ensgsi!
Ecole Nationale Supérieure
en Génie des Systèmes et de l'Innovation

UNIVERSITÉ DE LORRAINE

MODELING AND SIMULATION OF WWTP

Universitat Jaume I September 2016

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C.N.R.S. / Université de Lorraine

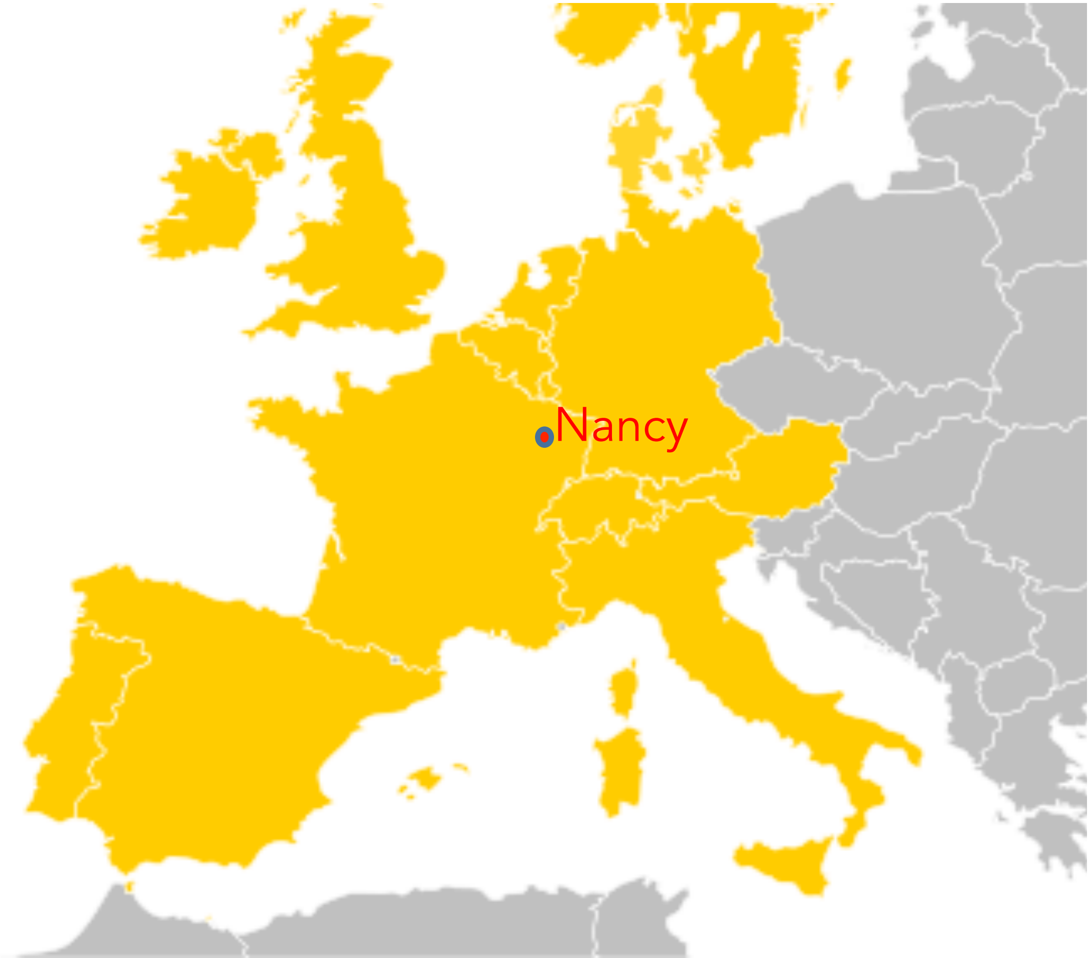
LRGP LABORATOIRE RÉACTIONS ET GÉNIE DES PROCÉDÉS

SFGP SOCIÉTÉ FRANÇAISE DE GÉNIE DES PROCÉDÉS La science des procédés face aux enjeux industriels et sociétaux

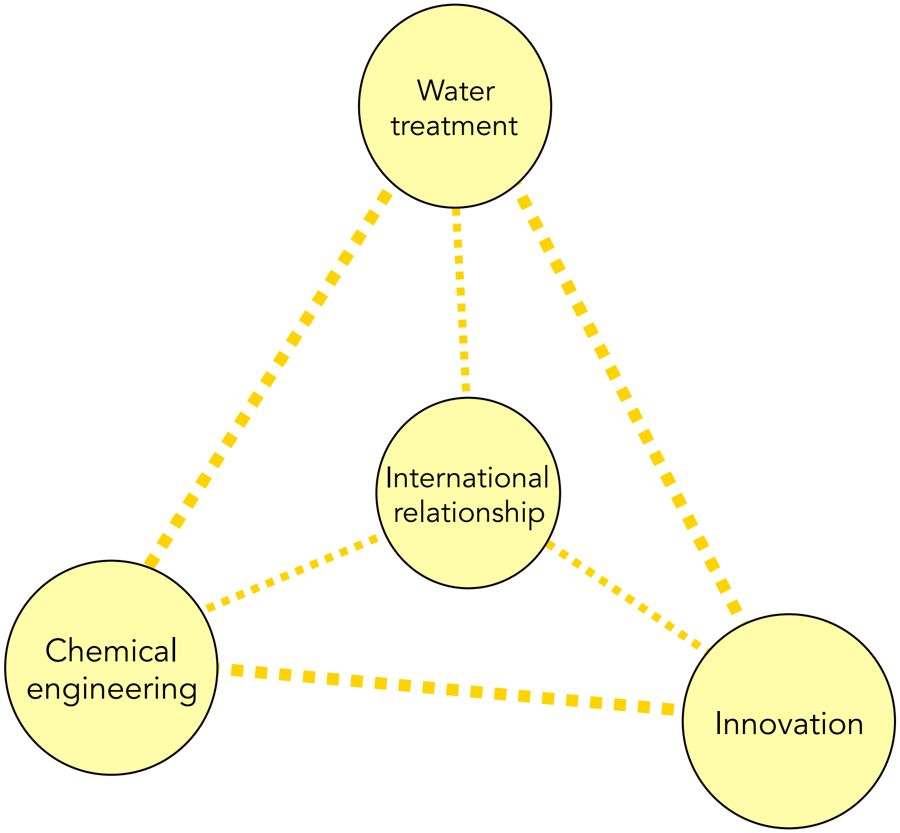
IWA the international water association

cnrs

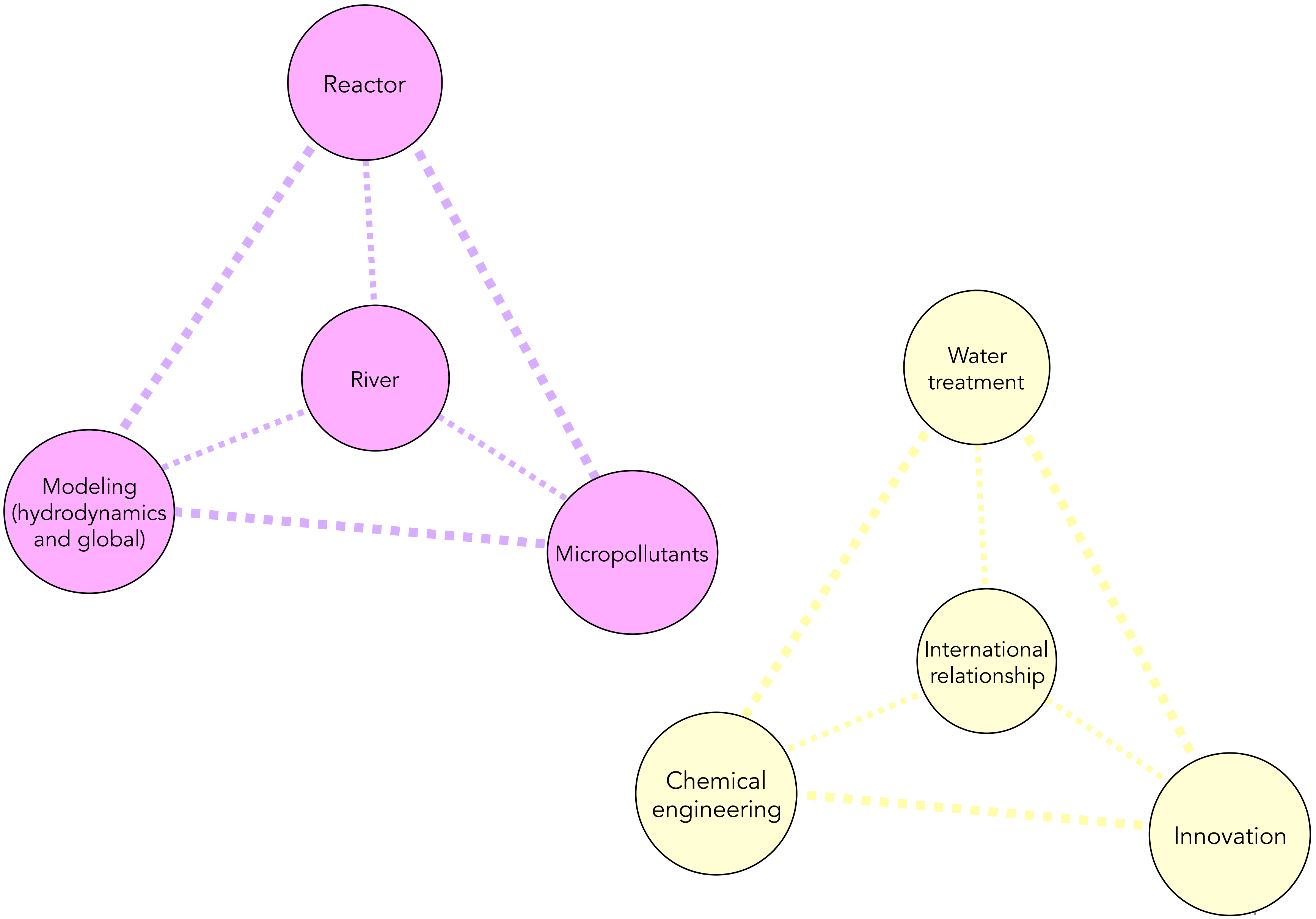
City of Nancy



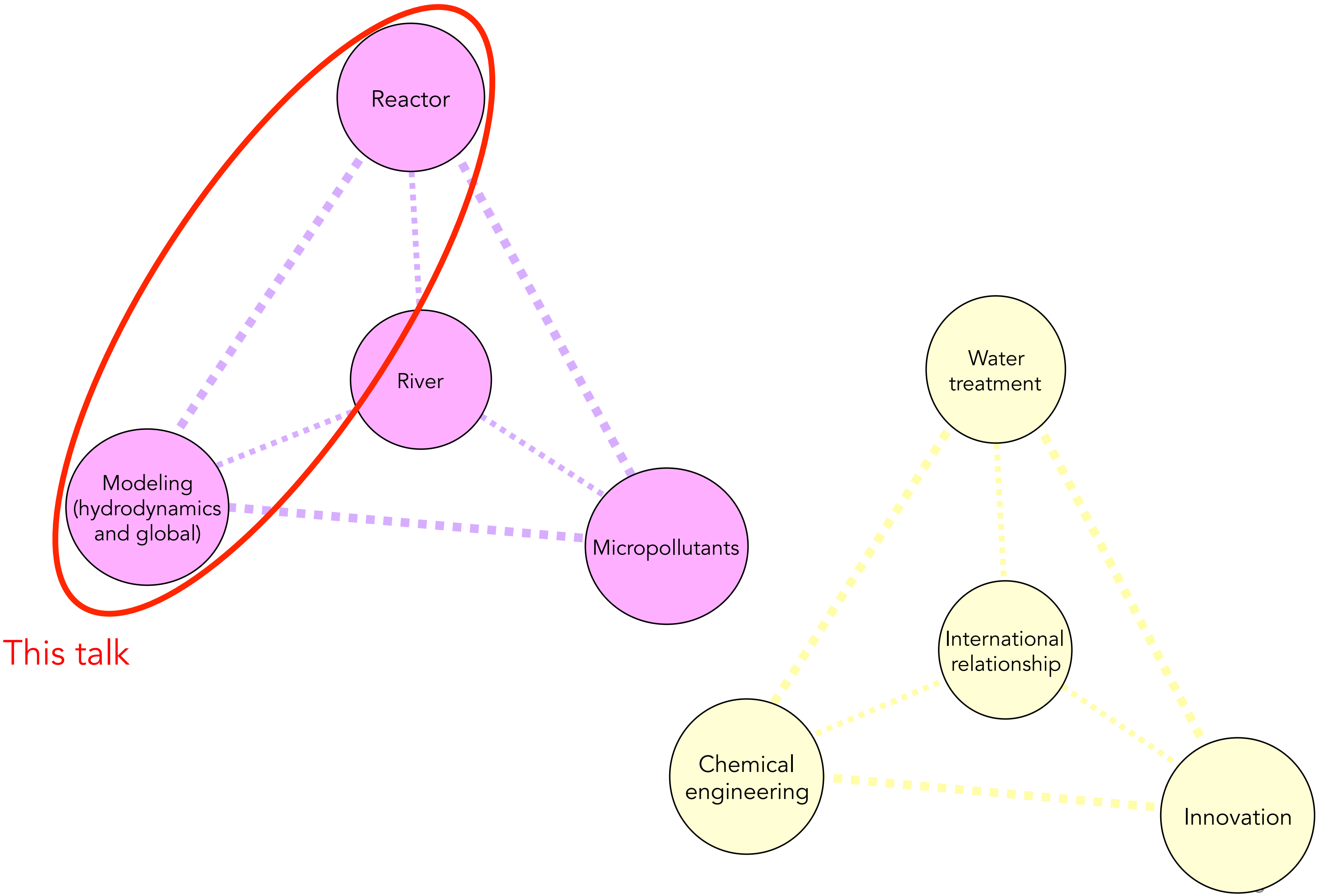
Personal interests



Personal interests



Personal interests



Why Modeling and Simulation?

