19 MAY 2023

10:00 CEST

IWA Specialist Group on Modelling and Integrated Assessment Webinar Series

Generalised Physicochemical Model (PCM) for Wastewater Processes

Speakers

- **Ulf Jeppsson** – Lund University
- **Damien Batstone** – The University of Queensland, Australia
- **Kimberly Solon** – Ghent University, Belgium
- **Sylvie Gillot** – INRAE, France
- **Christian Kazadi Mbamba** – The University of Queensland, Australia
- **Xavier Flores-Alsina** – University of Denmark, Demark
- **Paloma Grau** – University of Navarra, Spain
- **Tamara Fernández-Arévalo** – CEIT, Spain

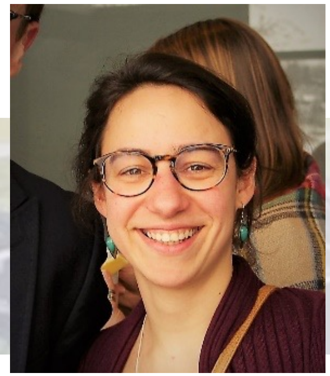
The webinar is going to be recorded and shared on the MIA SG Youtube channel afterward.

MIA Welcome Note

IWA Modelling and Integrated Assessment Specialist Group

Dr. Ulf Jeppsson (Chair of MIA SG)

Dr. Elena Torfs (Vice-chair of MIA SG)



inspiring change

LUND UNIVERSITY

UNIVERSITÉ LAVAL

MODELLING AND INTEGRATED ASSESSMENT SPECIALIST GROUP (MIA SG)

"This group targets people from research, consulting companies, institutions and operators to think along ***the use of models and computing tools to support the understanding, management and optimization of water systems****."*

PRIORITIES

- Interact with other IWA SGs and other professional organizations
- Organize specialized conferences, sessions and workshops
- Engage and activate YWPs in the domain.

CURRENTLY 2200 MEMBERS

How to find us

Website: http://iwa-mia.org/

https://iwa-connectplus.org

MIA SG: ACTIVITIES

Task Groups (TGs)

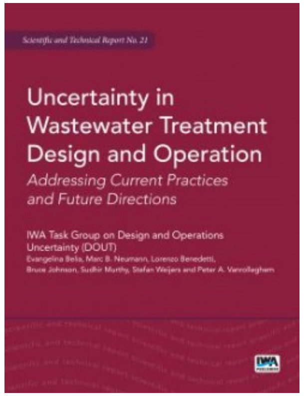
- Benchmarking of Control Strategies (BSM) AND Good Modelling Practice (GMP) AND Design and Operations Uncertainty (DOUT) AND Use of Modelling for Minimizing GHG Emissions (GHG) AND Generalised Physicochemical Modelling (PCM) (all five finished)
- Membrane Bioreactor Modelling and Control (MBR)
- Good Modelling Practice in Water Resource Recovery Systems (GMP2)

Working Groups (WGs)

- Integrated Urban Water Systems (IUWS)
- Computational Fluid Dynamics (CFD)
- Good Modelling Practice (GMP)

Conferences / Events

- WRRmod
- Watermatex



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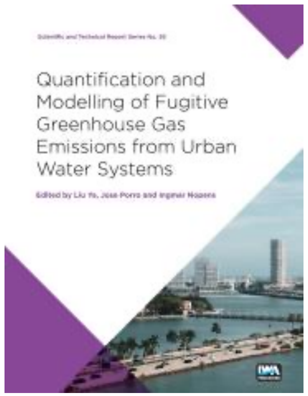
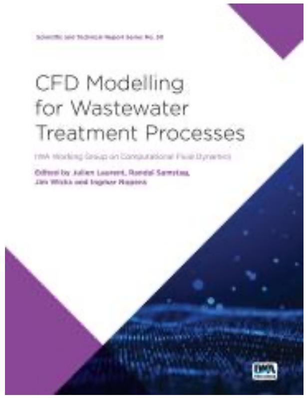
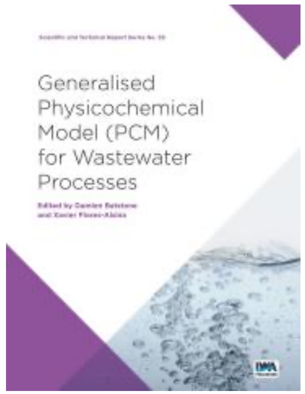


STR (2022, open access)



STR (2022)



STR (2022, open access)

MIA SG: UPCOMING CONFERENCES

11th Symposium on Modelling and Integrated Assessment (Watermatex2023)

- Location: Québec City, Canada, 23-27 Sept. 2023
- Chair/vice-chair: Prof. Peter Vanrolleghem (Univ. Laval)/Dr. Elena Torfs (Univ. Ghent)

9th Water Resource Recovery Modelling seminar (WRRmod2024)

- Location: Notre Dame, Indiana, USA, 6-10 April 2024
- Organisers: Adrienne Menniti, Leon Downing, Tom Johnson, Rob Nerenberg

- **CALL FOR WRRmod2026 soon to appear**

FIND MIA SG ON SOCIAL MEDIA

– https://www.iwaconnectplus.org/

- https://www.linkedin.com/company/iwa-mia-specialist-group-on-modelling-and-integrated-assessment

– https://twitter.com/iwa_mia_sg

– **MIA SG open web site** http://iwa-mia.org

Newsletters, push messages, MIA_YouTube channel, digital archive

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Q&A Session Moderator: *Damien Batstone (Uni. Queensland, Australia)*

