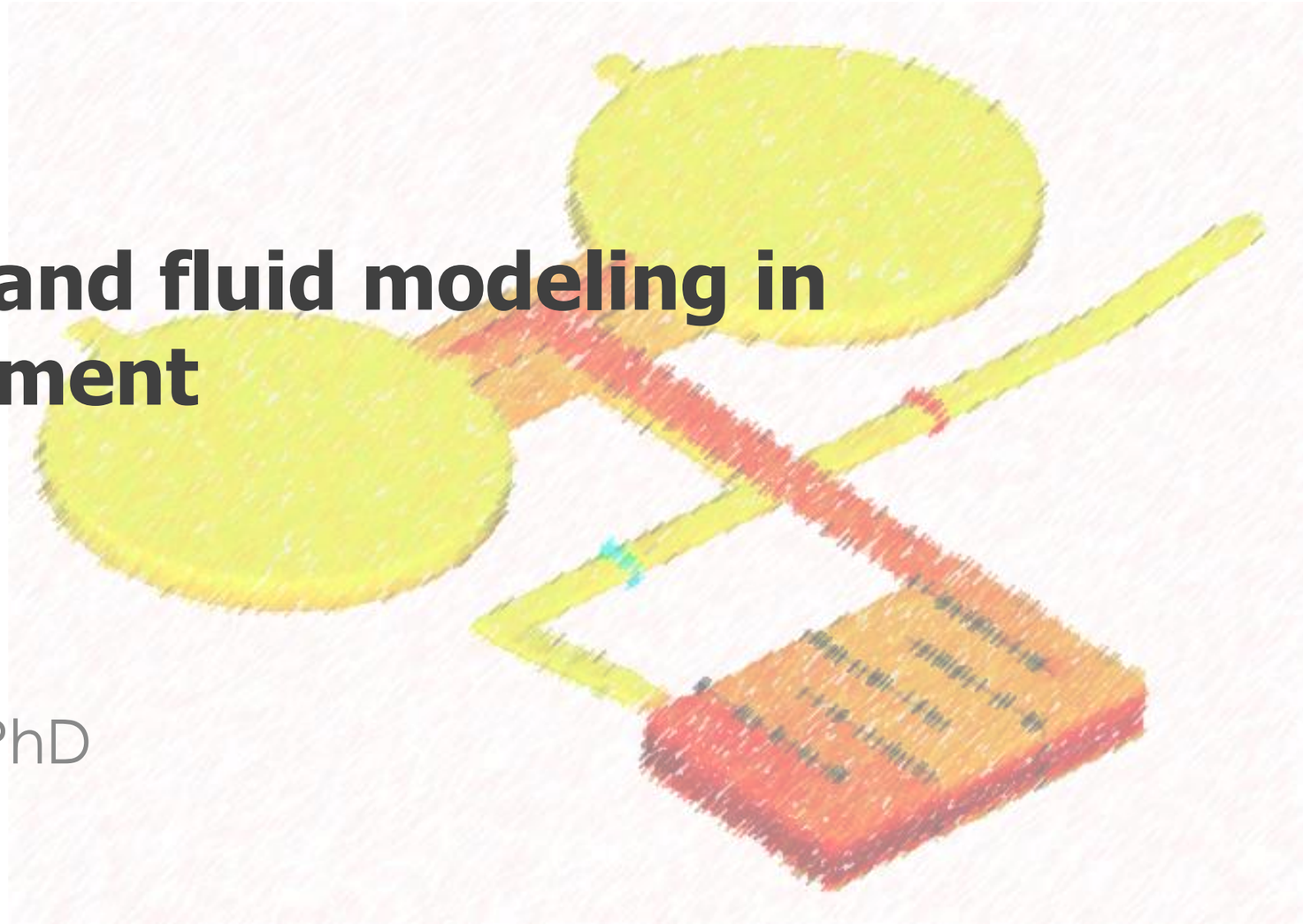
Activated sludge and fluid modeling in wastewater treatment



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Work in progress

About me

- Senior Computational Fluid Dynamics (CFD) Engineer at Flow Science, Inc., Santa Fe, USA since 2015
  - Head of global academic programs
  - Head of software verification and validation
  - Activated sludge model development and validation
- A 1.5 days of experience in SWMM

FLOW Science®

Senior Computational Fluid Dynamics Engineer

Stanford University

Master's in Fluid Mechanics and Computational Engineering

Bachelor's in Civil Engineering

About Flow Science Inc

- Founded in 1980 by Dr. C.W. "Tony" Hirt at Los Alamos National Lab
- International distributors in Europe, Asia, Australia and South America
- Users in 53 countries around the world
- ***FLOW-3D*** is a CFD software specializing in general purpose free surface and multi-physics simulations

Santa Fe, New Mexico

Why 3D?
Stereotypes about CFD

Zele WWTP, Belgium
The CFD model
Relevant physics and meshing
ASM-1 reaction kinetics
Preliminary verification
Assumptions and incomplete data
Simulation evolution
Results