- To simply simulate!
- To control the process.
- To try to optimize the whole processes; indeed, only to improve some parts of it.
- To forecast the released pollution.
- But also to deeply study the process and have a new tool for design.

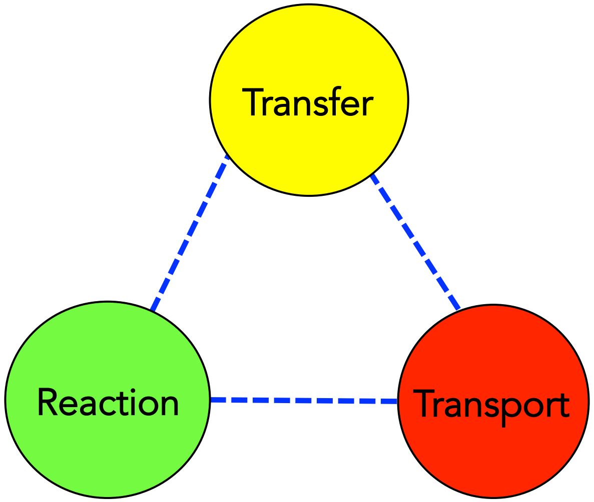
Keywords

The 3 keywords of Chemical engineering:

Transfer

Transport

Reaction



=> Hydrodynamics is really important

Hydrodynamics

It is very important to know the space distribution of the fluid; so where the Compounds are going to react.

But

Hydrodynamics

Hydrodynamics is not only a space distribution of compounds, which react at different places,

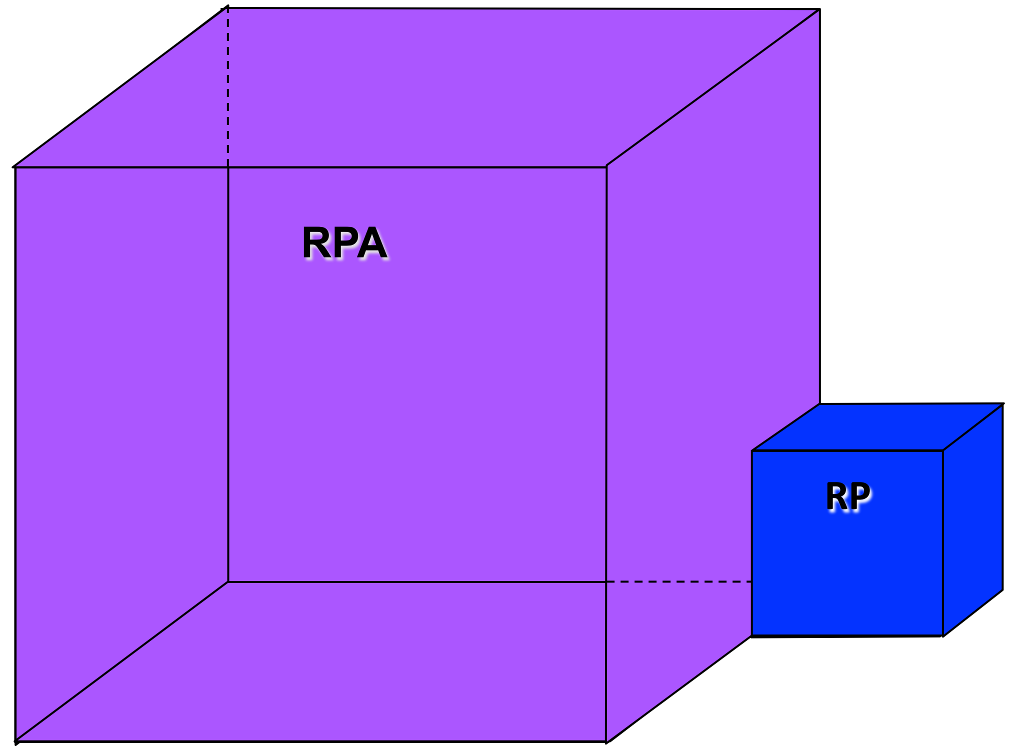
but also

a useful tool for optimization of the process design by "joining" effects of reactions and transport (and transfer).

Exemple :

- On traite 10 m³/h de solution de réactif A

- Réaction chimique d'ordre 1 (k = 4 h^{-1})
- Taux de conversion souhaité : 99 %



Opération continue dans un Réacteur Parfaitement Agité :

Le volume du réacteur RPA est donc : $V_{RPA} = \tau Q = 248 \text{ m}^3$

Opération continue dans un Réacteur Piston :

Le volume du réacteur piston est donc : $V_{RP} = \tau Q = 11{,}5 \text{ m}^3$

Ici : $\dfrac{V_{RPA}}{V_{RP}} \approx 22$

Hydrodynamics

Hydrodynamics is not only a space distribution of compounds, which react at different places,

but also

a useful tool for optimization of the process design by "joining" effects of reactions and transport (and transfer).

Therefore, Hydrodynamics is also a tool to improve the performance; increasing the reaction yields, reducing the reactor size and costs.

Hydrodynamics

Necessary to use an integrated approach using Reaction, Hydrodynamics and eventually Transfer;

theoretically, experimentally, and also with simulations.

Therefore, Hydrodynamics is also a tool to improve the performance; increasing the reaction yields, reducing the reactor size and costs.

Hydrodynamics

Necessary to use an integrated approach using Reaction, Hydrodynamics and eventually Transfer;

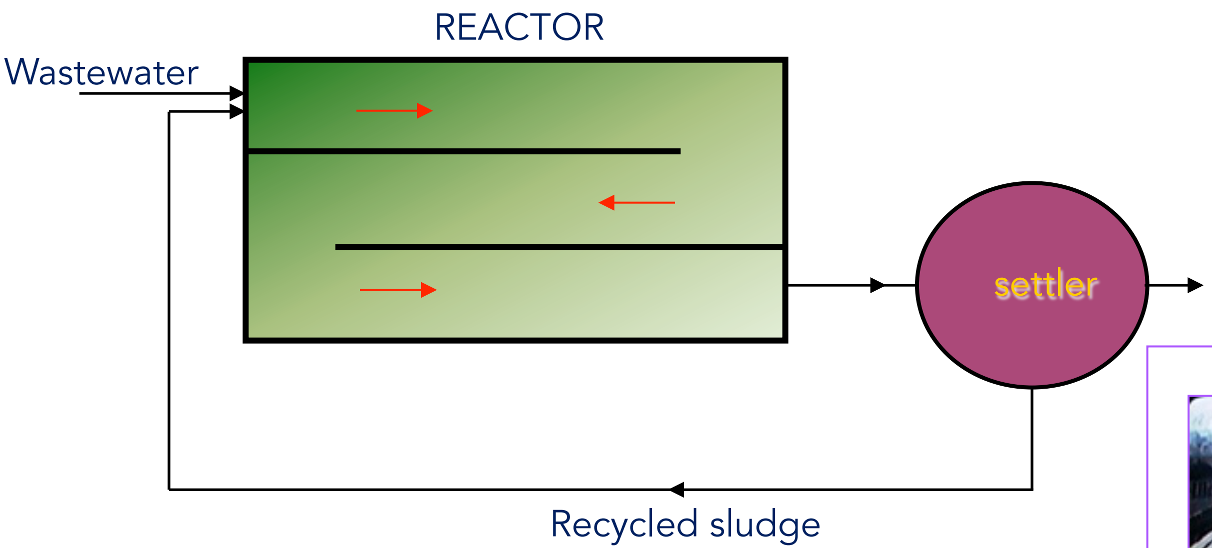
theoretically, experimentally, and also with simulations.

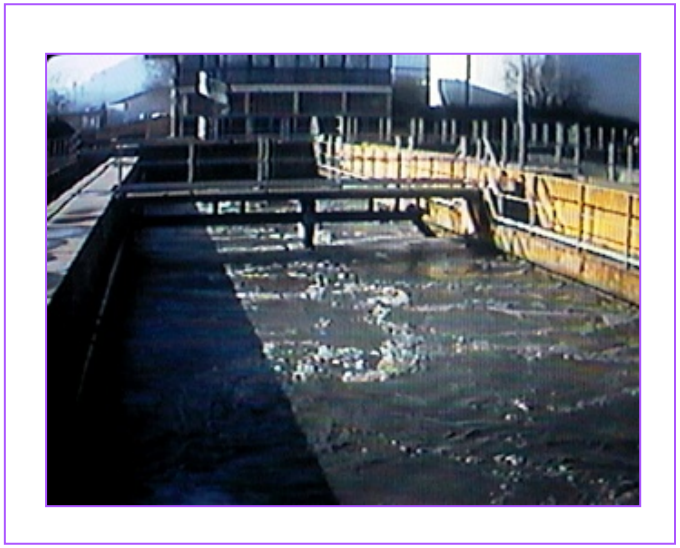
But first,

it is necessary to understand and model the hydrodynamics.

Therefore, Hydrodynamics is also a tool to improve the performance; increasing the reaction yields, reducing the reactor size and costs.

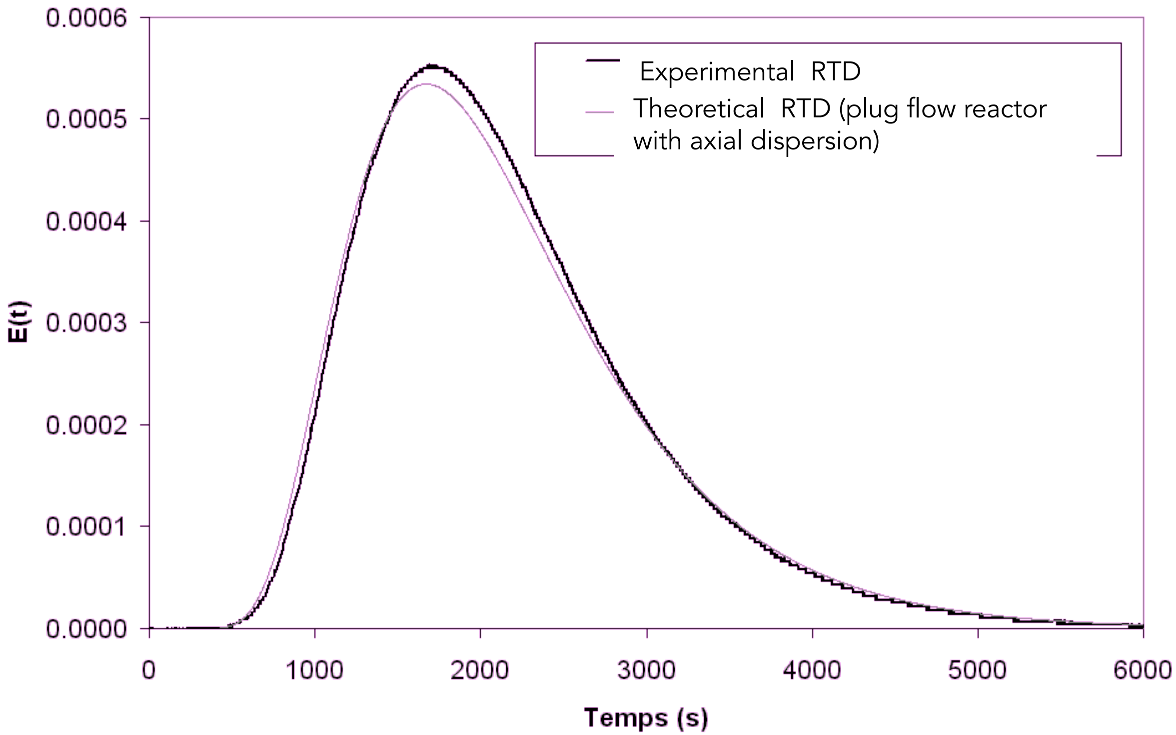
Wastewater treatment reactors





Example of the channel reactor:
volume 3300 m^3, total length 102 m, width 9 m, depth 3.6 m

Tracing in the full-scale plant of Nancy: residence time distributions



Hydrodynamic model : Series of CSTR or Plug flow reactor with axial dispersion

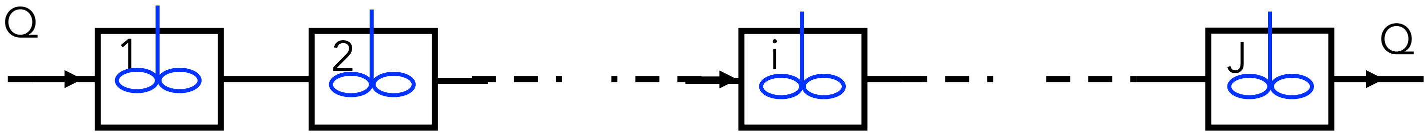
Le Moullec et al. Chemical Engineering Science 63 (2008) 2436–2449