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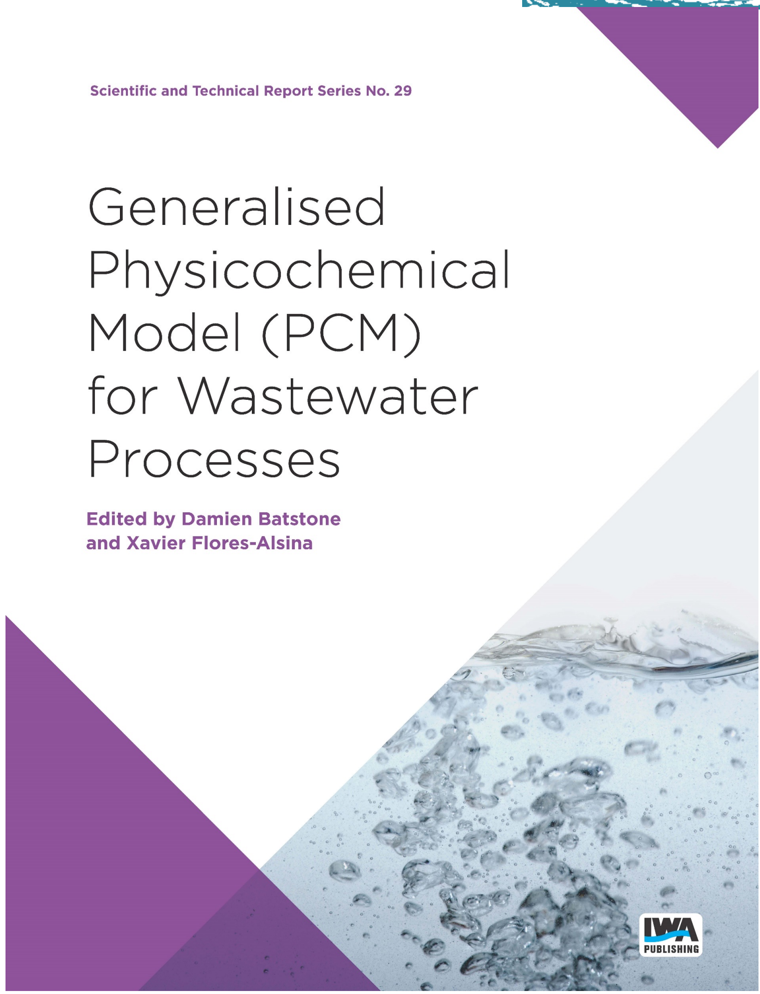
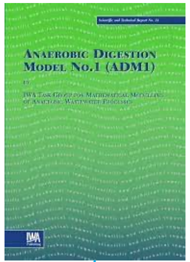
- Microphones and cameras have been disabled due to the large number of attendees;
- The normal chat function is disabled;
- Please put any questions and comments you may have in the Q&A (icon to the low right in Zoom) and we will do our best to answer them during the session (in writing or orally).

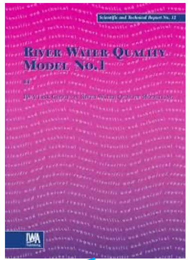
PCM1 AIMS

- Represent spontaneous (chemical) reactions across the (waste) water cycle for plant wide (or more) modelling
- Ion concentrations up to the % level (non-ideal behavior)
- Allow phosphorous modelling in ASM/ADM
- Capable for resource recovery
- Describes theory applicable to wastewater



https://iwaponline.com/ebooks/book/865/Generalised-Physicochemical-Model-PCM-for



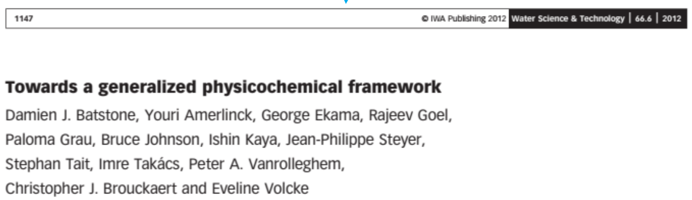


Commercial
Modelling
Packages

WWTMod 2010

PHREEQC

MINTEQA2


1147 © IWA Publishing 2012 Water Science & Technology | 66.6 | 2012

Towards a generalized physicochemical framework

Damien J. Batstone, Youri Amerlinck, George Ekama, Rajeev Goel, Paloma Grau, Bruce Johnson, Ishin Kaya, Jean-Philippe Steyer, Stephan Tait, Imre Takács, Peter A. Vanrolleghem, Christopher J. Brouckaert and Eveline Volcke

2013 TG Established

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FACULTY OF
BIOSCIENCE ENGINEERING

AQUEOUS PHASE CHEMISTRY

Kimberly Solon

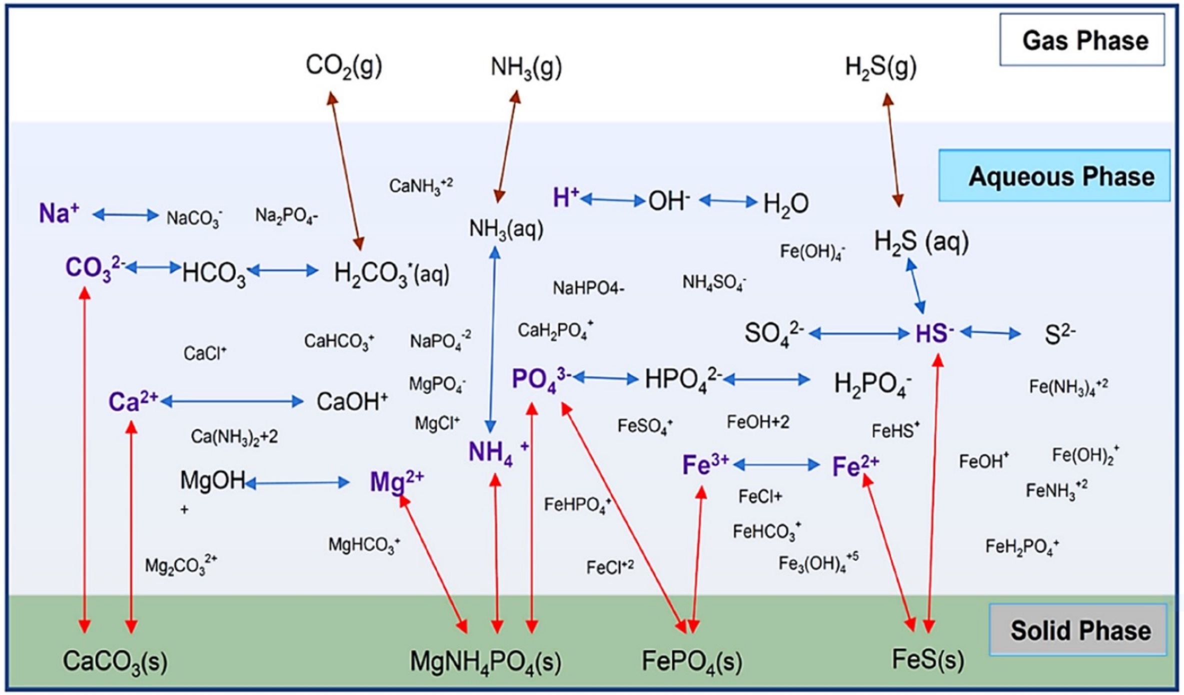
19 May 2023

GHENT
UNIVERSITY

PHYSICOCHEMICAL PROCESSES?

physico-chemical refers to both physical and chemical properties/aspects, as opposed to biochemical