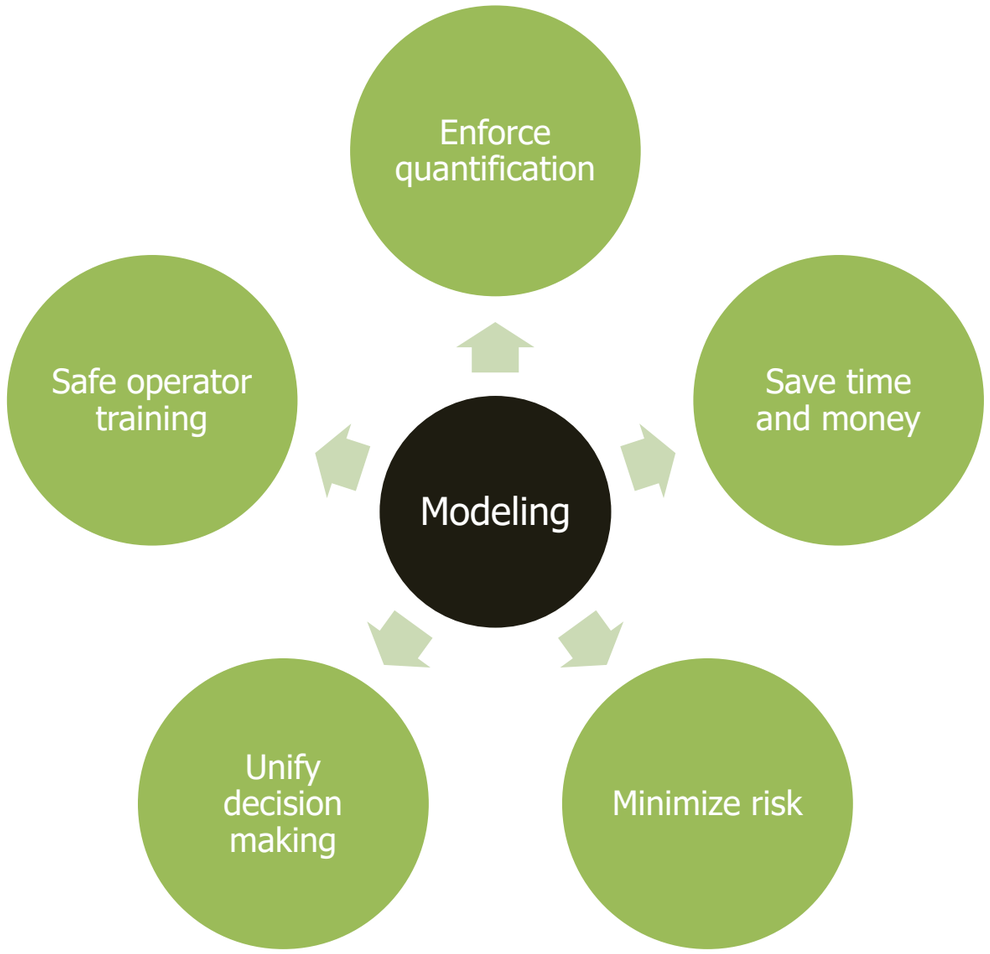
Conclusions
Future work

Why modeling in WWTP?

Enforce quantification	• Avoid comparisons such as “better”, “larger” and “higher” • Objective process decisions
Save time and money	• Better comparisons between different plant designs • Quantified upgrade decisions based on effluent quality, oxygen requirements, etc.
Minimize risk	• “What if?” scenarios can be examined quantitatively • “What will happen if the influent rate doubles?” • “What will happen if the industrial waste percent increases?”
Unify decision making	• A common mathematical context allows interdisciplinary decision making
Safe operator training	• Safely investigate the consequences of an action in the treatment process

Biological Wastewater Treatment, Principles, Modelling and Design, Henze m., Lossdrecht M.C.M., Ekama G.A., Brdjanovic D., IWA publishing 2008

Why modeling in WWTP? Why 3D?



- 3D models account for important physics such as
  - Complex mixing and turbulence
  - Particle settling
  - Non-Newtonian fluid dynamics
  - Free surface aeration
- Activated sludge processes have reaction orders greater than zero
  - Reactions are sensitive to the hydrodynamics

Stereotypes about CFD

CFD is too expensive financially.