Hydrodynamic model

Plug flow reactor with axial dispersion
Characterized by the Peclet number (Pe)

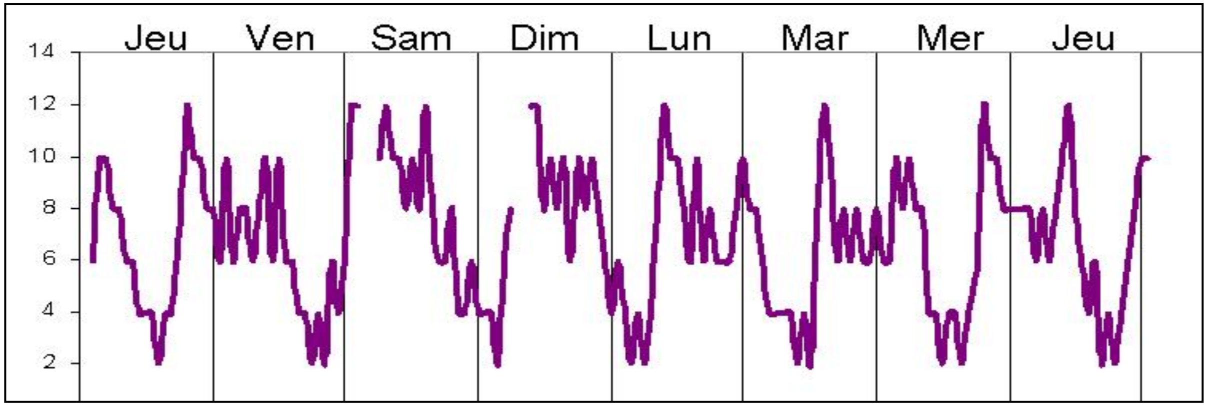
$$Pe = \frac{u.L}{D}$$

Series of CSTR
Characterized by J



Potier et al. Water Research 39 (2005) 4454–4462

Wastewater flowrate variation



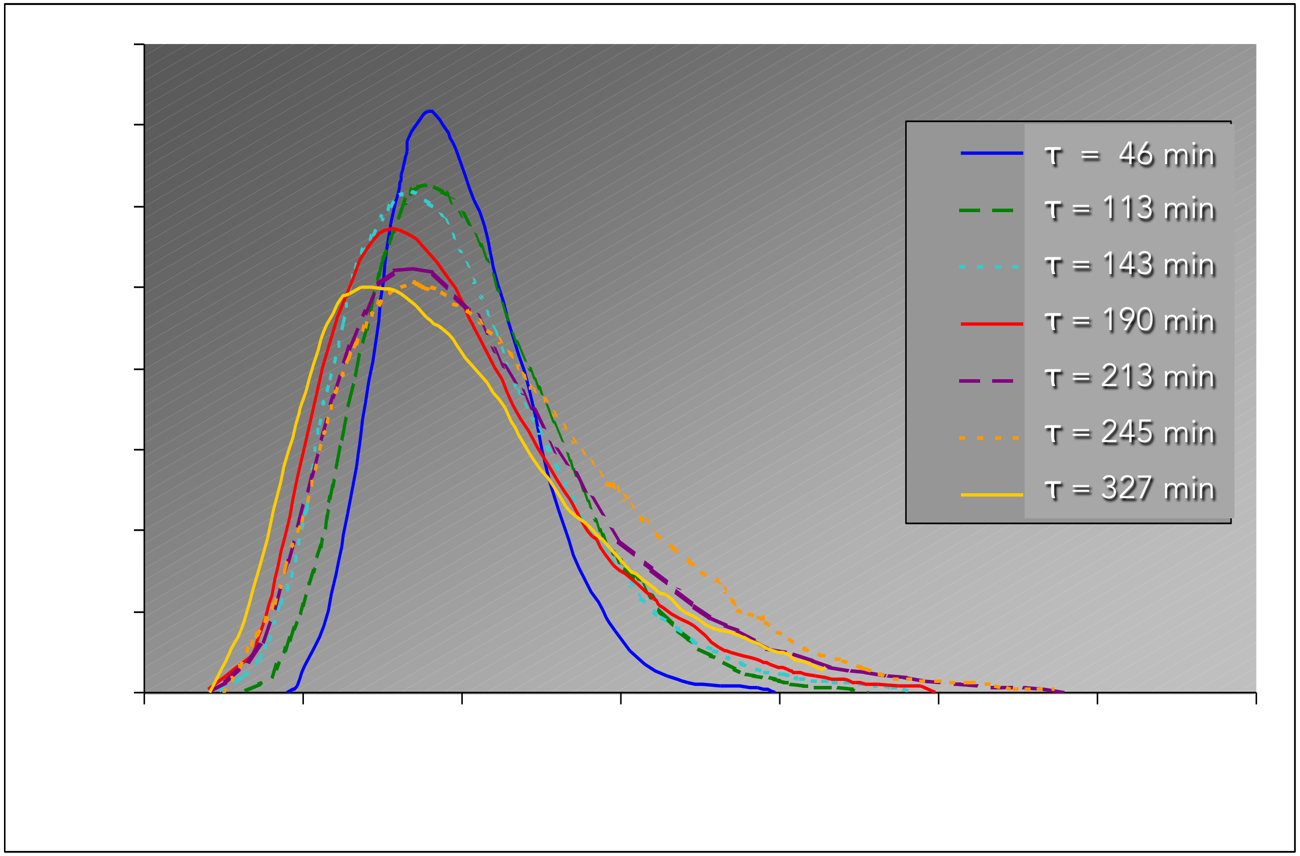
Wastewater treatment reactors

Modeling the hydrodynamic variation
(effect of flowrate)

Forecasting the reactor hydrodynamic without having expensive tracer experiments

Residence Time Distributions for different space-times (τ) in a channel reactor pilot plant

With same geometry (same width w, same height H) and same gas flowrate



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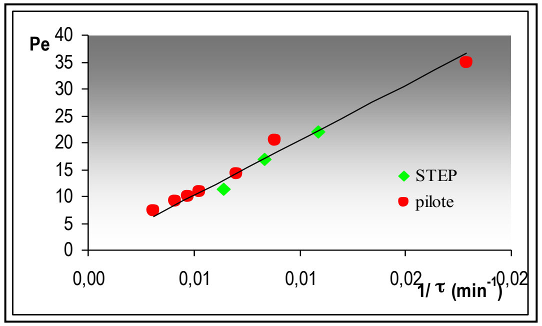
Comparison between theoretical curve and experimental data

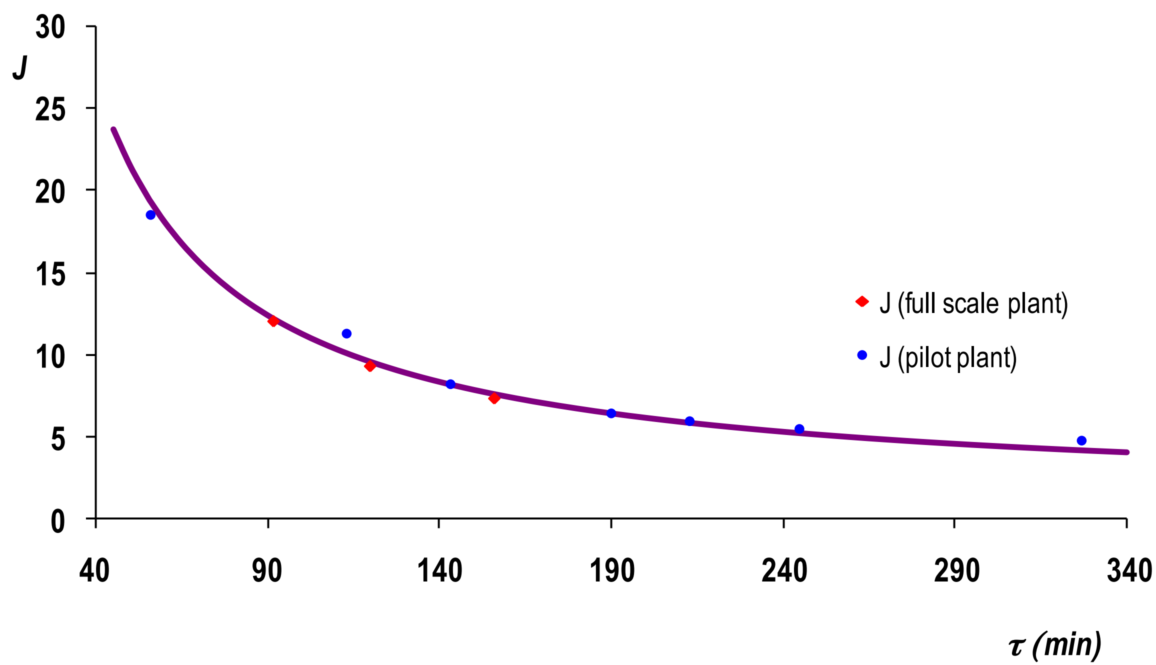
Plug flow reactor with axial dispersion

$$P = \frac{u.L}{D} = \frac{L^2}{D.\tau}$$



Series of CSTR

$$J \cong \frac{L^2}{2D\tau} + 1$$ $$J \cong 1 + \frac{K}{\tau}$$ with $$K = \frac{L^2}{2D}$$



Potier et al. Water Research 39 (2005) 4454–4462

Reactor hydrodynamic modeling

- 3 pilot plants
- 1 WWTP (Nancy)
- 194 data from the literature

Correlation

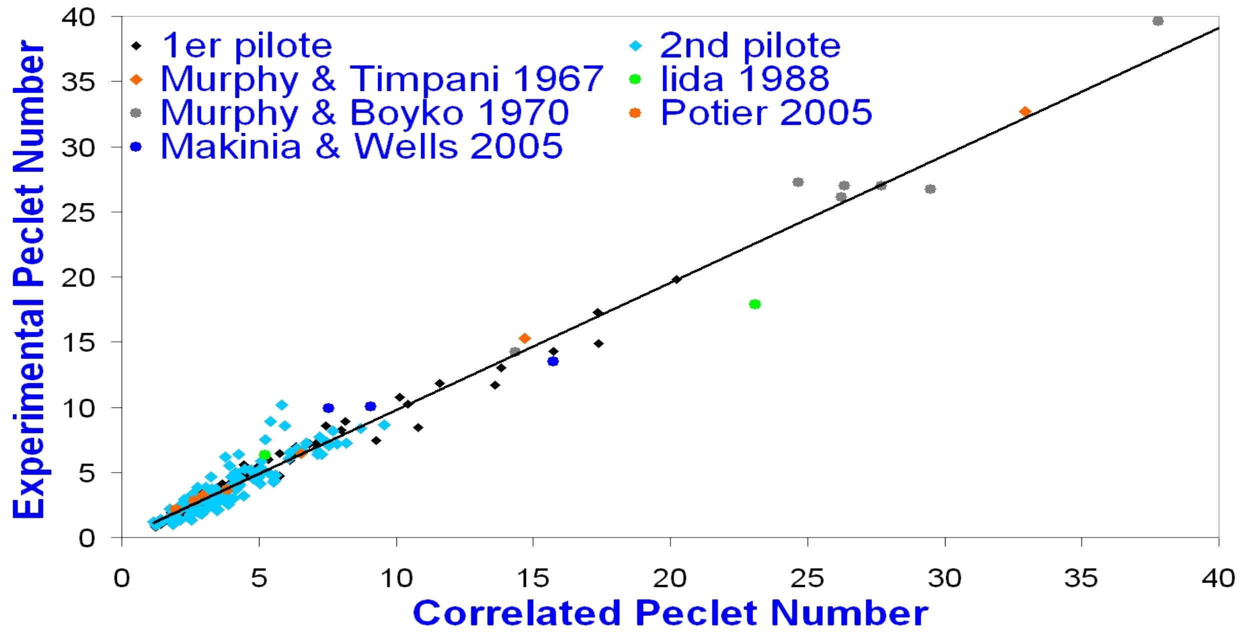
P = f (adimensional numbers)

Modeling using the Buckingham π Theorem

$$Pe = 0,0264\left(\frac{\mu_L.DH_h}{Q_L\rho_L}\right)^{-0.102}\left(\frac{DH_h}{DH_v}\right)^{-0,908}\left(\frac{g.DH_h^5}{Q_L^2}\right)^{0,309}\left(\frac{Q_G}{Q_L}\right)^{0,468}\left(\frac{l_{aération}}{l}\right)^{0,438}$$