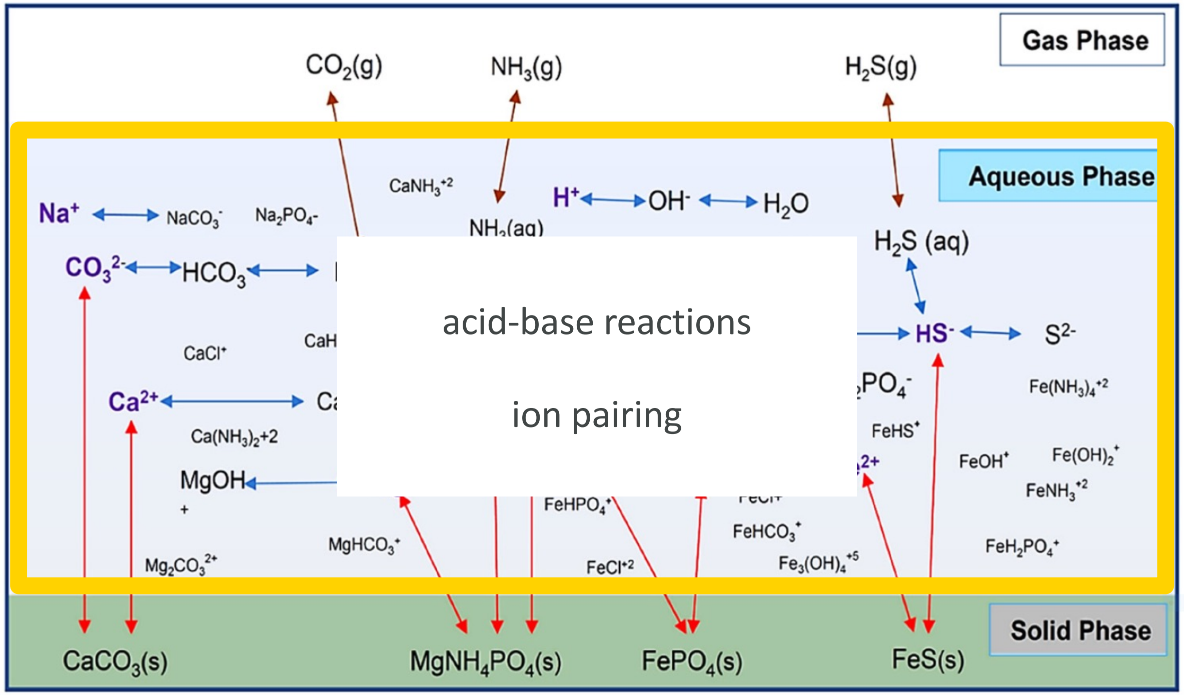
non-biologically mediated



AQUEOUS PHASE CHEMISTRY?

Physicochemical model

- liquid - liquid
- solid - liquid
- gas - liquid



WHY MODEL AQUEOUS PHASE CHEMISTRY?

Limitations to IWA Activated Sludge Models

Plant-wide optimisation

Resource recovery

Commercial software has generally led academic research into implementation of aqueous phase chemistry modelling

AQUEOUS PHASE CHEMISTRY CONSISTS OF …

ACID-BASE REACTIONS

association and dissociation of solute species with protons and hydroxide ions

ION PAIRING

solute species can associate with other solute species to form ion pairs

Reaction:

$$\mathrm{HA} \leftrightarrow \mathrm{A}^- + \mathrm{H}^+$$

$$\mathrm{NaHCO}_{3,\mathrm{aq}} \Leftrightarrow \mathrm{Na}^+ + \mathrm{HCO_3}^-$$

Equilibrium equation:

$$K_\mathrm{A} = \frac{\{\mathrm{A}^-\}\{\mathrm{H}^+\}}{\{\mathrm{HA}\}}$$

$$K_{\mathrm{NaHCO_3}} = \frac{\{\mathrm{Na}^+\}\{\mathrm{HCO_3}^-\}}{\{\mathrm{NaHCO_3}\}}$$

HOW TO REPRESENT EQUILIBRIUM SYSTEMS?

TABLEAU APPROACH

COMPONENTS & SPECIES

Species (i) ↓	Components→ (TOT_j)	TOTH* 1	S_{IC} 2	S_{AC} 3	S_{Na} 4	S_{Cl} 5	S_{IN} 6	TOT (H_2O)	−log(K_i)
1	H^+	1							
2	CO_3^{2-}		1						
3	Ac^-			1					
4	Na^+				1				
5	Cl^-					1			
6	NH_4^+						1		
	(H_2O)							1	
7	OH^-	−1							14.18
8	HCO_3^-	1	1						10.33
9	$CO_2(aq)/H_2CO_3$	2	1					−1	16.68
10	HAc	1		1					4.76
11	NH_3	−1					1		−9.24
12	$NaCO_3^-$		1		1				1.27
13	$NaHCO_{3(aq)}$	1	1		1				10.03
14	$NaAc_{(aq)}$			1	1				−0.12
15	$NaOH_{(aq)}$	−1			1				−13.9

Component = Sum of species

$$0 = \mathrm{TOT_J} - \sum_{i=1}^{N_S} v_{i,j}[S_i] \quad i = 1 \ldots N_C$$

$$0 = S_{IC} - [CO_3^{2-}] - [HCO_3^-] - [CO_2] - [NaCO_3^-] - [NaHCO_3]$$

Equilibrium equation for each species:

$$0 = \{S_i\} - K_i \prod_{j=1}^{N_C} \{S_j\}^{v_{i,j}} \quad i = N_{C+1} \ldots N_S$$

$$0 = \{HCO_3^-\} - 10^{10.33}\{H^+\}\{CO_3^{2-}\}$$

$$0 = \{CO_2\} - 10^{16.68}\{H^+\}\{CO_3^{2-}\}^2$$

$$0 = \{NaCO_3^-\} - 10^{1.27}\{Na^+\}\{CO_3^{2-}\}$$

$$0 = \{NaHCO_3\} - 10^{10.03}\{H^+\}\{Na^+\}\{CO_3^{2-}\}$$

ION ACTIVITY?

the electrostatic interactions of ions in solution, measured *via* ionic strength, reduces their effective concentration

Application of activity corrections at $I > 0.2\ mol \cdot L^{-1}$

Correction to apply to achieve pH error of <5%

Level	Ionic Strength (M)	Wastewater Type	Approach
1	<0.001	Drinking water, clean natural fresh water	No correction required – assume ideal
2	<0.1	Weak industrial WW. All domestic WWTP.	Non-iterative simple correction. Non-ion specific activity coefficient. $K'_A = K_A \gamma_A{}^1$
3	<1 (only ionic species corrected)	Brackish, anaerobic digesters	Full iterative calculation of ion activity using appropriate activity coefficient calculation.
4	<1 (all species corrected)	As above, with gas transfer	As above, with addition of uncharged specie correction
5	<5	Strong industrial, landfill leachate, RO brine	Requires specific ion interaction (SIT) corrections