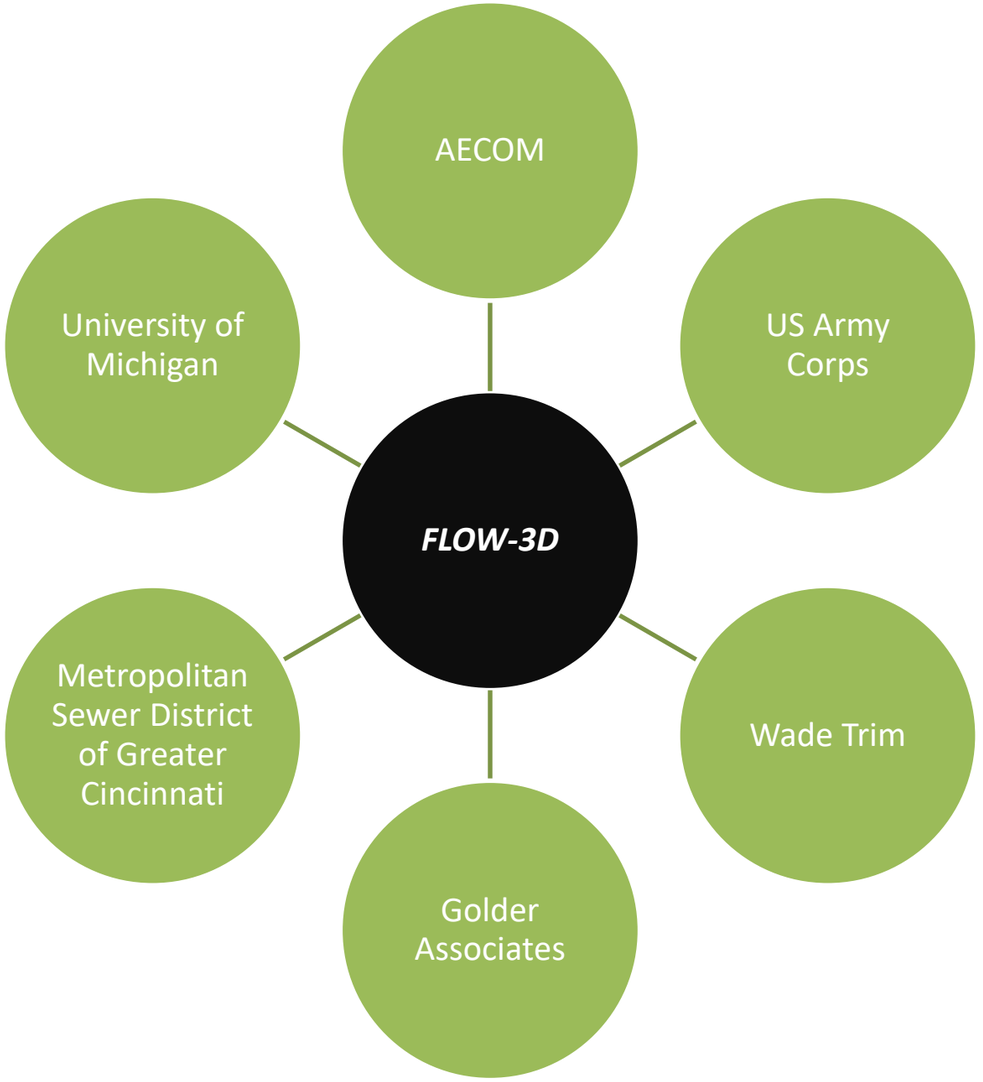
- Depends on efficiency gains to investment ratio
- In many cases the efficiency gains can be higher than the investment

CFD is too expensive computationally.

- Depends on the long-term time savings vs the immediate modeling time investment
- Depends on physics and accuracy requirements
- Advances in computer technology has made CFD a more widespread tool

CFD requires a steep learning curve.

- No, if the CFD software is designed keeping the end users in mind
- No, if the software comes with good onboarding and support