Le Moullec et al. Water Research 39 (2008) 1767–1777

Reactor hydrodynamic modeling



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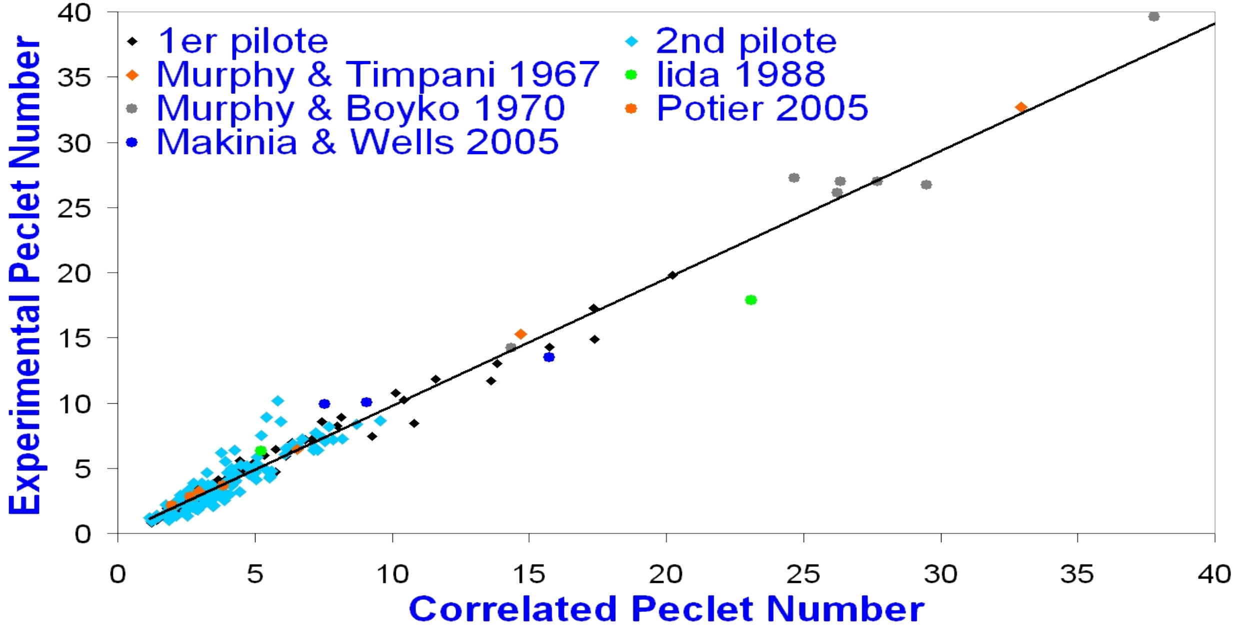
Le Moullec et al. Water Research 39 (2008) 1767–1777

Reactor hydrodynamic modeling



$$D = \frac{2}{3}\frac{h}{h+w}\sqrt{\frac{Q_G . w_{aeration}\left(L+w\right)}{2}}$$

Le Moullec et al. Water Research 39 (2008) 1767–1777

Wastewater Treatment: Approach to Modeling Transport, Transfer and Reactions

Wastewater Treatment: Approach to Modeling Transport, Transfer and Reactions

Reactor

Systemic approach

CFD with reaction

Compartmental methodology

Objectives

Modeling and Simulate Transport, Transfer, and Reactions comparing 3 approaches:

- Systemic model obtained by tracing

  Generally 5 to 20 elementary cells (CSTR)

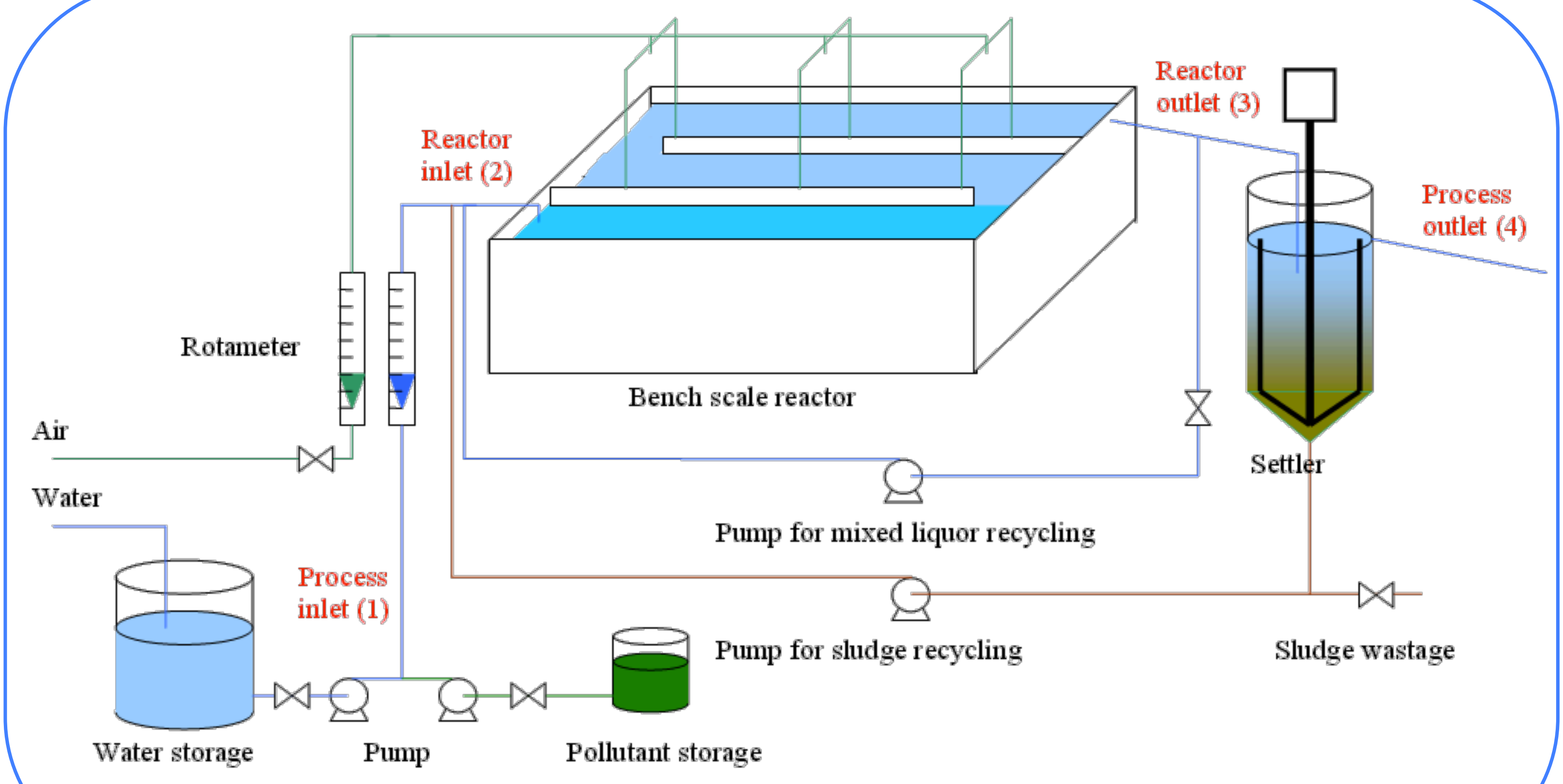
- Computational Fluid Dynamics (CFD) with reactions

