Improving WWTP Design and Operations Through 3D CFD Modeling (Application of CFD to Wastewater Process Engineering)

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"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 *Chemical Reaction Engineering* (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.

Hydraulic Model

Continuity (mass conservation)

 $\frac{\partial \rho}{\partial t} + \frac{\rho \partial U_i}{\partial X_i} = 0$

Hydraulic Model

- Continuity (mass conservation)
- Momentum transport

$$\frac{\partial \rho}{\partial t} + \frac{\rho \partial U_i}{\partial X_j} = 0$$
$$\rho \frac{\partial U_i}{\partial t} = -\rho U_j \frac{\partial U_i}{\partial X_j} - \frac{\partial P}{\partial X_i} + \frac{\partial}{\partial X_j} (v_t \frac{\partial U_i}{\partial X_j}) + F_i$$

Hydraulic Model

- Continuity (mass conservation)
- Momentum transport
- k-epsilon turbulence model

$$\frac{\partial \rho}{\partial t} + \frac{\rho \partial U_i}{\partial X_j} = 0$$

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$$\mathbf{v}_t = C_{\mu} \frac{k^2}{\varepsilon}$$

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial X_i} (\rho k U_i) = \frac{\partial}{\partial X_j} \left[\left(\mu + \frac{\mu_i}{\sigma_k} \right) \frac{\partial k}{\partial X_j} \right] + P_k + P_b - \rho \varepsilon - Y_M + S_b$$

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

Hydraulic Model

- Continuity (mass conservation)
- Momentum transport
- k-epsilon turbulence model
- Control volume solution scheme

$$\frac{\partial \rho}{\partial t} + \frac{\rho \partial U_i}{\partial X_j} = 0$$

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

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

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

But CFD can also be used as to track solids flow and reactions in the tank.



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 ϕ_{in}

 $\phi_{\rm out}$

 $\frac{\partial \phi}{\partial t} = \frac{-U_i \partial \phi}{\partial X_i} + \frac{\partial}{\partial X_i} \left(\frac{v_t}{\sigma_s} \frac{\partial \phi}{\partial X_i}\right) + S_i$

3D Solids Transport Model Individual Control Volume



3D transport models can be implemented by user defined functions (UDF) in Fluent or other commercial software.

Solids transport UDF – Solids Transport

$$\frac{\partial C}{\partial t} = \frac{-U_i \partial C}{\partial X_i} + \frac{\partial}{\partial X_i} \left(\frac{v_t}{\sigma_s} \frac{\partial C}{\partial X_i}\right) + V_s \frac{\partial C}{\partial z}$$

3D transport models can be implemented by user defined functions (UDF) in Fluent or other commercial software.

- Solids transport UDF
 - Solids Transport
 - Vesilind settling

$$\frac{\partial C}{\partial t} = \frac{-U_i \partial C}{\partial X_i} + \frac{\partial}{\partial X_i} \left(\frac{v_t}{\sigma_s} \frac{\partial C}{\partial X_i}\right) + V_s \frac{\partial C}{\partial z}$$
$$V_s = V_o * \exp(-k * C)$$

3D transport models can be implemented by user defined functions (UDF) in Fluent or other commercial software.

- Solids transport UDF
 - Solids Transport
 - Vesilind settling
 - Density couple

$$\frac{\partial C}{\partial t} = \frac{-U_i \partial C}{\partial X_i} + \frac{\partial}{\partial X_i} \left(\frac{v_t}{\sigma_s} \frac{\partial C}{\partial X_i} \right) + V_s \frac{\partial C}{\partial z}$$
$$V_s = V_o * \exp(-k * C)$$
$$\rho = \rho_w / (1 - C * (1 - \rho / \rho_w))$$

3D transport models can also be implemented for reactions in the fluid.

Biokinetic Models

- IWA Activated Sludge Models (ASM)
- Advanced oxidation models
- Disinfection models



Figure 5c. Nitrate

Sobremisana, Ducoste, de los Reyes III (2011)

CFD is well established for analysis of hydraulic components.





ew112wwtmod.ai

Often flows are split between parallel treatment components. Proper flow split can have important process consequences.

Pump Stations – Optimize Intake Hydraulics

Adverse Hydraulics:

Vortices

Pre-rotation

Turbulence

Velocity Distribution

Lead to:

Decreased capacity

Cavitation

Excessive wear



Screening / Headworks

CFD can optimize design Screen channel flow balance Screen flow distribution Infer grit deposition from velocity profiles



Grit Management

Vortex grit system efficiency is a function of approach and exit velocity

Aerated grit tanks require proper sizing and baffling to prevent short circuiting

Grit deposition can be inferred from velocity profiles and neutral density particle tracking



Flow Splitting

Flow Splitting is critical to optimize the capacity of parallel treatment components

CFD analysis can be rigid lid or free surface





olateWaterWave.pptx

Head losses through complex systems with nonuniform approach conditions can be investigated.



But CFD can also be used for analysis of transport processes.





These are processes where reactions happen as well as hydraulics.

Primary Clarification

- CFD can be used to investigate geometric influences on solids removal.
- CFD can be used to investigate sludge consolidation problems.





Aeration Tanks

Multiphase modeling can be used to investigate water-air flows.

Dissolved air transfer models can be incorporated.

Solids transport and biokinetic models can be incorporated.



Secondary Sedimentation

Clarifiers require effective inlet energy dissipation.

Baffles can aid in sedimentation.

Density currents dominate flow field, therefore a custom transport model is required.

CFD analysis of activated sludge sedimentation is very well established.