Case study: Zele WWTP, Belgium

Validate effluent concentrations

Secondary treatment

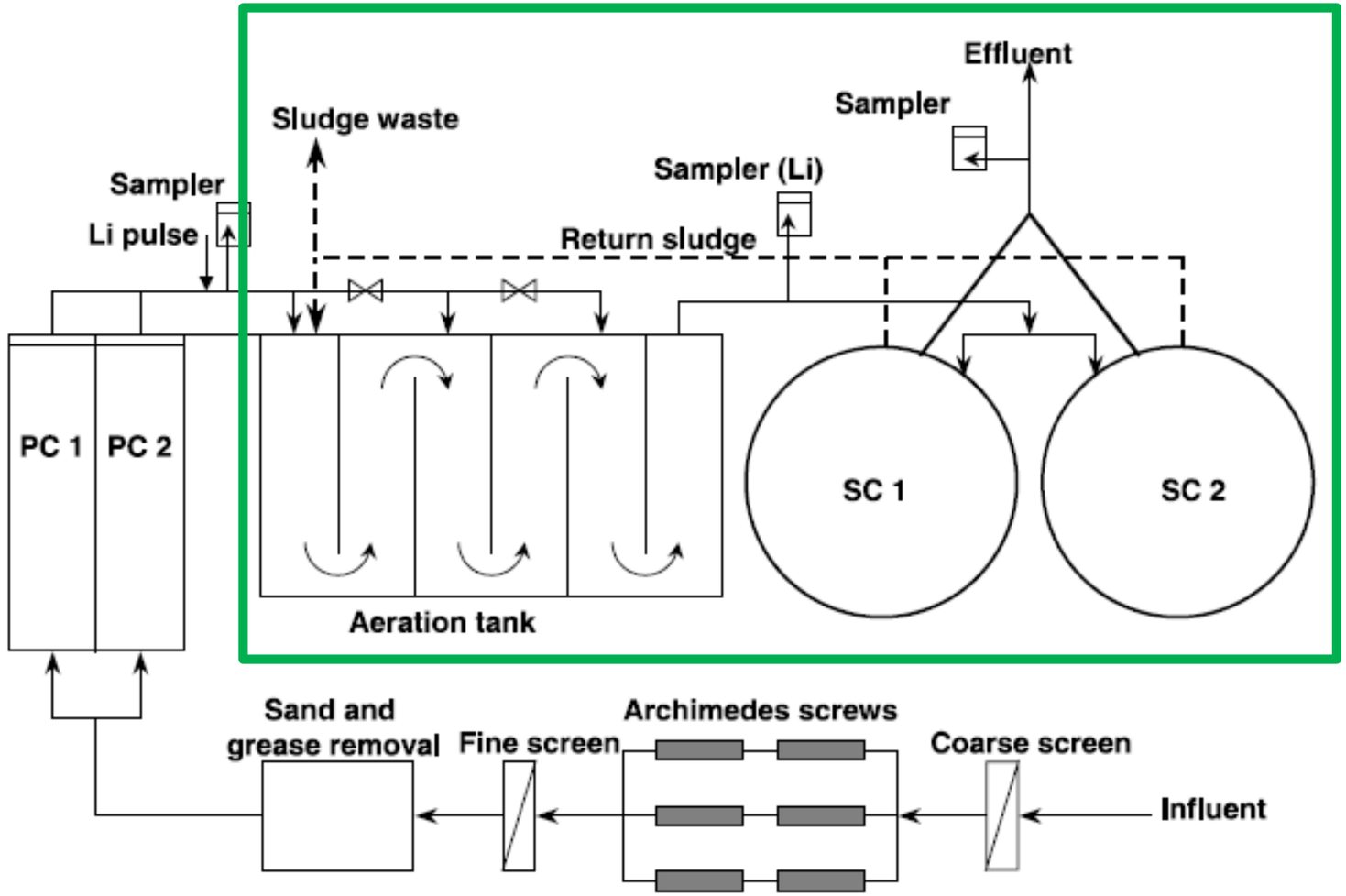
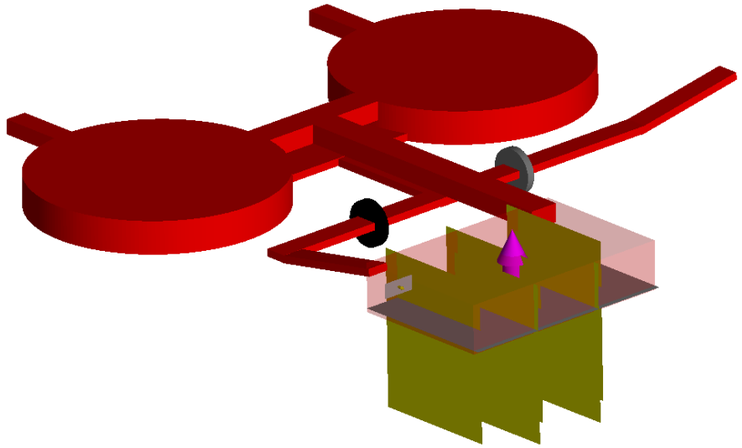
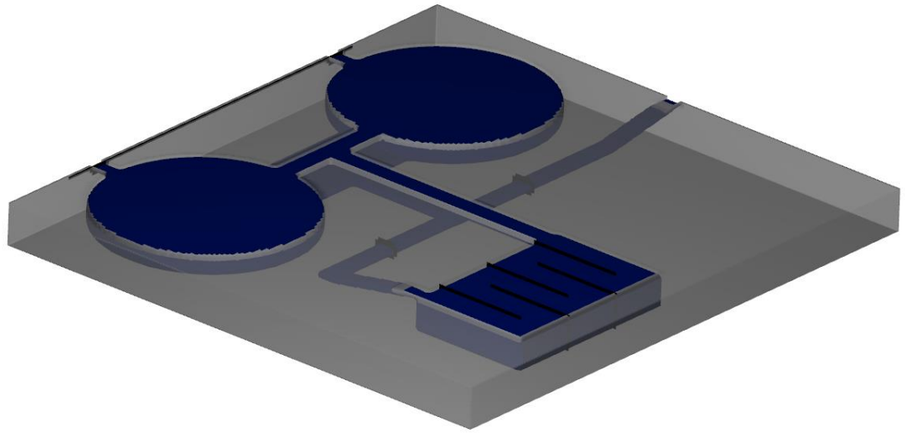
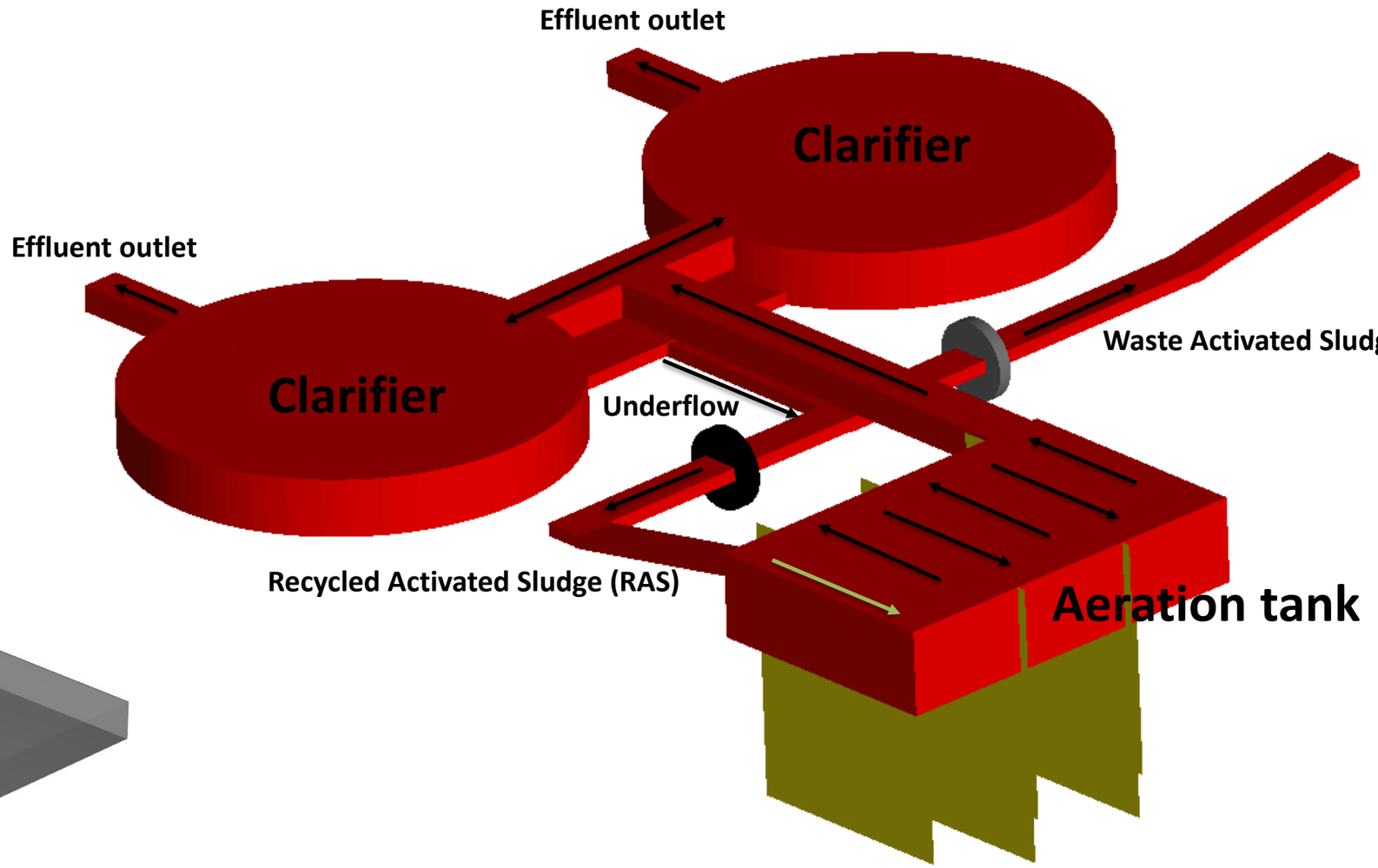