  High number of cells

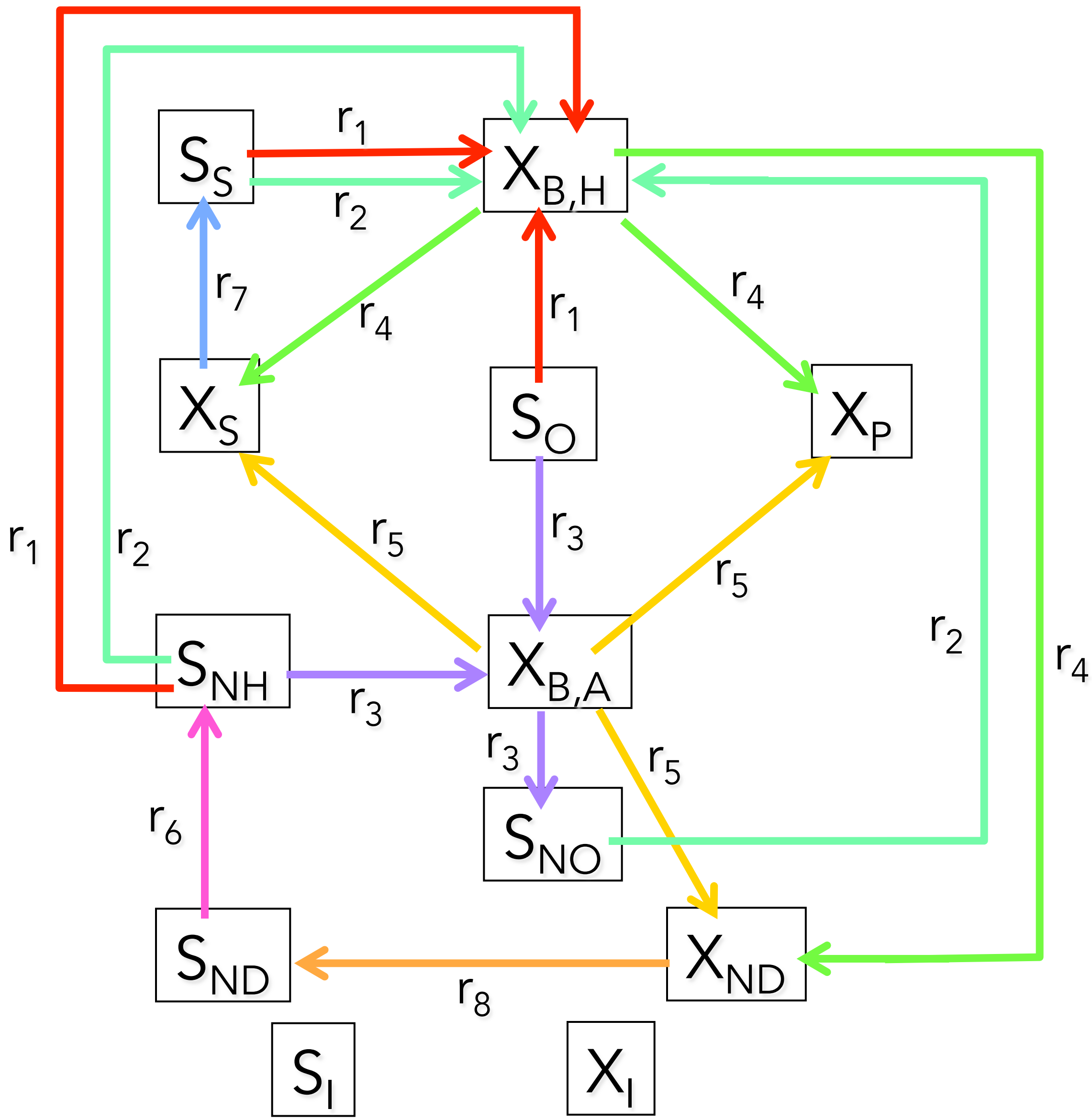
- New approach: compartmental modeling

  New discretization method: 10 to 2000 cells

Reactor and biological reaction



Kinetics modeling ASM1



S_I : Soluble inert organic matter

S_S : Readily biodegradable substrate

X_I : Particulate inert organic matter

X_S : Slowly biodegradable substrate

$X_{B,H}$: Active heterotrophic biomass

$X_{B,A}$: Active autotrophic biomass

X_P : Particulate products arising from biomass decay

S_O : Oxygen

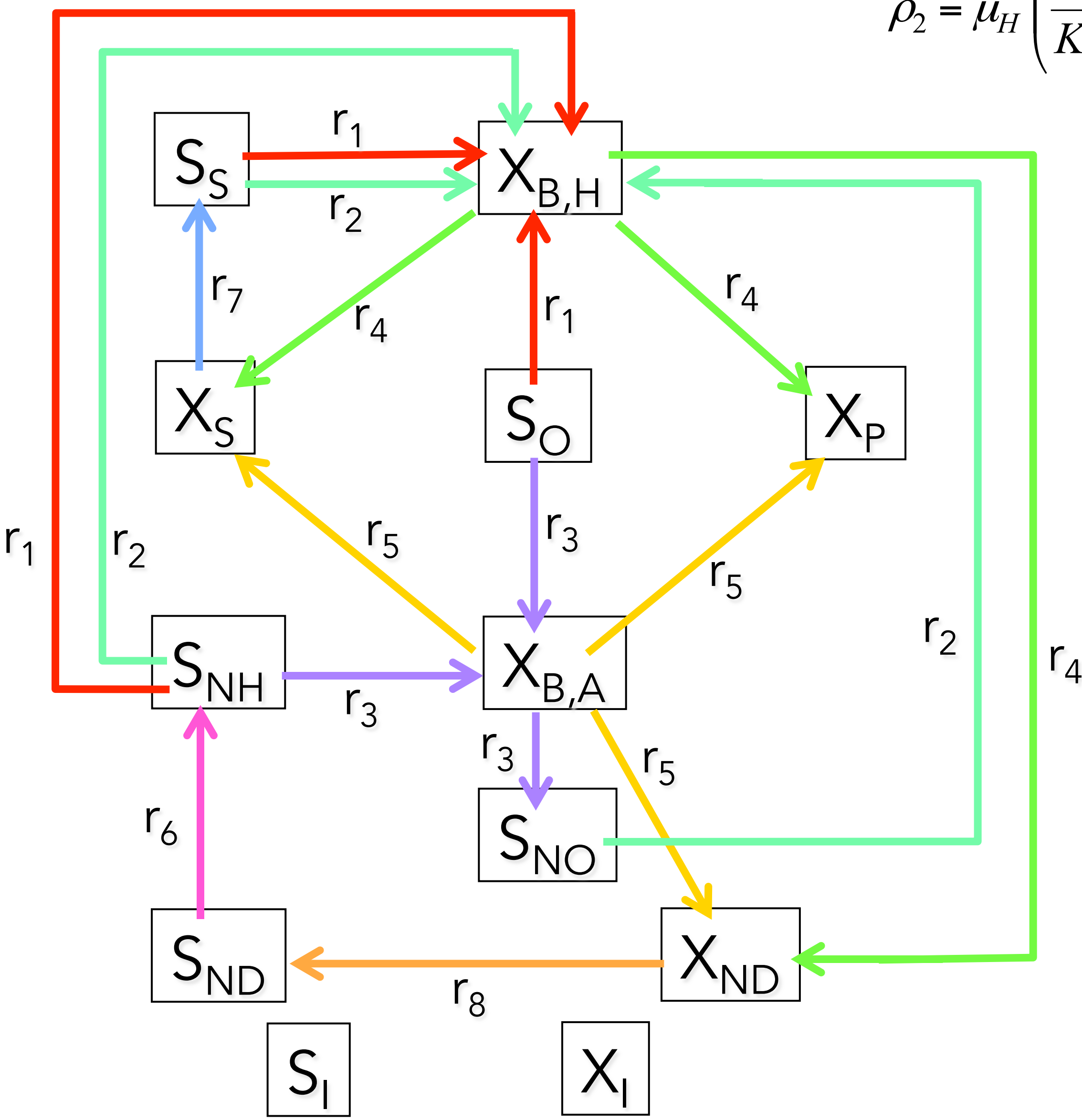
S_{NO} : Nitrate and nitrite nitrogen

S_{NH} : NH_4^+ and NH_3 nitrogen

S_{ND} : Soluble biodegradable organic nitrogen

X_{ND} : Particulate biodegradable organic nitrogen

Kinetics modeling ASM1



Anoxic growth of heterotrophs

$$\rho_2 = \mu_H \left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{N0}}{K_{NO}+S_{NO}}\right)\eta_g \, X_{B,H}$$

Aerobic growth of heterotrophs

$$\rho_1 = \mu_H \left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_0}{K_{O,H}+S_O}\right) X_{B,H}$$

Aerobic growth of autotrophs

$$\rho_3 = \mu_A \left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_0}{K_{O,A}+S_O}\right) X_{B,A}$$

Decay of heterotrophs

$$\rho_4 = b_H \, X_{B,H}$$

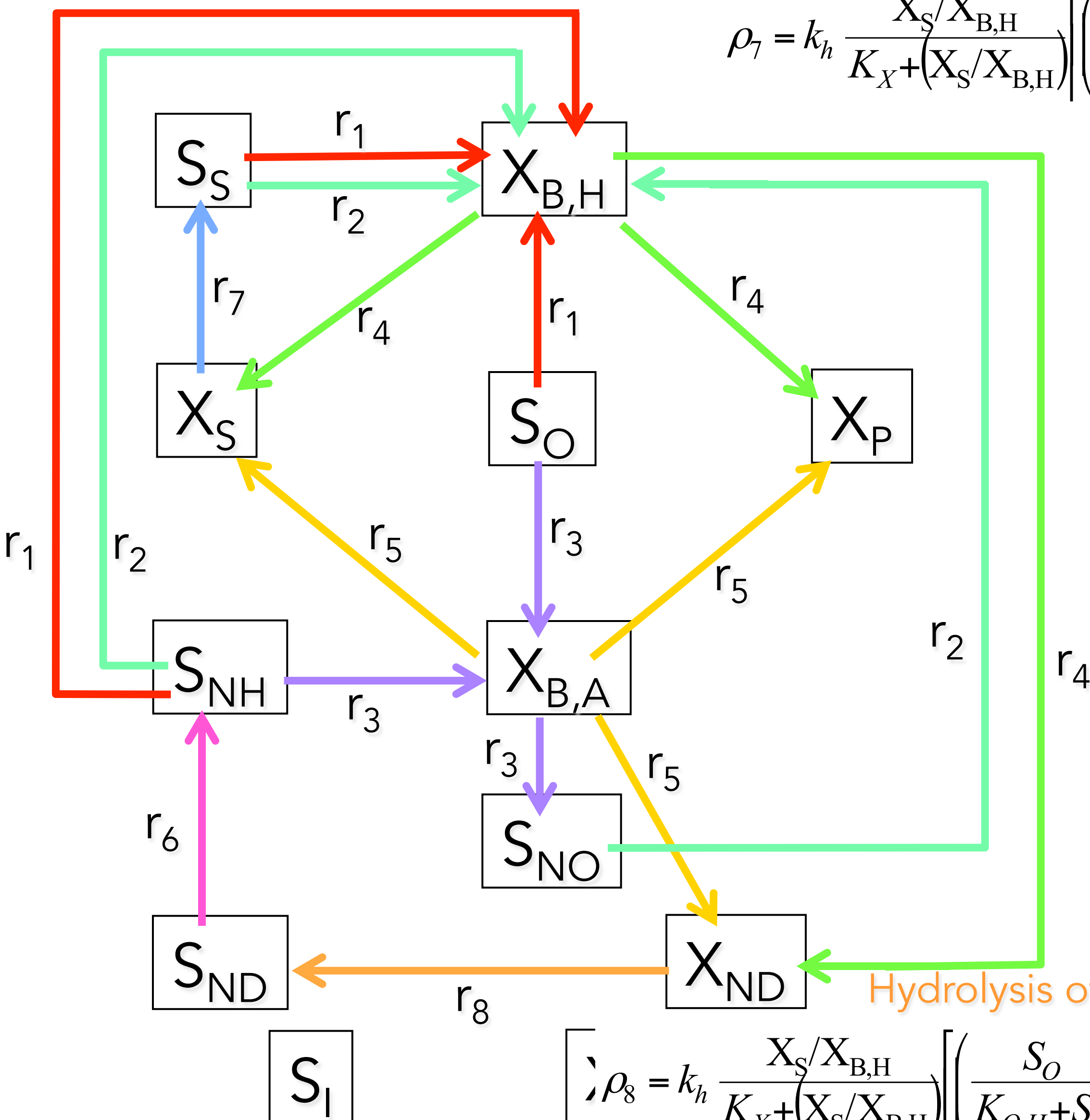
Decay of autotrophs

$$\rho_5 = b_A \, X_{B,A}$$

Ammonification of soluble organic nitrogen

$$\rho_6 = k_a \, S_{ND} \, X_{B,H}$$

Kinetics modeling ASM1



Hydrolysis of entrapped organics

$$\rho_7 = k_h \frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{N0}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$$

Hydrolysis of entrapped organic nitrogen

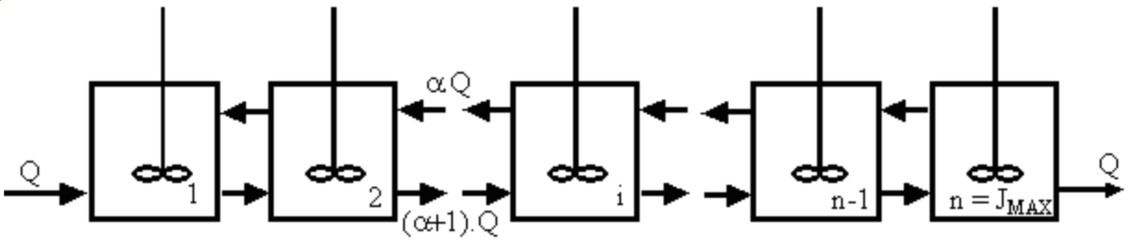
$$\rho_8 = k_h \frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{N0}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}(X_{ND}/X_S)$$

Simulation with reactions

systemic approach

Systemic modeling

CSTR in series with backmixing, enabling to take into account the hydrodynamics changes



$$G(s) = (1+\alpha)\left[\frac{1+\alpha}{\alpha}\right]^{J_{\max}-1}\left\{\frac{2\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha B}\right\} \quad (16)$$

with

$$B = \left(\frac{1+\alpha}{\alpha}\right)\left\{\left(\frac{\gamma-\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right)^{J_{\max}-2} Y_- - \left(\frac{\gamma+\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right)^{J_{\max}-2} Y_+\right\} \quad (17)$$

and

$$\gamma = 1 + 2\alpha + \frac{\tau.s}{J_{\max}}, \quad (18)$$

$$Y_- = \left[1+\alpha+\frac{\tau.s}{J_{\max}} - \alpha\frac{\gamma+\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right]\left[(1+\alpha)-\left(1+\alpha+\frac{\tau s}{J_{\max}}\right)\frac{\gamma-\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right],$$

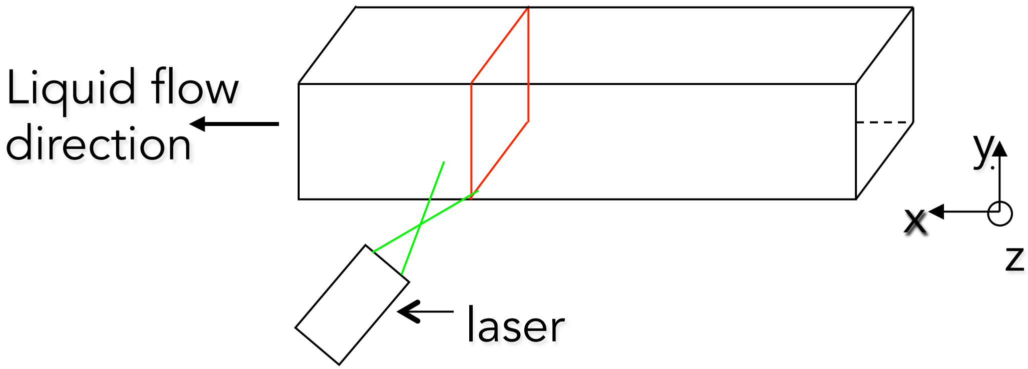
$$Y_+ = \left[1+\alpha+\frac{\tau s}{J_{\max}} - \alpha\frac{\gamma-\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right]\left[(1+\alpha)-\left(1+\alpha+\frac{\tau s}{J_{\max}}\right)\frac{\gamma+\sqrt{\gamma^2-4\alpha(1+\alpha)}}{2\alpha}\right]$$

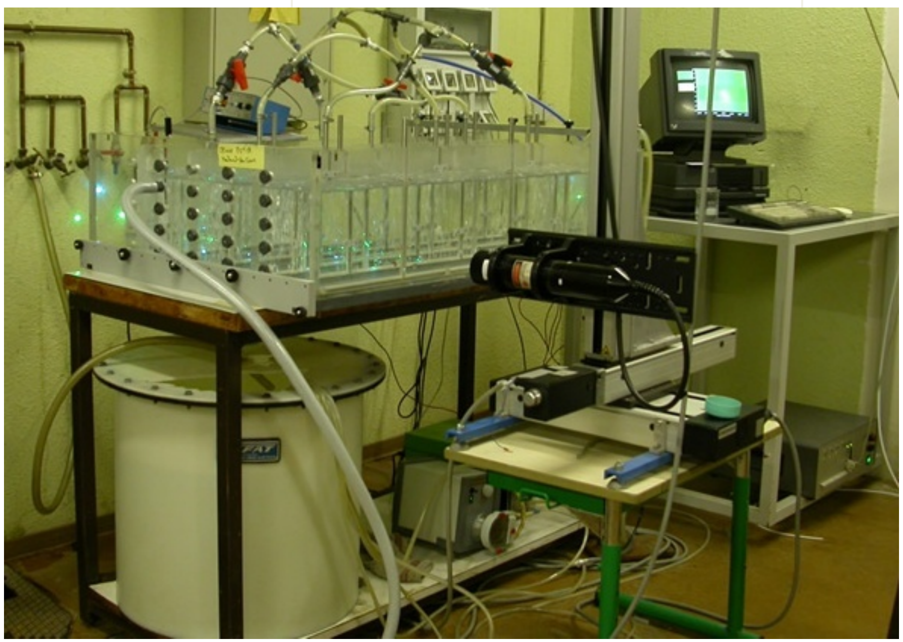
$$\alpha = \frac{1}{2}\left[(J_{\max}-1)-\left(1+J_{\max}^2\left(1-\frac{2}{J_{\text{app}}}\right)\right)^{1/2}\right]$$

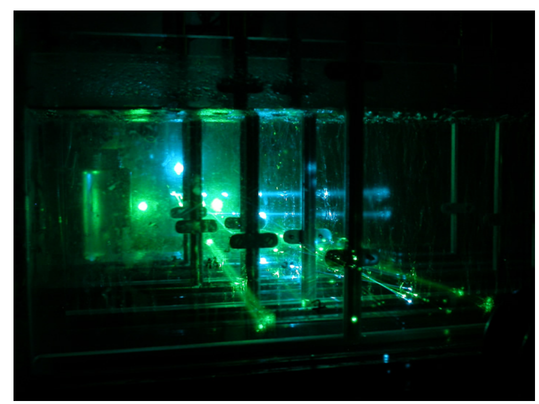
Potier et al. Water Research 39 (2005) 4454–4462