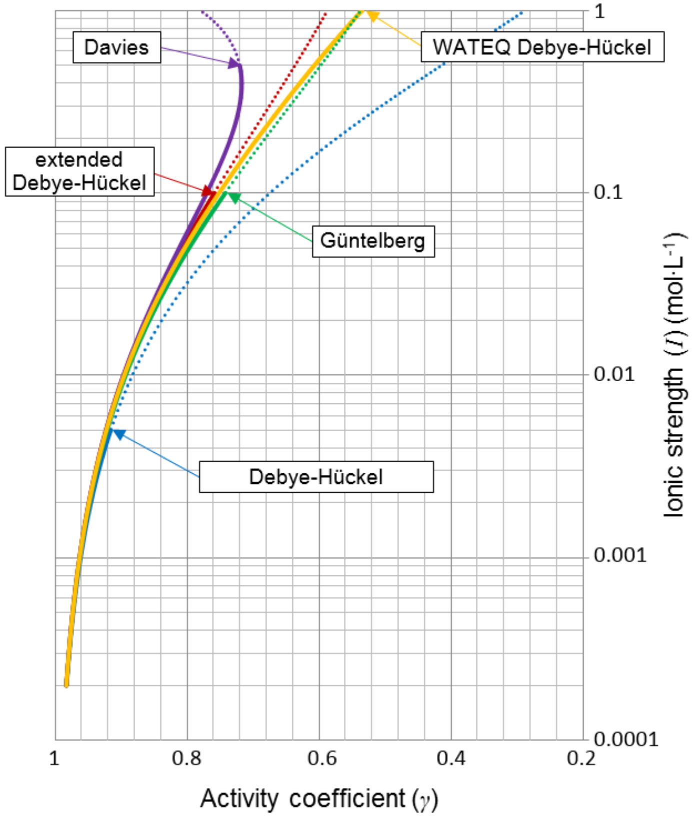
HOW TO CALCULATE ION ACTIVITY?

Ionic strength (I)	$I = \frac{1}{2}\sum[S_i]z_i^2$ [ ] = concentration, z = valency
Activity correction factor (γ)	(see table below)
Activity (a)	$\{a_i\} = \gamma_i[S_i]$

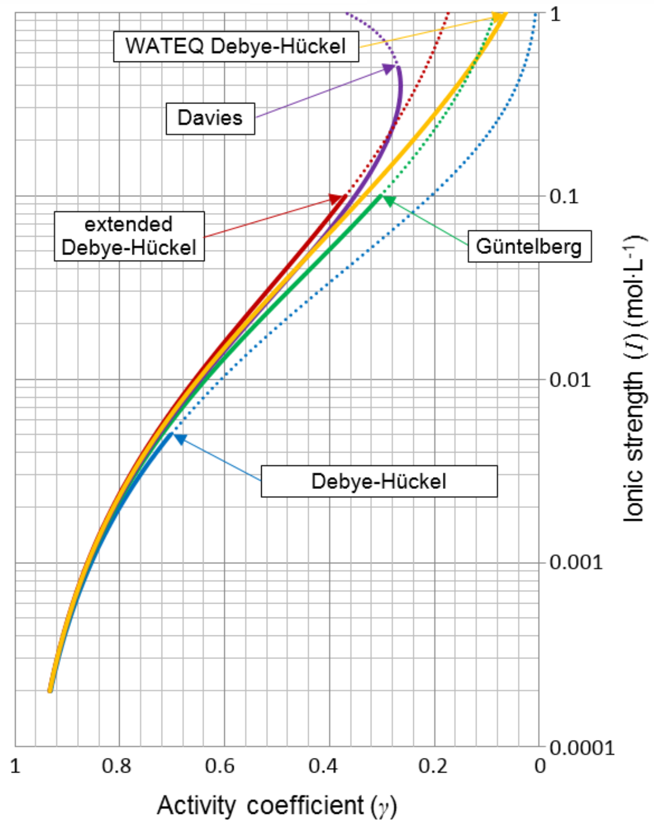
Level	Type	Model	Ionic Strength
1	Debye Hückel	$\log(\gamma_i) = -Az_i^2\sqrt{I}$	0–0.05
	Günterberg	$\log(\gamma_i) = -Az_i^2\left(\frac{\sqrt{I}}{1+1.4\sqrt{I}}\right)$	0–0.1
	Davies	$\log(\gamma_i) = -Az_i^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right)$	0–0.7
2	Extended Debye Hückel[1] (PHREEQC)	$\log(\gamma_i) = -Az_i^2\left(\frac{\sqrt{I}}{1+Bc_i\sqrt{I}}\right)$	0–0.5
	Extended Debye Hückel (WATEQ)[1] (also in PHREEQC)	$\log(\gamma_i) = -Az_i^2\left(\frac{\sqrt{I}}{1+Bc_i\sqrt{I}} - d_iI\right)$	0–1
4	SIT	$\log(\gamma_i) = -Az_i^2\left(\frac{\sqrt{I}}{1+B\sqrt{I}}\right) - \sum b_{ij}[S_j]$	>>1 Solubility limit for high solubility salts
	Pitzer[2]	Extends SIT for second- and higher-order interactions	>>1 Solubility limit for high solubility salts
N/A	Non-ionic species	$\log(\gamma_i) = d_iI$ $d_i \sim 0.1$	All

EFFECT ON ACTIVITY COEFFICIENTS? mono vs multivalent

monovalent: Na^{+}



multivalent: Mg^{2+}



Greater influence at higher ionic strengths.

Greater influence of multivalent ions.

CONCLUSIONS & PERSPECTIVES

Ionic strength influences pH in a plant-wide model.

Valency of ions affects the species distribution, and in turn affects plant-wide performance.

All acid-base and ion pairing equations and parameters are fundamental.

The acid-base and ion pairing model developed is generally applicable across the majority of the water and wastewater processes.

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THANK YOU FOR YOUR ATTENTION!