Image source:
Peterson B., Vanrollenghem P.A., Gernaey K., Henze M., Evaluation of an ASM1 model calibration procedure on a municipal–industrial wastewater treatment plant, Journal of Hydroinformatics (2002) 4 (1): 15-38.

Case study: The CFD model

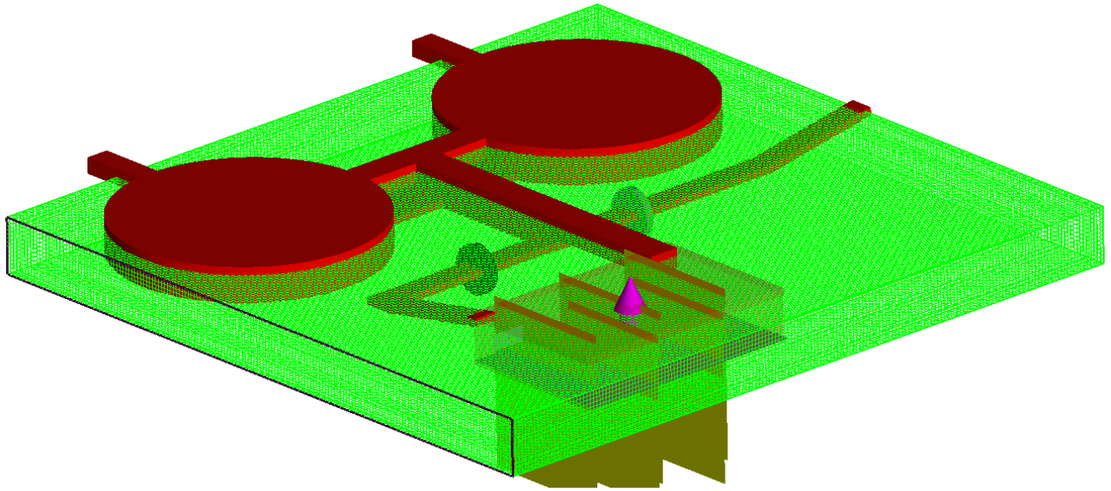


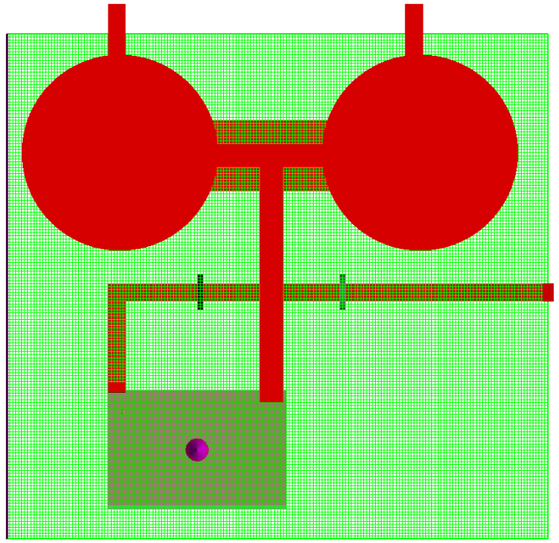




Case study: Relevant physics and meshing

- Fluid dynamics
  - Complete mass and momentum conservation (Navier-Stokes equations)
- Activated sludge
  - Scalars advection
  - Reaction kinetics
  - Oxygen dissolution and air entrainment
  - Density evaluation
- Meshing
  - Simple structured grid