LDA and CFD Simulation with reactions

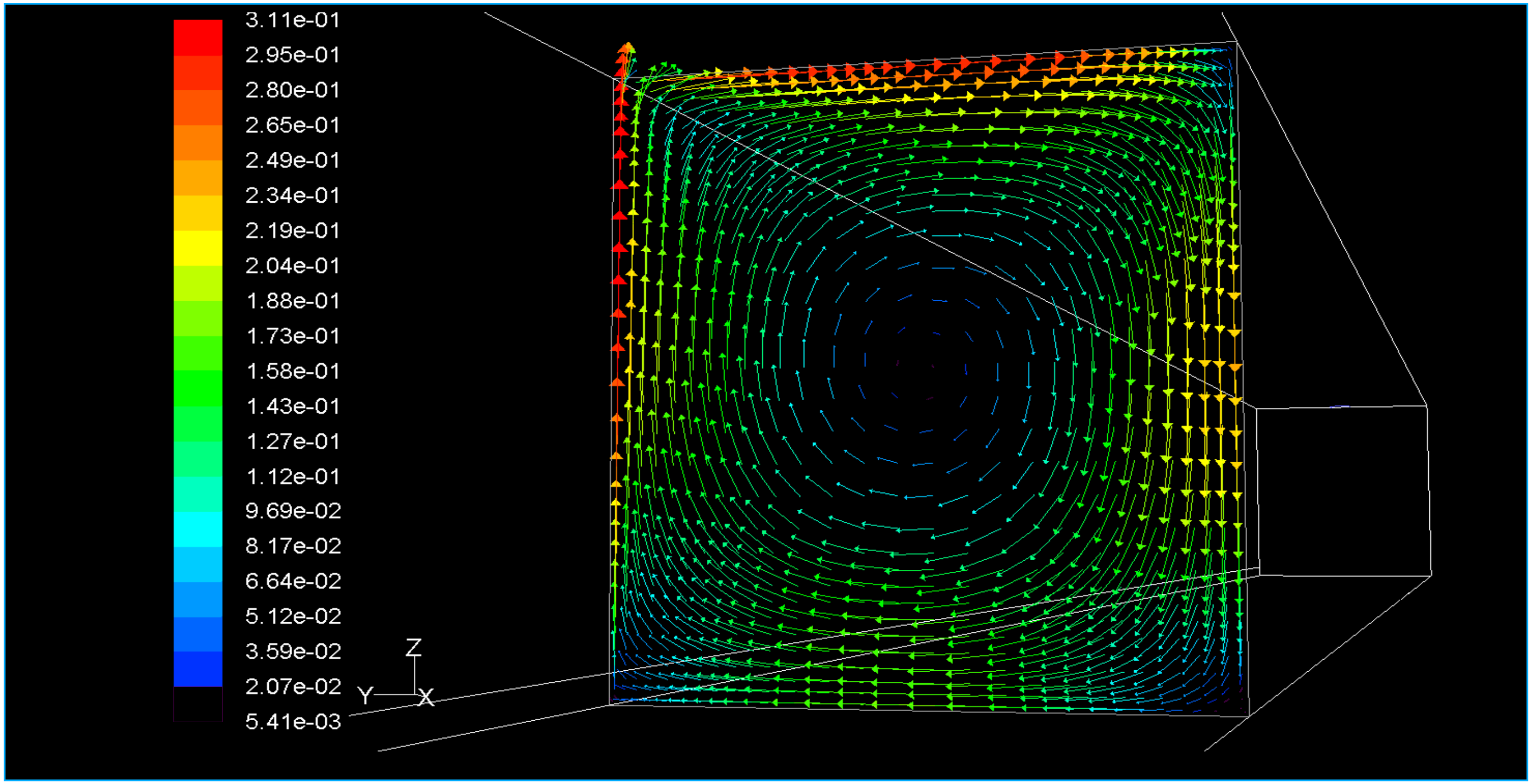
Laser Doppler Anemometry





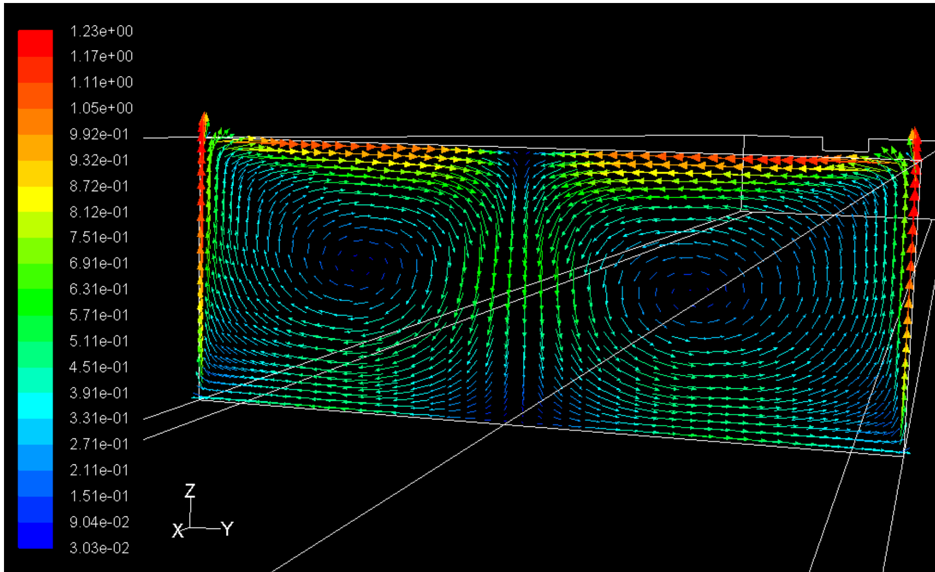


CFD modeling

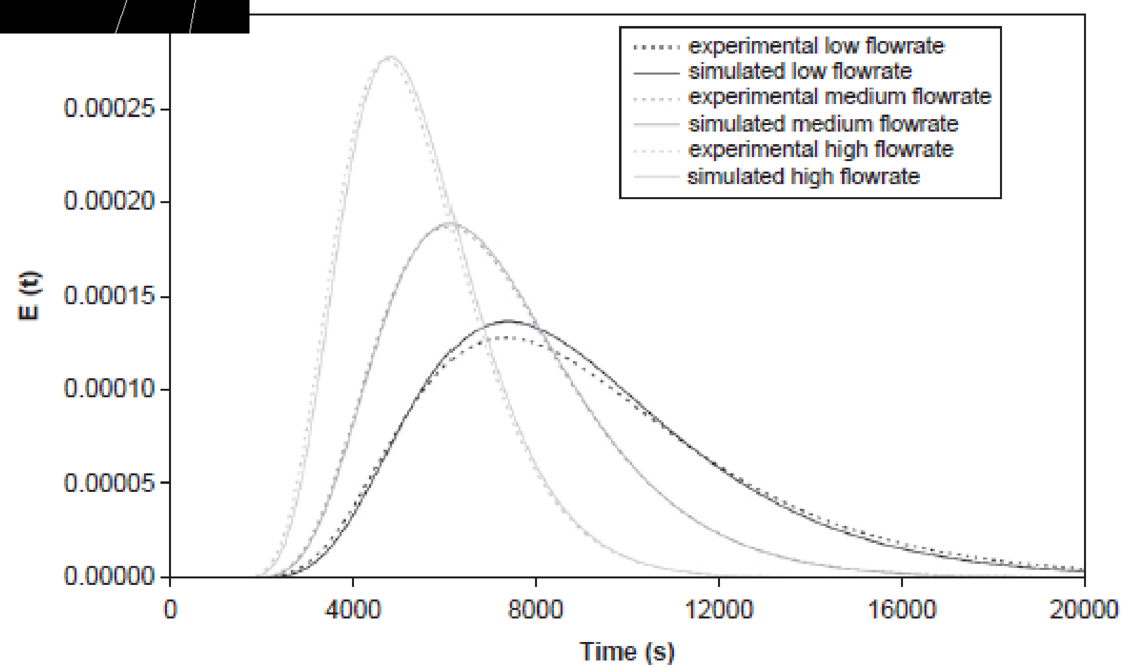


Le Moullec et al. Chemical Engineering Science 63 (2008) 2436–2449

CFD modeling



WWTP Nancy-Maxéville



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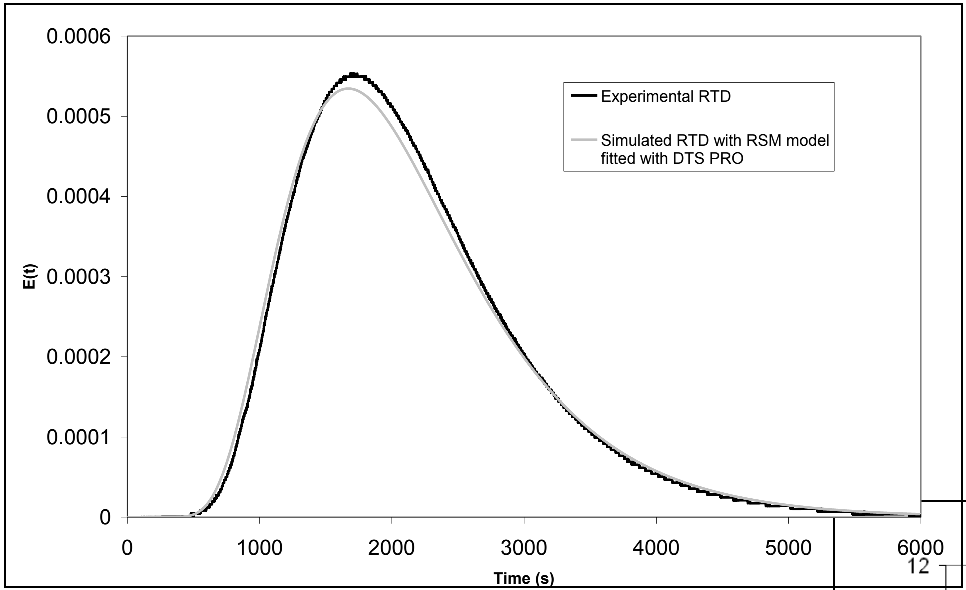
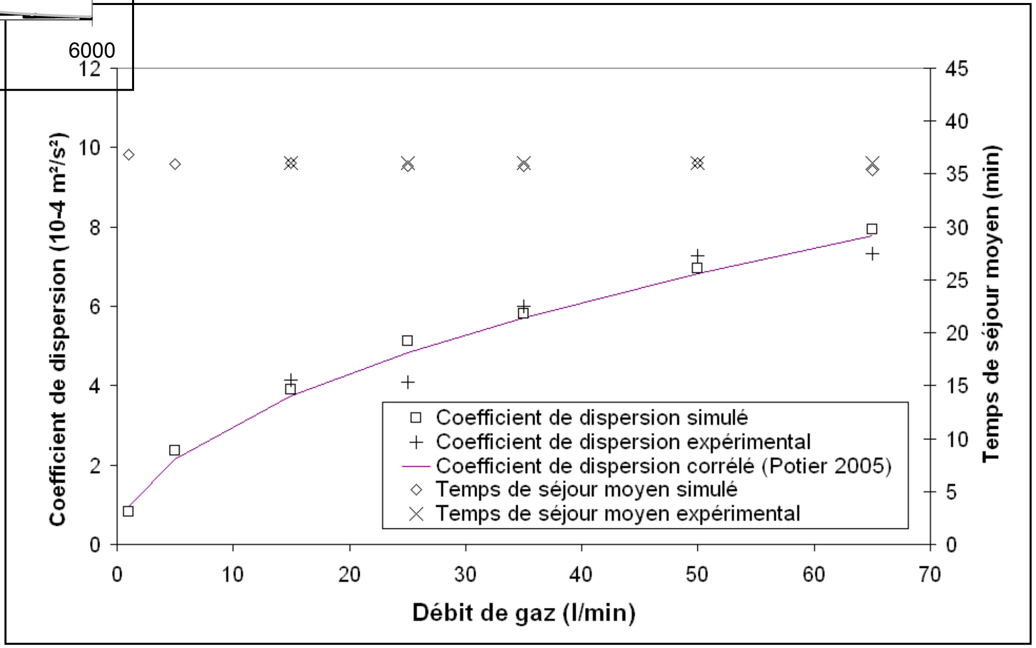
CFD modeling – Residence Time Distribution