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RÉPUBLIQUE FRANÇAISE
Liberté
Égalité
Fraternité

INRAE

GAS/LIQUID MASS TRANSFER

Sylvie Gillot (sylvie.gillot@inrae.fr)
INRAE

A ubiquitous process

Many reactions depend on L/G or G/L mass transfer processes

Oxygen supply

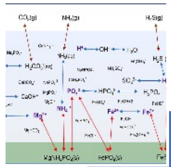
Key process

Energy intensive

GHG emissions

CH_4

N_2O



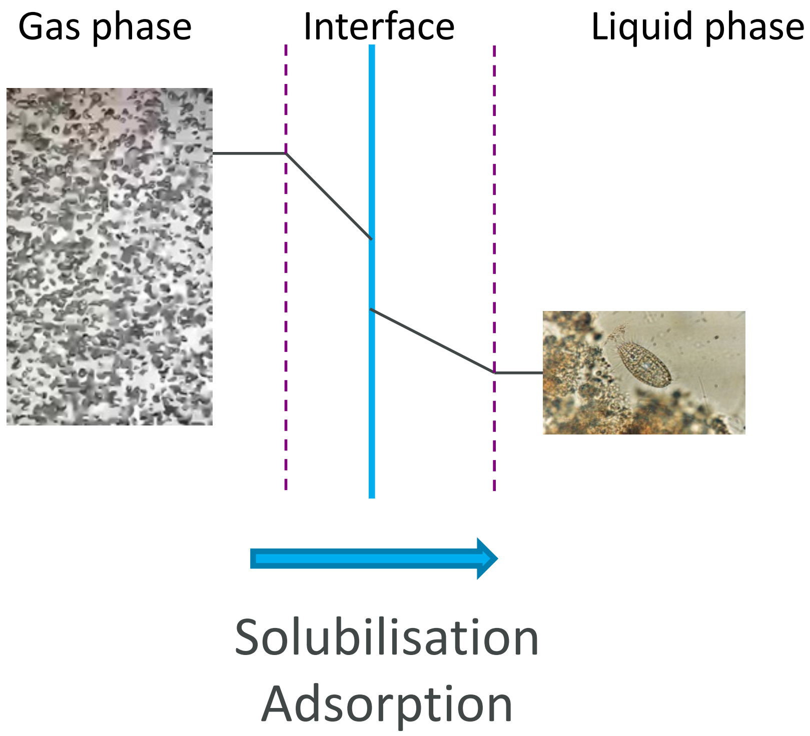
Liquid phase

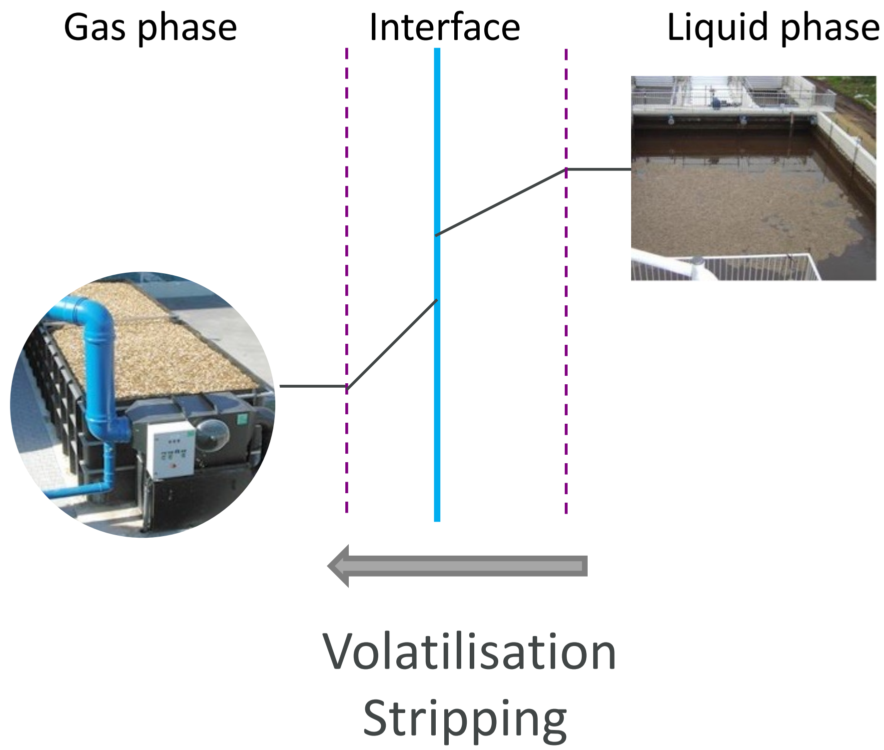
Acid-base equilibria

Inhibition

(O_2, H_2S, NH_3)

A few terms





Active ≠ passive gas exchange

Fundamentals

Ficks' first law – one phase

$$J_i = k\ \Delta[S_i]$$

the mass flux of i (J_i) diffusing in one direction is the product of a transfer coefficient by a concentration gradient

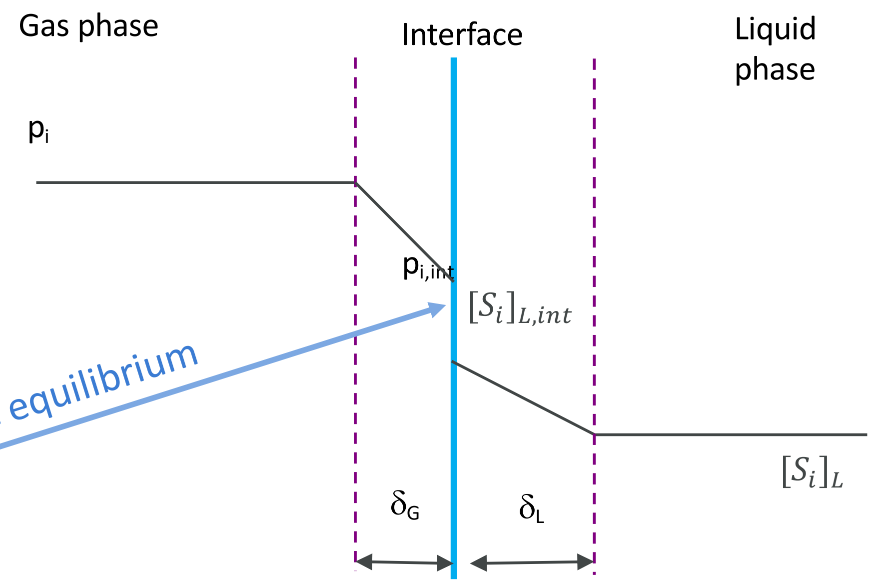
Henry's law

$$K_{H,i} = \frac{p_{i,int}}{\{S_i\}_{L,int}}$$

the activity of the dissolved gas i $\{S_i\}_L$ is proportional to its activity in the gas phase $p_{i,int}$