Case study: ASM-1 reaction kinetics

- System of coupled partial differential equations (PDEs)
- Developed by International Water Association (1987)

Component → i / j Process ↓	1 S_I	2 S_S	3 X_I	4 X_S	5 $X_{B,H}$	6 $X_{B,A}$	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	11 S_{ND}	12 X_{ND}	13 S_{ALK}	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1 Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H}$
2 Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\times\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
3 Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
4 'Decay' of heterotrophs				$1-f_P$	−1		f_P					$i_{XB}-f_P i_{XP}$		$b_H X_{B,H}$
5 'Decay' of autotrophs				$1-f_P$		−1	f_P					$i_{XB}-f_P i_{XP}$		$b_A X_{B,A}$
6 Ammonification of soluble organic nitrogen										1	−1		$\frac{1}{14}$	$k_a S_{ND} X_{B,H}$
7 'Hydrolysis' of entrapped organics		1		−1										$k_h\frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$
8 'Hydrolysis' of entrapped organic nitrogen											1	−1		$\rho_7(X_{ND}/X_S)$
Observed Conversion Rates $[ML^{-3}T^{-1}]$	$r_i=\sum_j \nu_{ij}\rho_j$													
Stoichiometric Parameters: Heterotrophic yield: Y_H Autotrophic yield: Y_A Fraction of biomass yielding particulate products: f_P Mass N/Mass COD in biomass: i_{XB} Mass N/Mass COD in products from biomass: i_{XP}	Soluble inert organic matter $[M(COD)L^{-3}]$	Readily biodegradable substrate $[M(COD)L^{-3}]$	Particulate inert organic matter $[M(COD)L^{-3}]$	Slowly biodegradable substrate $[M(COD)L^{-3}]$	Active heterotrophic biomass $[M(COD)L^{-3}]$	Active autotrophic biomass $[M(COD)L^{-3}]$	Particulate products arising from biomass decay $[M(COD)L^{-3}]$	Oxygen (negative COD) $[M(-COD)L^{-3}]$	Nitrate and nitrite nitrogen $[M(N)L^{-3}]$	$NH_4^+ + NH_3$ nitrogen $[M(N)L^{-3}]$	Soluble biodegradable organic nitrogen $[M(N)L^{-3}]$	Particulate biodegradable organic nitrogen $[M(N)L^{-3}]$	Alkalinity—Molar units	Kinetic Parameters: Heterotrophic growth and decay: $\hat{\mu}_H$, K_S, $K_{O,H}$, K_{NO}, b_H Autotrophic growth and decay: $\hat{\mu}_A$, K_{NH}, $K_{O,A}$, b_A Correction factor for anoxic growth of heterotrophs: η_g Ammonification: k_a Hydrolysis: k_h, K_X Correction factor for anoxic hydrolysis: η_h

Henze, M., Grady, C. P. L. Jr., Gujer, W., Marais, G. v. R. & Matsuo, T. 1987 *Activated Sludge Model No. 1.* IAWPRC Scientific and Technical Reports No. 1. London, UK.

Case study: ASM-1 system of PDEs

$$\begin{bmatrix} \dfrac{\partial S_I}{\partial t} = 0 \\ \dfrac{\partial S_S}{\partial t} = -\left(\dfrac{1}{Y_H}\right)\hat{\mu}_H\left(\dfrac{S_S}{K_S+S_S}\right)\left(\dfrac{S_O}{K_{O,H}+S_O}\right)X_{B,H} - \left(\dfrac{1}{Y_H}\right)\hat{\mu}_H\left(\dfrac{S_S}{K_S+S_S}\right)\left(\dfrac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\dfrac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_B X_{B,H} \\ \vdots \\ \dfrac{\partial X_{ND}}{\partial t} = (i_{XB}-f_p i_{XP})(b_H X_{B,H}) + (i_{XB}-f_p i_{XP})(b_A X_{B,A}) - \rho_7\left(\dfrac{X_{ND}}{X_S}\right) \end{bmatrix} \quad \begin{matrix} \\ (1) \\ (2) \\ \\ (12) \end{matrix}$$