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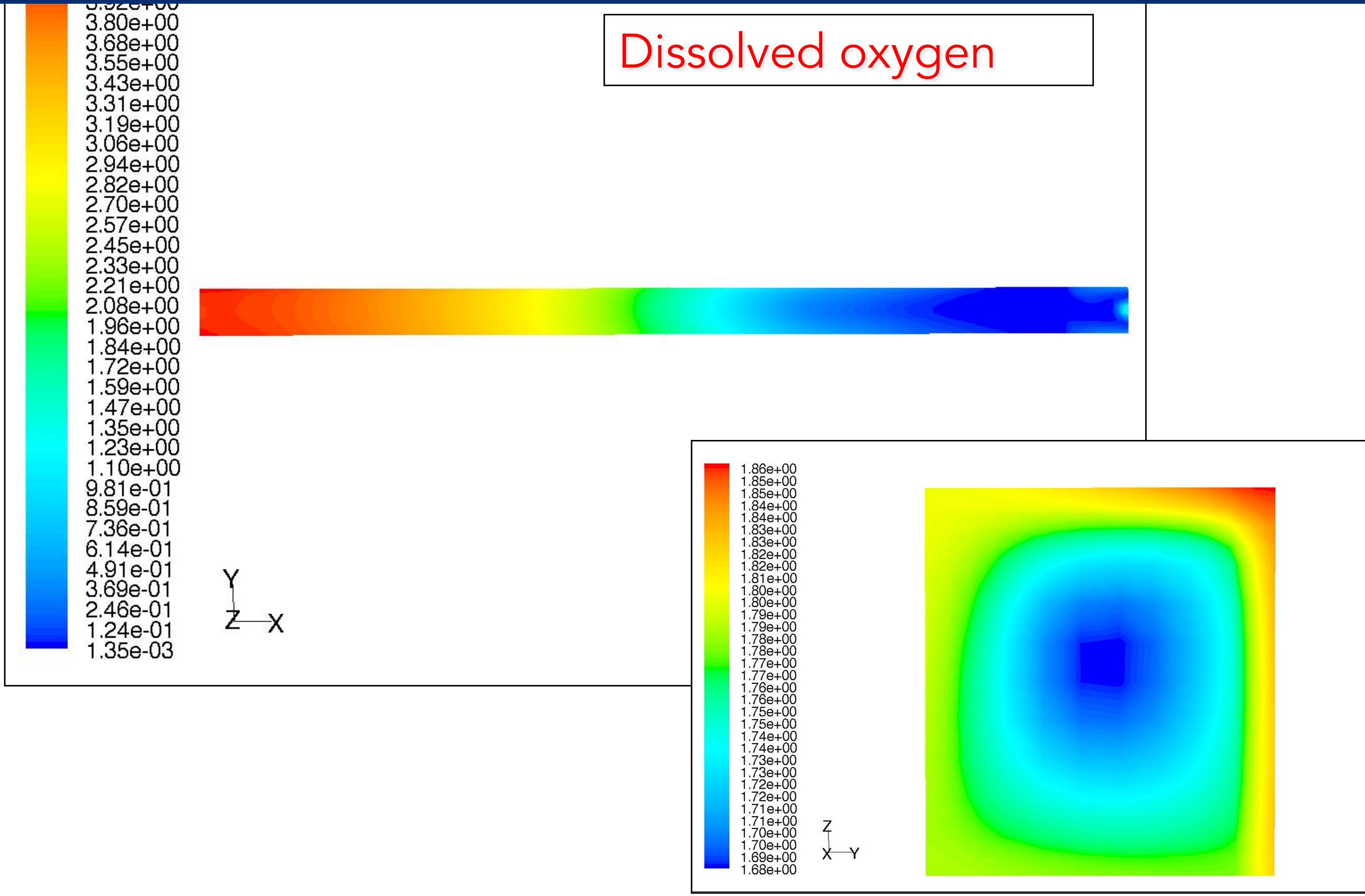
CFD with Reactions

CFD with reactions

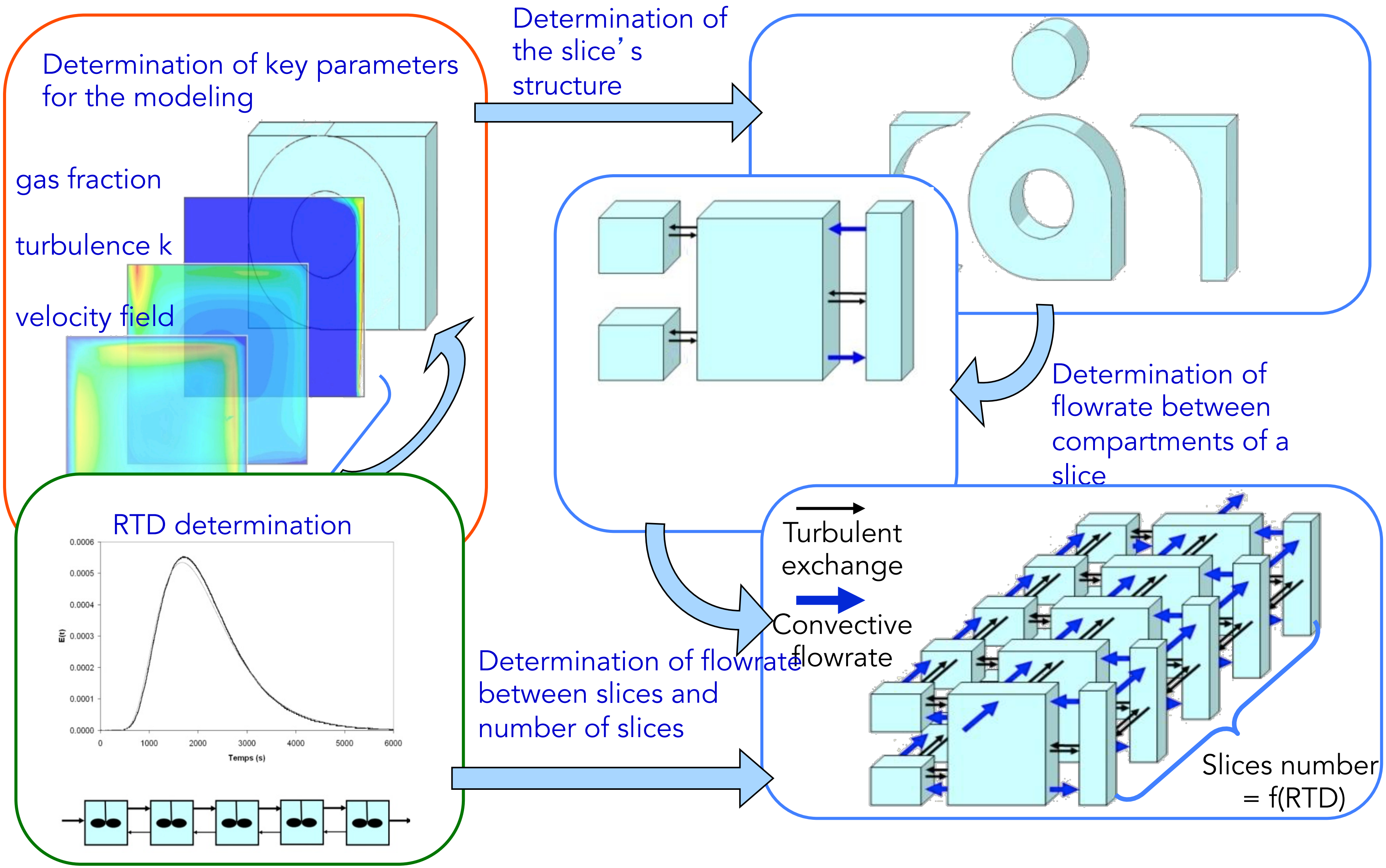
Dissolved oxygen



Le Moullec et al. Chemical Engineering Science 65 (2010) 492-498

Compartmental modeling

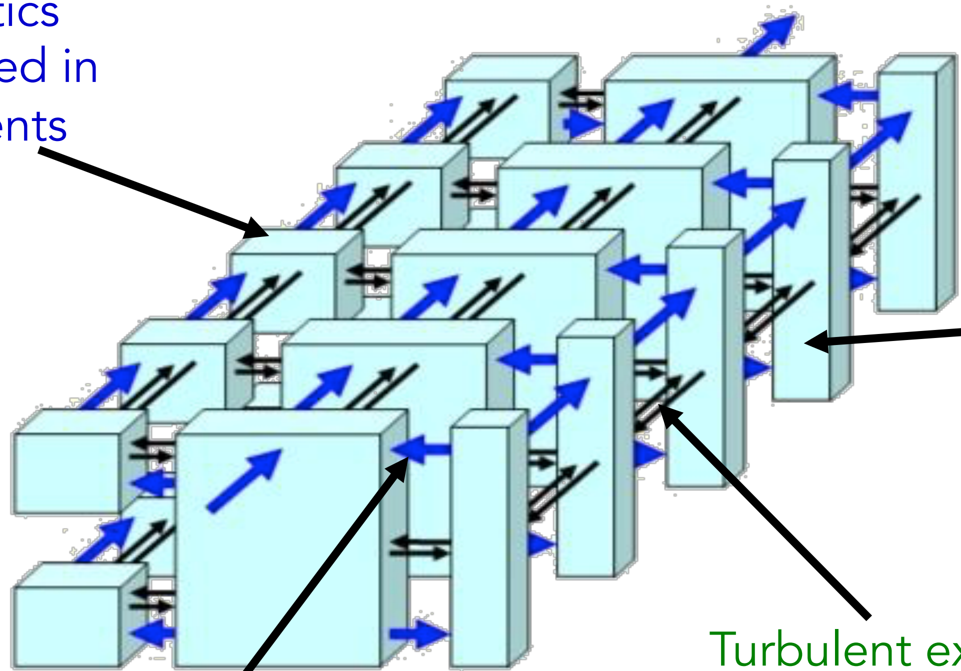
Compartmental approach



Le Moullec et al. Chemical Engineering Science 65 (2010) 343-350

Compartmental approach: summary

ASM1 kinetics model added in compartments



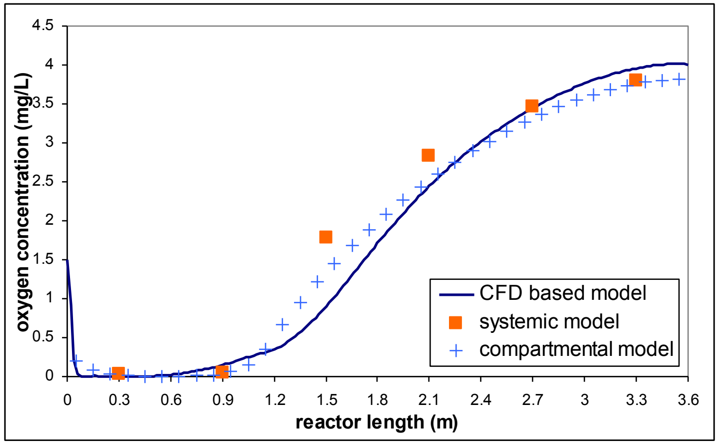
Gas-liquid transfer added in rich-gas compartments

Convective flowrate calculated from CFD mean velocity fields

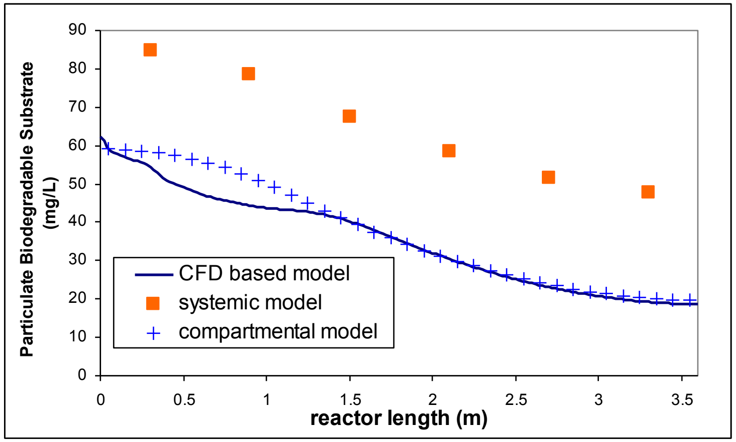
Turbulent exchange flowrates and number of slices calculated from simulated turbulence and RTD (by an iterative procedure)

Le Moullec et al. Water research 45 (2011) 3085-3097

Comparison of models

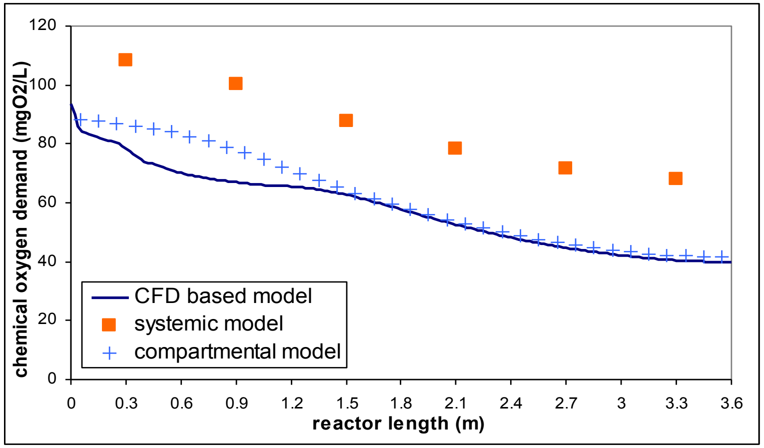


Three models give almost the same results for dissolved oxygen concentration



For X_S (slowly biodegradable substrate)

$$DCO = S_I + S_S + X_I + X_S$$



- The three models follow the same trend
- CFD and compartment model look very similar

Le Moullec et al. Chemical Engineering Science 65 (2010) 343-350

Compartmental modeling; another approach

Towards better models for describing mixing using compartmental modelling: a full-scale case demonstration