Thermodynamic equilibrium

Two-film theory – transfer through an interface



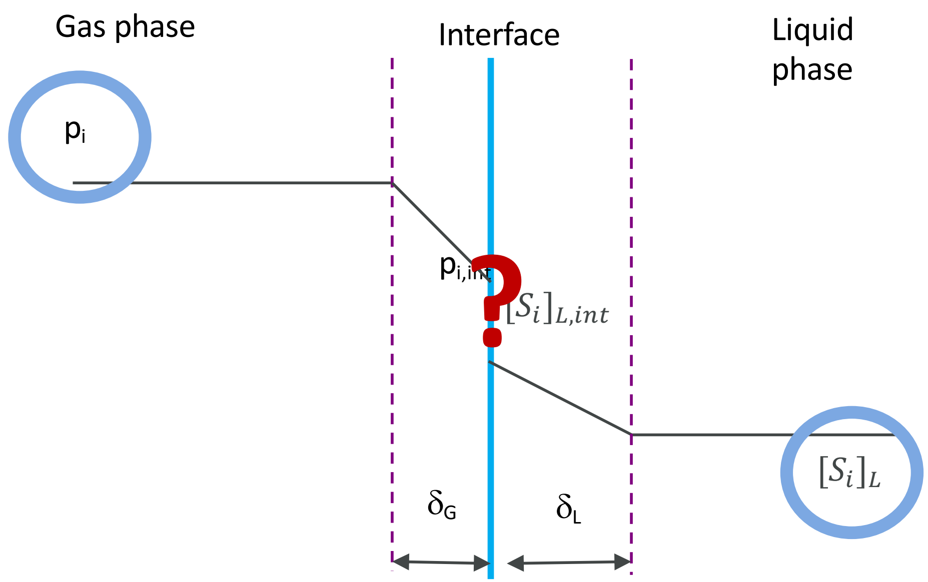
Lewis and Whitman (1924)

a thin layer of stagnant fluid exists on each side of the interface where diffusion takes place

Overall mass transfer coefficient

$$J^{\circ} = k_{ov,G}(p_i - p_i^*)$$

$$J^{\circ} = k_{ov,L}([S_i]_L{}^* - [S_i]_L)$$



$$\frac{1}{k_{ov,L}} = \frac{1}{k_L} + \frac{1}{\gamma_i K_H k_G}$$

Overall resistance to mass transfer

Resistance in the liquid film

Resistance in the gas film

Gas/Liquid mass transfer

Generalised expression of the mass transfer rate

$$r_{t,i} = k_{ov,L,i}\, a \left(\frac{p_i}{\gamma_i K_{H_i}} - [S_i]_L\right)$$

The overall liquid-side mass transfer coefficient

The concentration gradient
> 0 in case of gas solubilisation (absorption)
< 0 in case of gas volatilisation (stripping)

The interfacial area a = A/V_L

Gas/Liquid mass transfer

$$r_{t,i} = k_{ov,L,i}\, a\, \left(\frac{p_i}{\gamma_i K_{H_i}} - [S_i]_L\right)$$

The overall mass transfer coefficient

Empirical equations

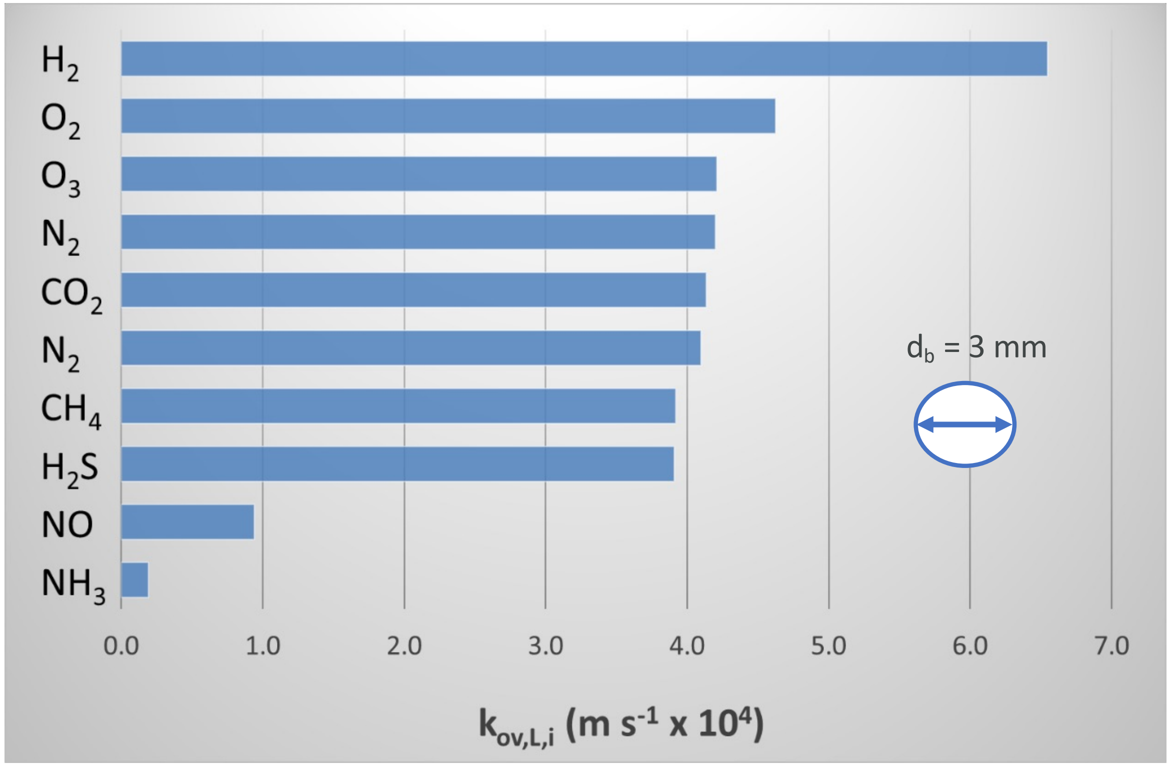
- Ex. Higbie (1935)

$$k_{L,i} = 2 \cdot \sqrt{\frac{D_{L,i} \cdot v_r}{\pi \cdot d_b}}$$

- Ex. Sharma & M (1968)

$$\mathrm{Sh_G} = \frac{k_{G,i} d_b}{D_{G,i}} = 6.58$$

$$\psi = \frac{k_{L,i}}{k_{L,j}} = \left(\frac{D_{L,i}}{D_{L,j}}\right)^n$$



Validity of the equations

Gas/Liquid mass transfer

$$r_{t,i} = k_{ov,L,i}\, a \left(\frac{p_i}{\gamma_i K_{H_i}} - [S_i]_L\right)$$

The overall mass transfer coefficient	The interfacial area	The concentration gradient