The 13th scalar, S_{alk} not measured

Case study: Preliminary verification

- System: Single species, Monod

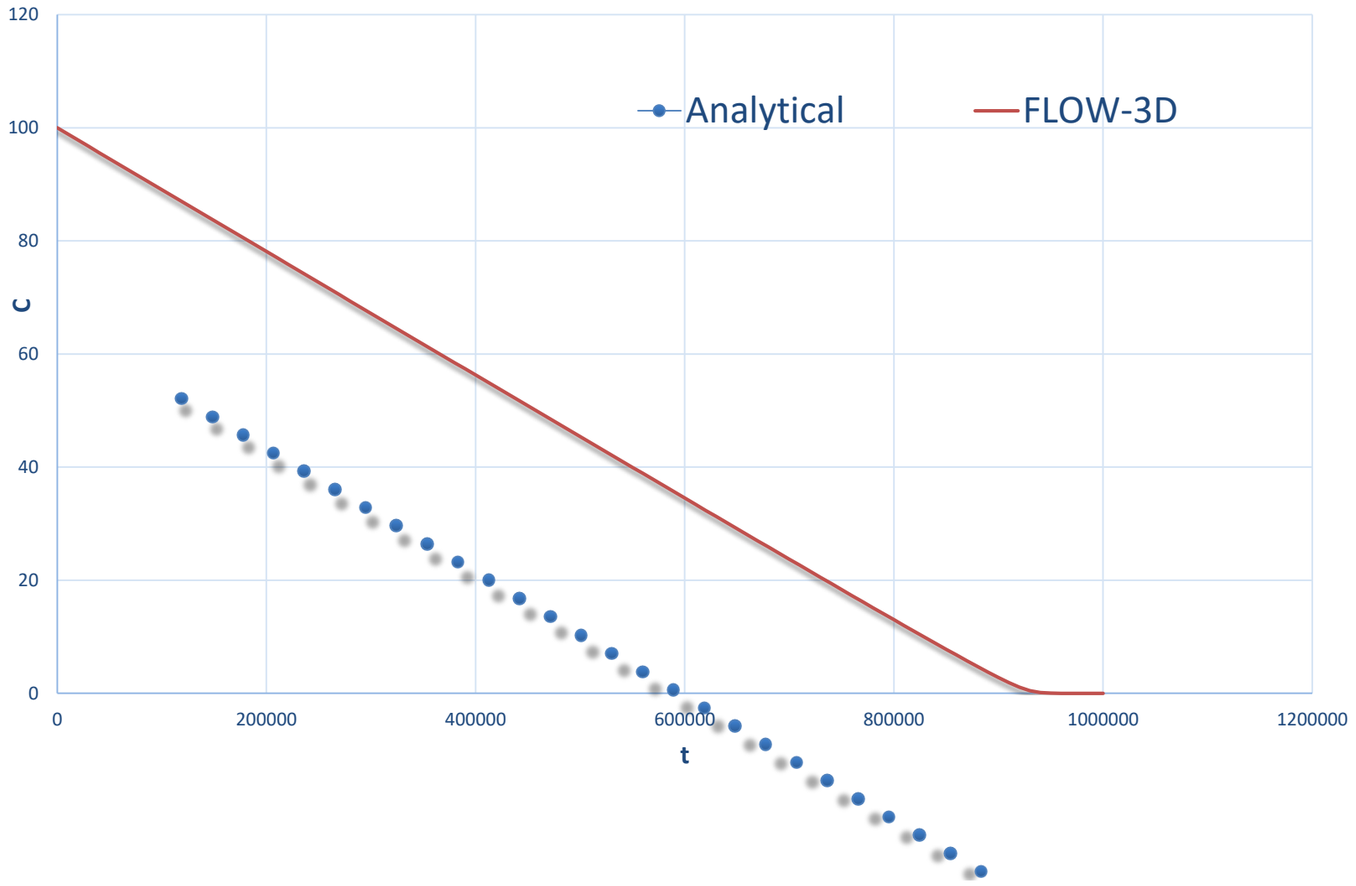
$$\frac{\partial C}{\partial t} = k\frac{C}{a + C}$$