Usman Rehman[1], Chaim De Mulder[1], Youri Amerlinck[1], Marina Arnaldos[2], Stefan R. Weijers[3], Olivier Potier[4], and Ingmar Nopens[1]

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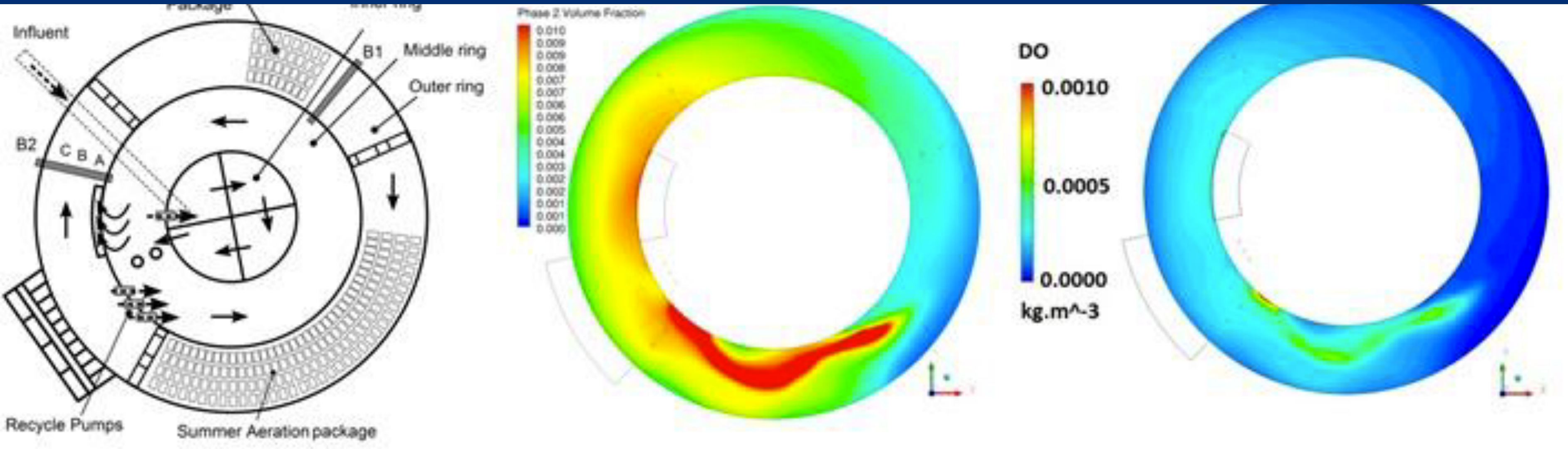
2 Acciona Agua S.A., R&D Department, Av. De les Garrigues 22, 08820 El Prat del Llobregat (Barcelona), Spain
3 Waterschap De Dommel, Bosscheweg 56, 5283 WB Boxtel, Postbus 10.001, Netherlands
4 Laboratoire Réactions et Génie des Procédés, LRGP, CNRS UMR 7274, Université de Lorraine, 1 rue Grandville, BP 20451, 54001 NANCY cedex, France

WWTmod 2016

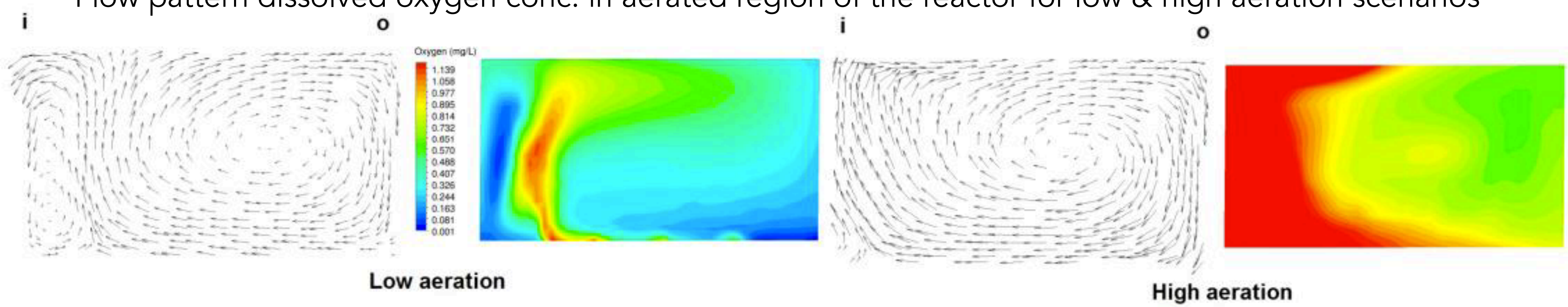
Compartmental modeling; another approach.
Usman Rehman's PhD



(a) (b) (c)

(a) Reactor configuration (b) Gas fraction distribution in the reactor (c) Dissolved oxygen concentration in the reactor

Flow pattern dissolved oxygen conc. in aerated region of the reactor for low & high aeration scenarios



Rehman et al. WWTmod 2016

Working Group on
Computational Fluid Dynamics (CFD) & Wastewater

WG Members

- WG composed of :
  - Consultants
  - Academics
  - People from Europe, Northern and Latin America, Australia

- Chair : Julien Laurent (University of Strasbourg, France)
- Vice-Chair : Jim Wicks (The Fluid Group, UK; vice-chair)
- Secretary : Randal Samstag (Independent Consultant, USA; secretary)
- Damien Batstone (AWMC, Australia)
- Joel Ducoste (NC State, USA)
- Alonso Griborio (Hazen & Sawyer, USA)
- Genevieve Kenny (R.V. Anderson Associates, Canada)
- Ingmar Nopens (Ghent University, Belgium; past-chair)
- Anna Karpinska Portela (University of Birmingham, England)
- Olivier Potier (LRGP, CNRS - Université de Lorraine, France)
- Nicolas Ratkovich (University of Los Andes, Columbia)
- Stephen Saunders (Ibis Group, USA)
- Ed Wicklein (Carollo Engineers, USA)

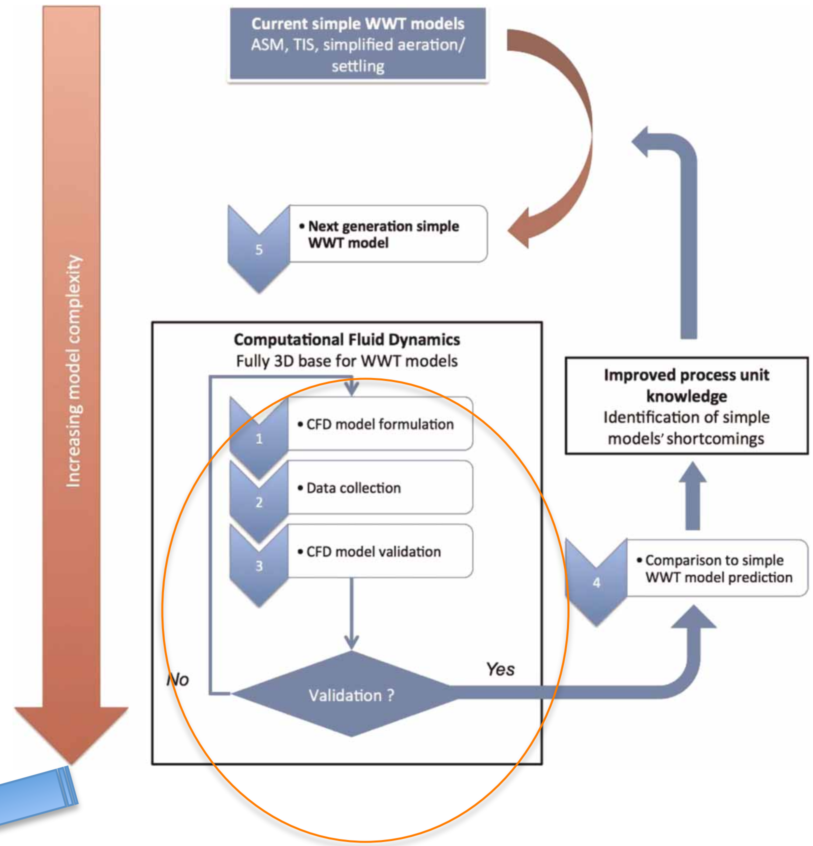
WG motivations & objectives

- No guidelines regarding GMP
- Lack of CFD training & education within environmental sector

- promote the exchange of ideas and experiences regarding the use of CFD in the field of water and wastewater treatment
- build a network of experts in the field

Use of CFD in WRRF

- Troubleshooting (e.g. clarifiers)
- Hydraulics – Flow splitting
- Design improvement (clarifiers, reactors ?)
- Next generation models development



GMP required

Good modelling practice in applying computational fluid dynamics for WWTP modelling

Edward Wicklein, Damien J. Batstone, Joel Ducoste, Julien Laurent, Alonso Griborio, Jim Wicks, Stephen Saunders, Randal Samstag, Olivier Potier and Ingmar Nopens

Water Science and Technology 73 (5), 969-982

IWA Working Group on Computational Fluid Dynamics (CFD) & Wastewater

Publications

A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling

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ABSTRACT

To date, computational fluid dynamics (CFD) models have been primarily used for evaluation of hydraulic problems at wastewater treatment plants (WWTPs). A potentially more powerful use, however, is to simulate integrated physical, chemical and/or biological processes involved in WWTP unit processes on a spatial scale and to use the gathered knowledge to accelerate improvement in plant models for everyday use, that is, design and optimized operation. Evolving improvements in computer speed and memory and improved software for implementing CFD, as well as for integrated processes, has allowed for broader usage of this tool for understanding, troubleshooting, and optimal design of WWTP unit processes. This paper proposes a protocol for an alternative use of CFD in process modelling, as a way to gain insight into complex systems leading to improved modelling approaches used in combination with the IWA activated sludge models and other kinetic models.

Key words | biokinetic models, CFD, complex systems, fluid motion, multi-phase flow, transport models

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Good modelling practice in applying computational fluid dynamics for WWTP modelling

Water Science and Technology 73 (5), 969-982

Edward Wicklein, Damien J. Batstone, Joel Ducoste, Julien Laurent, Alonso Griborio, Jim Wicks, Stephen Saunders, Randal Samstag, Olivier Potier and Ingmar Nopens

IWA Working Group on Computational Fluid Dynamics (CFD) & Wastewater

Complete flow of a CFD modelling process

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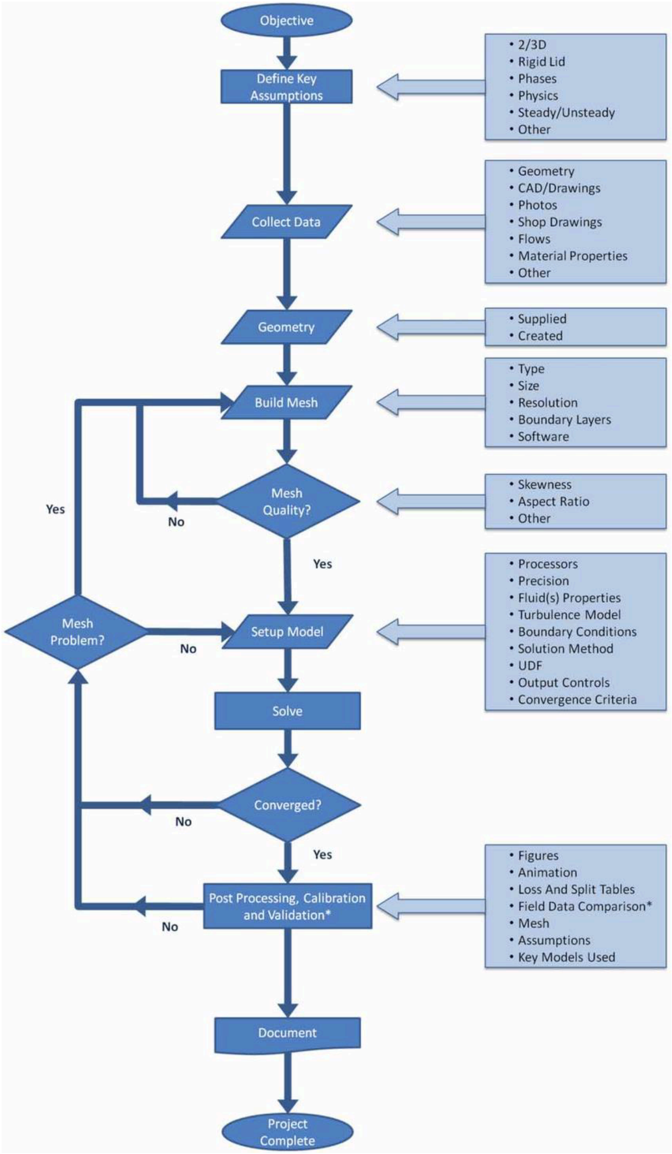

IWA Working Group on Computational Fluid Dynamics (CFD) & Wastewater

Coming soon…

- CFD for Wastewater Treatment: An Overview
- Scientific & Technical Report
- Student book

Being aware it is only modeling

We try for being close to the reality with the simplest models,

but not the more simplistic ones.

Merci de votre attention !

Gràcies per la seva atenció!