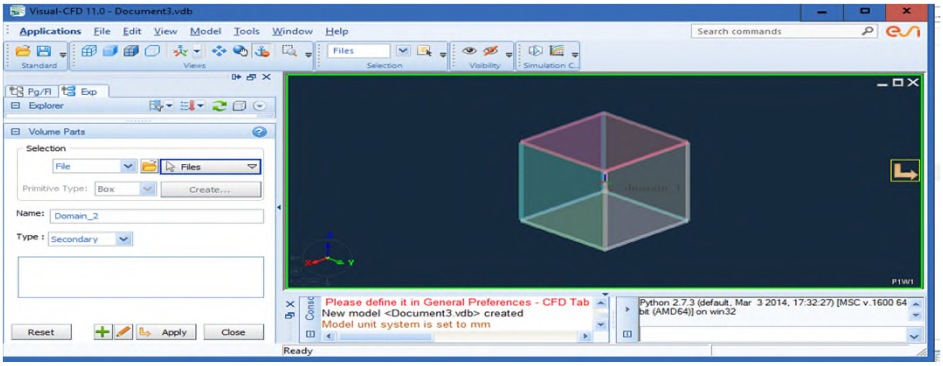
Fluent Interface



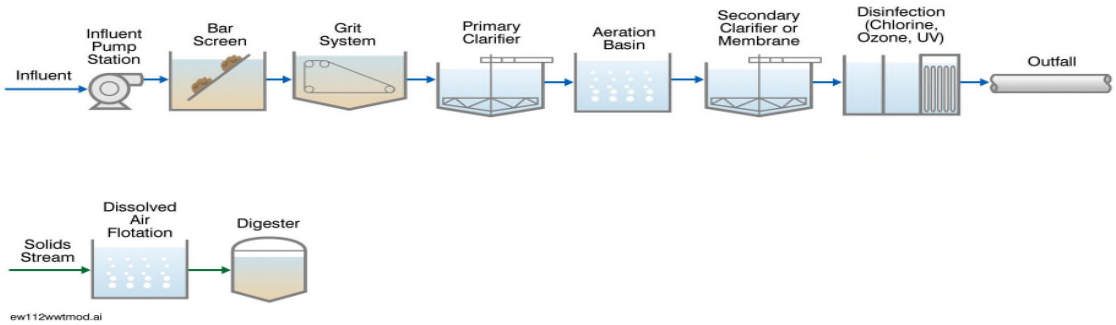
blueCFD-Core Windows OpenFOAM Interface



Visual-CFD Interface for OpenFOAM



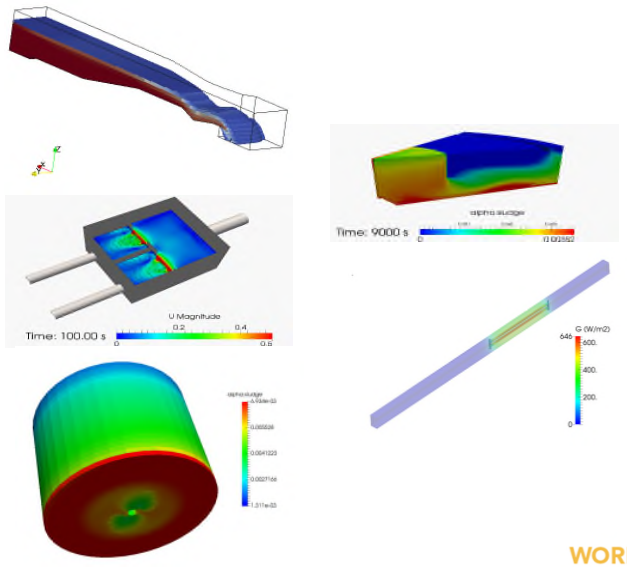
What can be done with CFD? Wastewater Treatment Examples



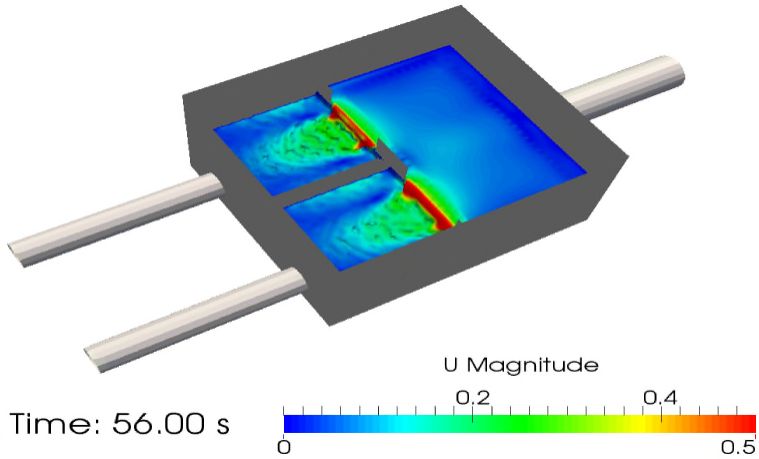
Samstag et al. (2016) CFD for Wastewater: An Overview, Water Science and Technology, 74 (3), 549–563.

Examples you will learn to simulate in these workshops:

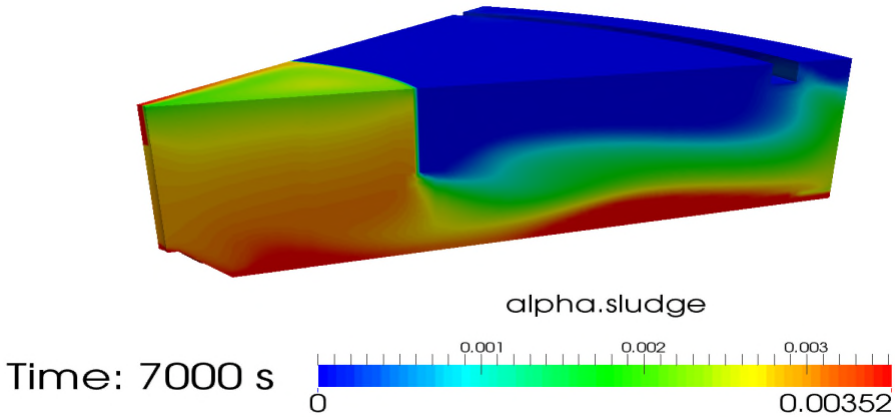
- Parshall Flume (Day 1)
- Splitter Box (Day 1)
- Mixing Tank (Day 2)
- Clarifier (Day 2)
- UV Disinfection (Day 2)



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

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- Wicklein, E., Batstone, D.J., Ducoste, J., Laurent, J., Griborio, A., Wicks, J., Saunders, S., Samstag, R., Potier, O. and Nopens, I. 2016 Good modelling practice in applying computational fluid dynamics for WWTP modelling. *Water Science and Technology*. **73** (5) 969-982.
- R. W. Samstag, J. J. Ducoste, A. Griborio, I. Nopens, D. J. Batstone, J. D. Wicks, S. Saunders, E. A. Wicklein, G. Kenny and J. Lauren (2016) CFD for Wastewater: An Overview, *Water Science and Technology,* **74** (3), 549–563.

Thank you!
Questions?

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