- Analytical solution

$$C_t = aW\left(\frac{C_0 e^{\frac{C_0 + kt}{a}}}{a}\right)$$

$W \rightarrow$ Lambert W function

$$W(xe^x) = x$$

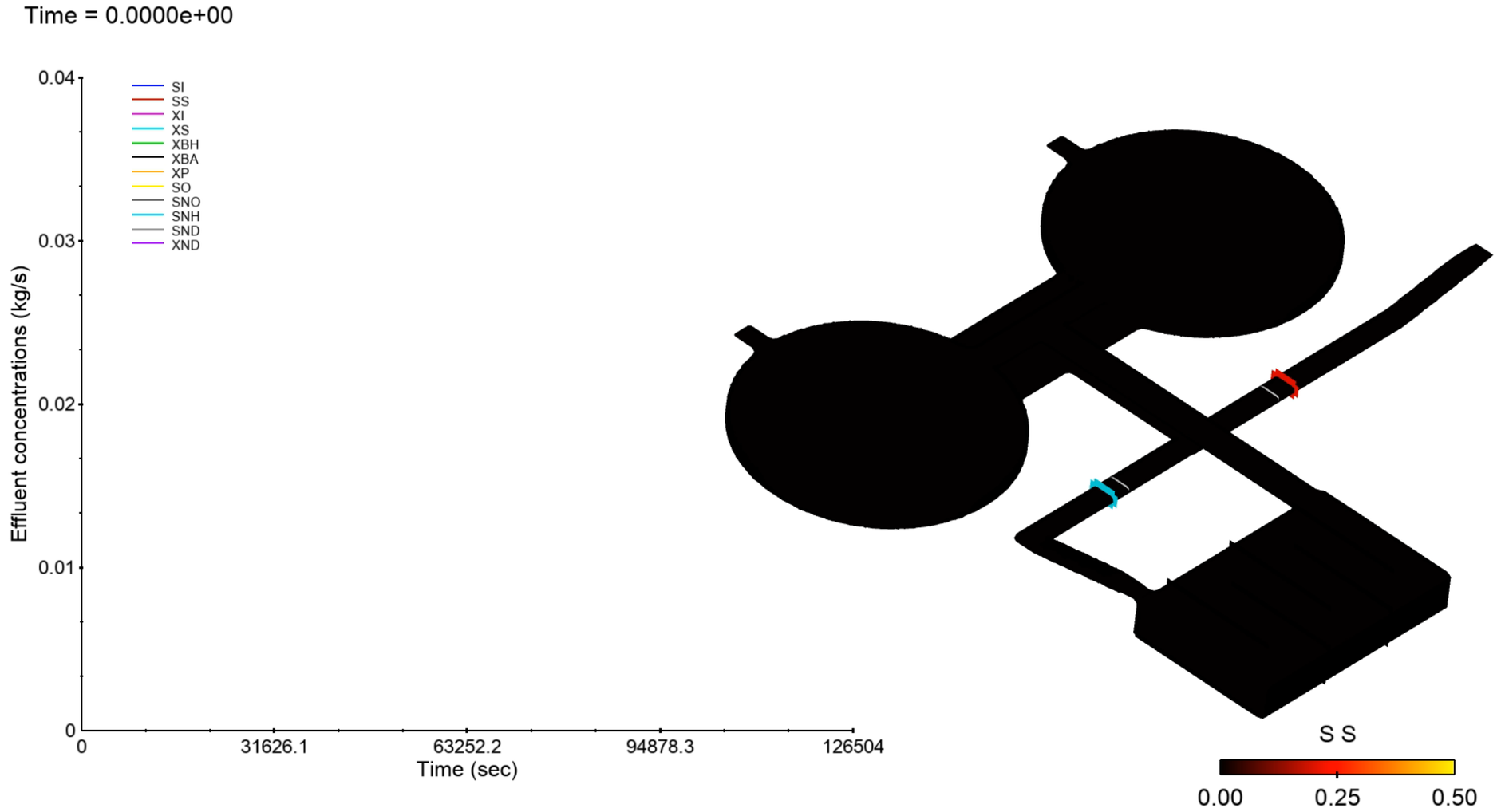


Case study: Assumptions and incomplete data

- Some uncertainty with the measured scalar quantities in the influent
  - Affects the scalar quantities in the effluent
- Missing initial concentrations in the WWTP
  - Affects scalar evolution
- Some uncertainty with geometry specifications
  - Affects hydrodynamics inside the domain
  - Missing oxygen spargar specification
- Some uncertainty with the settling properties for the particulate material
  - Affects the scalar quantities in the effluent

Influent scalar	Concentration (mg/l)
SI	7.5
SS	400.0
XI	40.0
XS	40.0
XB,H	120.0
XB,A	5.0
XP	0.0
SO	0.0
SNO	0.0
SNH	15.0
SND	8.2
XND	11.3
Salk	N/A

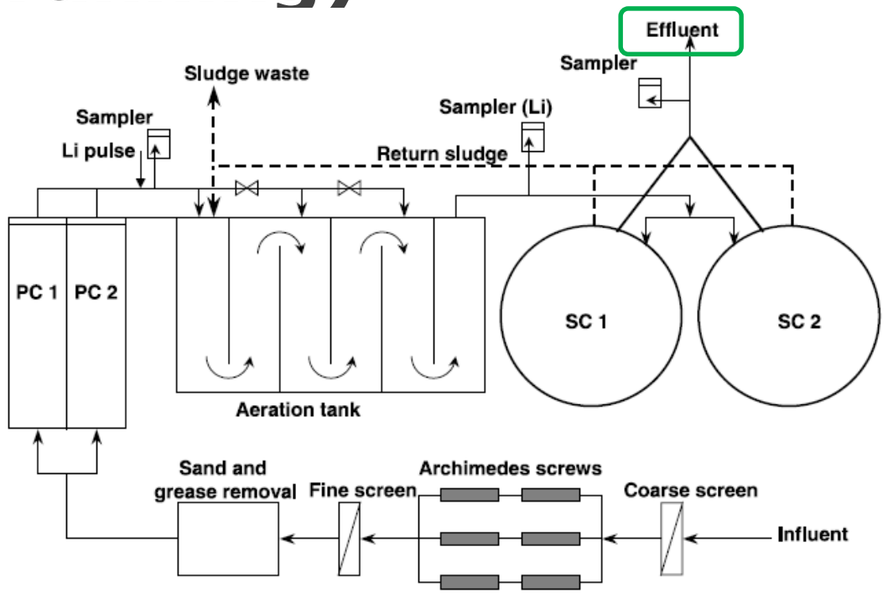
Case study: Simulation evolution



FLOW-3D®

Case study: Results (not final, still running)

- Measured effluent scalar quantities
  - $COD_{tot} = SI + SS + XI + XS$
  - $COD_{sol} \sim SS$
  - SNH
  - SNO
  - $TKN \sim XND + SND + SNH$



Effluent quantities	Measured concetration (mg/l)	FLOW-3D concentration (mg/l)
CODtot	60.0	264.04
CODsol	60.0	198
SNH	4.0	30.34
SNO	2.5	1.86
TKN	11.0	37.28
SI	7.5	7.28

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SND	8.2
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Salk	N/A

Summary

- Conclusions
  - CFD and ASM modeling are successfully coupled
  - Fairly accurate predictions even with incomplete data and geometry specifications
- Future work
  - Add mixing and turbulence
  - Procure validation with complete specifications

Work in progress

Contact

Model inquiries, validations, development suggestions, academic use

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धन्यवाद

thank you

merci

dankie

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