Disinfection - UV

Hydraulics are critical:

Flow split between trains

Flow distribution

Head losses

Dose models can be incorporated when developing new designs.



Mixing Systems

Mixing Used When:

Combining Fluid Streams Chemical Additions Minimizing Stagnation

Typical Mixing Systems Natural Diffusion Passive Baffles Aeration Mechanical Pumped Jets



emplateWaterWave.ppt

Digesters

Good mixing is critical to performance Improved kinetics → more gas production Reduces foaming Efficient mixing saves power







Case Studies Using Transport Modeling

Activated sludge lamella clarifiers Use of UDF model to evaluate sedimentation inlets Use of UDF models to evaluate activated sludge mixing

Sedimentation Case Study: Activated Sludge Lamellas*



*Samstag, Wicklein, Lee (2012)

The Boycott Effect has been used as the basis for the PNK theory.

Boycott (1920) observed a difference in apparent batch settling rate of blood in slanted tubes.

PNK theory: Settling is enhanced by the ratio of the projected area of inclined plates or tubes.



Does this apply to flow-through activated sludge lamella clarifiers?

Coarse Grid Custom Model

2D and 3D Commercial Models



/e.ppt



RAS Outlet 10 Distance (m)

Distance (m)

Results: No difference between tanks with and without lamella plates!



With lamella plates



Without lamella plates

o TemplateWaterWave.pptx

Sedimentation Case Study: Clarifier Inlet Comparison Existing Configuration



Clarifier Inlet Comparison Existing Configuration



Alternative Inlet Configurations



Alternative Velocity Vector Plans



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Alternative Velocity Plans



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Alternative Velocity Profiles



Comparison Solids Profiles



Mixing Case Study: Jet mixing and aeration in a sequencing batch reactor (SBR)*

- 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, Wicklein, et al. (2012)



Mesh projected onto model surfaces.

Velocity profiles for pumped mixing and aeration



Comparison of pumped mix velocity profiles for increasing jet velocities



Comparison of solids profiles for increasing jet velocities



Min / Max Deviations from Average

Average TSS Concentration (mg/L)

2.5 m/sec	3.0 m/sec	3.5 m/sec	4.0 m/sec
1,208	1,404	2,102	2,155
2,385	2,331	2,280	2,285
2,519	2,374	2,322	2,308
2,538	2,422	2,448	2,387
2,554	2,518	2,526	2,443
2,604	2,620	2,511	2,456
3,008	2,806	2,559	2,500
2,402	2,353	2,392	2,362
50%	40%	12%	9%
	2.5 m/sec 1,208 2,385 2,519 2,538 2,554 2,604 3,008 2,402 50%	2.5 m/sec3.0 m/sec1,2081,4042,3852,3312,5192,3742,5382,4222,5542,5182,6042,6203,0082,8062,4022,35350%40%	2.5 m/sec3.0 m/sec3.5 m/sec1,2081,4042,1022,3852,3312,2802,5192,3742,3222,5382,4222,4482,5542,5182,5262,6042,6202,5113,0082,8062,5592,4022,3532,39250%40%12%

TemplateWaterWave.ppt

Comparison of Power Levels at Different Jet Velocities

Jet Velocity	Mix Criterion	Power Level (hp/MG)	Power Level (W/m ³)
2.5 m/sec jet velocity	50% Max Deviation	39	7.7
3.0 m/sec jet velocity	40% Max Deviation	66	13.0
3.5 m/sec jet velocity	12% Max Deviation	105	20.7
4.0 m/sec jet velocity	<10% Max Deviation	156	30.8

To meet a 10 percent deviation criterion would require four times more power than currently installed.

Comparison of Power Levels to Other Mixing Devices

			Power Level (hp/	Power Level (W/
Mixer	Reference	Mix Criterion	MG)	m ³)
4.0 m/sec jet	This study	< 10% Max Deviation	156	30.8
Large Propeller in Racetrack	Carollo Field Visit	Little MLSS separation	5	~1
Surface Mixing Impeller	Carollo Witnessed Test	0.6 m/sec (2 fps) bottom velocity	39	7.6
Hydrofoil mixer	Otun et al. (2009)	< 30% Max Deviation	39	7.6
Hyperboloid mixer	Otun et al. (2009)	< 11% Max Deviation	20	4.0

Frequent CFD practice for mixing is to assume neutral density.

- The influence of solids on the velocity pattern is ignored.
- A velocity profile is then calculated assuming clear water.
- It is then assumed that a given minimum velocity (2.5 ft/min) will be sufficient to provide mixing.
- But it is SOLIDS that we are trying to mix. They aren't typically modeled.

3.40E-102 3.28E-402 3.28E-402 3.28E-402 2.368E-402 2.368E-402 2.38E-402 2.38E-402 2.48E-402 2.48E-402 2.48E-402 2.48E-402 2.48E-402 2.48E-402 2.48E-402 1.38E-402		
Z Y X	B280285.agi - A1 Average-Velocity (Inc Turb) (Ft/Min)	Jul 29 2011 Fluent 4.56 Fluent Inc.

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.



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 overpredicted measured solids mixing.



Comparison of density-coupled and neutral density simulations



Neutral density simulation dramatically over-predicts the degree of mixing.

CFD and Process Engineering Conclusions

CFD is well established and important for analysis of hydraulic components.

There is growing appreciation that CFD can be a powerful tool for analysis of the impact of geometry and hydrodynamics on process performance.

Results from studies of lamella settlers, radial flow clarifier inlets, and activated sludge mixing show that CFD can establish important conclusions for process engineering.