The overall mass transfer coefficient

Empirical equations

- Ex. Higbie (1935)

$$k_{L,i} = 2 \cdot \sqrt{\frac{D_{L,i} \cdot v_r}{\pi \cdot d_b}}$$

- Ex. Sharma & M (1968)

$$\mathrm{Sh_G} = \frac{k_{G,i} d_b}{D_{G,i}} = 6.58$$

$$\psi = \frac{k_{L,i}}{k_{L,j}} = \left(\frac{D_{L,i}}{D_{L,j}}\right)^n$$

The interfacial area

Passive gas exchange

$$a = \frac{A_{reactor}}{V_L}$$

Active gas exchange

$$a = \frac{6\epsilon_G}{(1-\epsilon_G)d_{bs}}$$

The concentration gradient

Liquid saturation concentration depends on:

- enrichment /depletion of gas in the bubbles
- Pressure (depth, open vs closed reactors)
- Chemical equilibrium composition

Validity of the equations

4 main cases

Active mass transfer

1

2

$$a = \frac{6\varepsilon_G}{d_b(1-\varepsilon_G)}$$

$$k_{ov,L,i} = k_{L,i} = \sqrt{\frac{4D_{L,i}.u}{\pi.d_b}}$$

$$k_{ov,L,i} = k_{G,i}K_{H,i} = \frac{6{,}58D_{G,i}}{d_b}K_{H,i}$$

Low gas solubility

+ Impact of pressure (closed reactors) and temperature

High gas solubility

O_2, N_2O, NO, CH_4, H_2, H_2S

NH_3

Aerobic conditions

$$k_{ov,L,i}a = k_{L,i}a = k_{L,O2}a\left(\frac{D_{L,i}}{D_{L,O2}}\right)^n$$

Anaerobic conditions

$$k_{ov,L,i}a = k_{L,i}a = k_{L,H2}a\left(\frac{D_{L,i}}{D_{L,H2}}\right)^n$$

Experimental determination of $k_{ovL,i}a$ required or use of a default value

3

4

$$a = \frac{A}{V_L}$$

Passive mass transfer

Adapted from Vaneeckhaute et al. (2018)

Oxygen transfer modelling

Clean water mass transfer coefficient

Activity correction

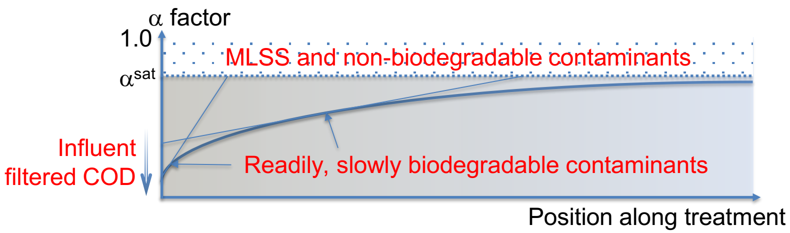
$$r_{t,O2} = \alpha F k_{ov,L,O2} a(20°C) \left(\beta \tau \Omega [O_2]^{*}_{L,20} - [O_2]_L \right) \theta^{T-20}$$

'Mysterious' alpha factor x fouling factor (F)

- Matrix dependent (surfactants, TSS)
- Reactor dependent (depth, velocity…)
- Dynamic behaviour

Water depth dependent

Adapted from Stenstrom & Gilbert (1981)



Bencsik et al., 2022

Thank you for your attention!

Chapter 4

Gas–liquid transfer

Sylvie Gillot[1], Eveline Volcke[2], Izarro Lizarralde[3], Youri Amerlink[4] and Damien J. Batstone[5]

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[3]University of Navarra, Manuel Lardizabal 15, 20018 Donostia/San Sebastián
[4]Aquafin NV, Belgium
[5]Australian Centre for Water and Environmental Biotechnology, The University of Queensland, St Lucia, Brisbane, QLD 4072, Australia

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Modelling Precipitation and Dissolution

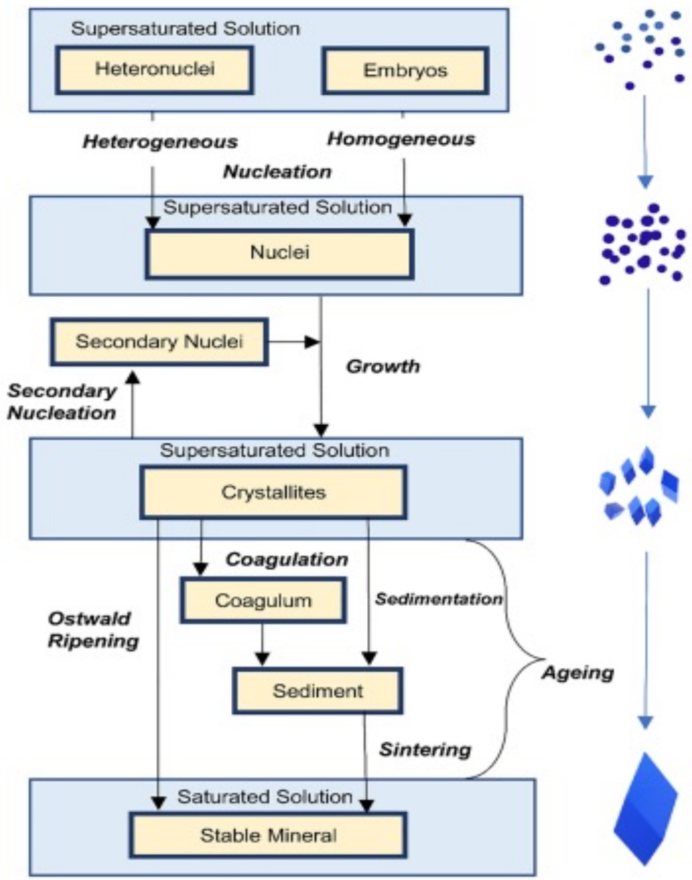
Christian Kazadi Mbamba, Paloma Grau, Stephan Tait, Xavier Flores-Alsina, Imre Takács and Damien J. Batstone

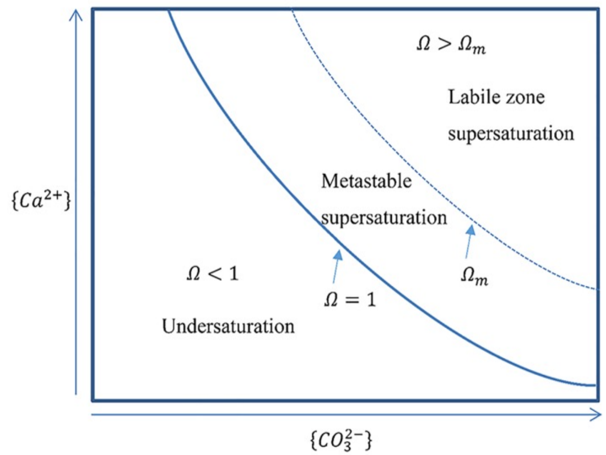
OVERVIEW OF **PRECIPITATION AND DISSOLUTION**

- Precipitation refers to the formation of a solid from solutes in a supersaturated solution under certain conditions.
- Precipitates may be amorphous or crystalline.
- Amorphous precipitates lack regular crystalline structure.
- Crystalline precipitates have a crystal structure.
- Solubility and equilibrium in precipitation

MECHANISMS OF MINERAL FORMATION

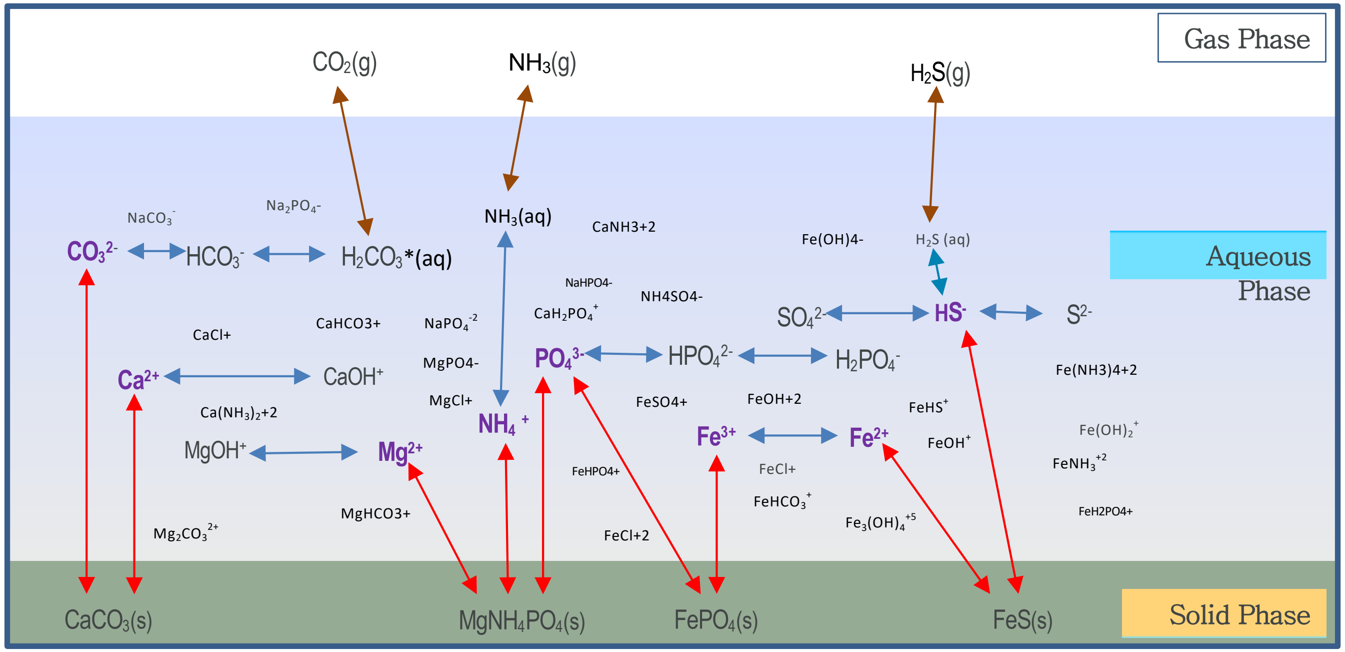
- Nucleation
- Metastability
- Particle growth
- Ageing





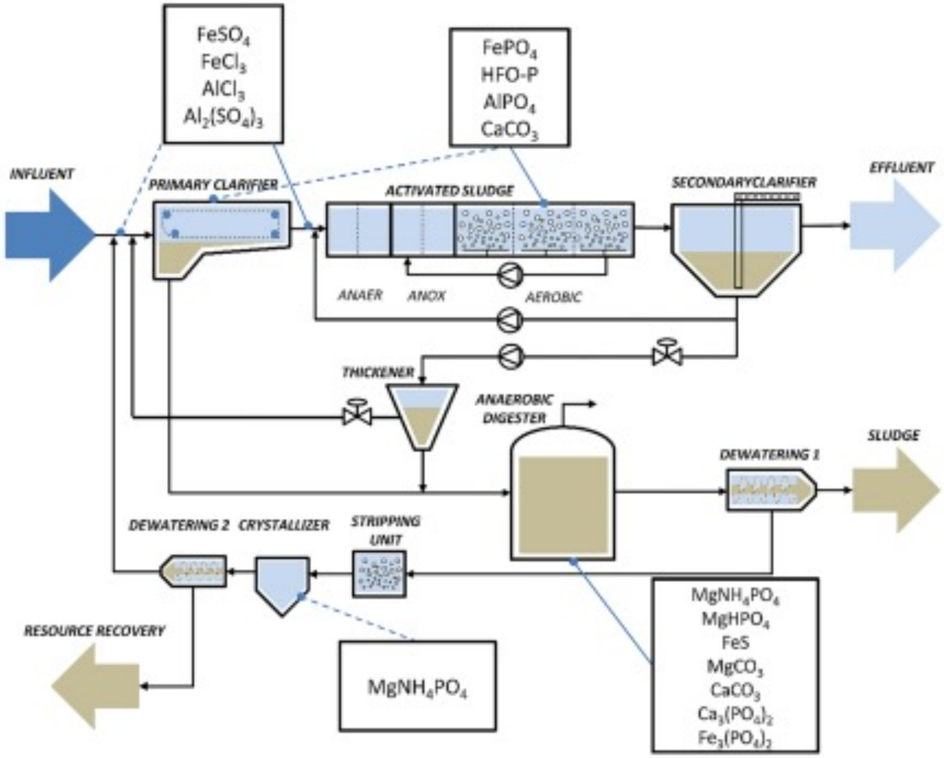
FACTORS AFFECTING MINERAL PRECIPITATION

- Saturation extent - SI
- pH
- Mixing liquid shear
- Temperature
- Impurities



TYPES OF MINERALS IN WASTEWATER

- Calcium and magnesium carbonates and phosphates



MODELLING APPROACHES

- General framework

$$SI = \log_{10}\left(\frac{S_{(\mathrm{Ca}^{2+})} \times S_{(\mathrm{CO}_3^{2-})}}{K_{\mathrm{sp,calcite}}}\right)$$

$SI < 0$ Solution is undersaturated

$SI = 0$ Solution is saturated

$SI > 0$ Solution is supersaturated

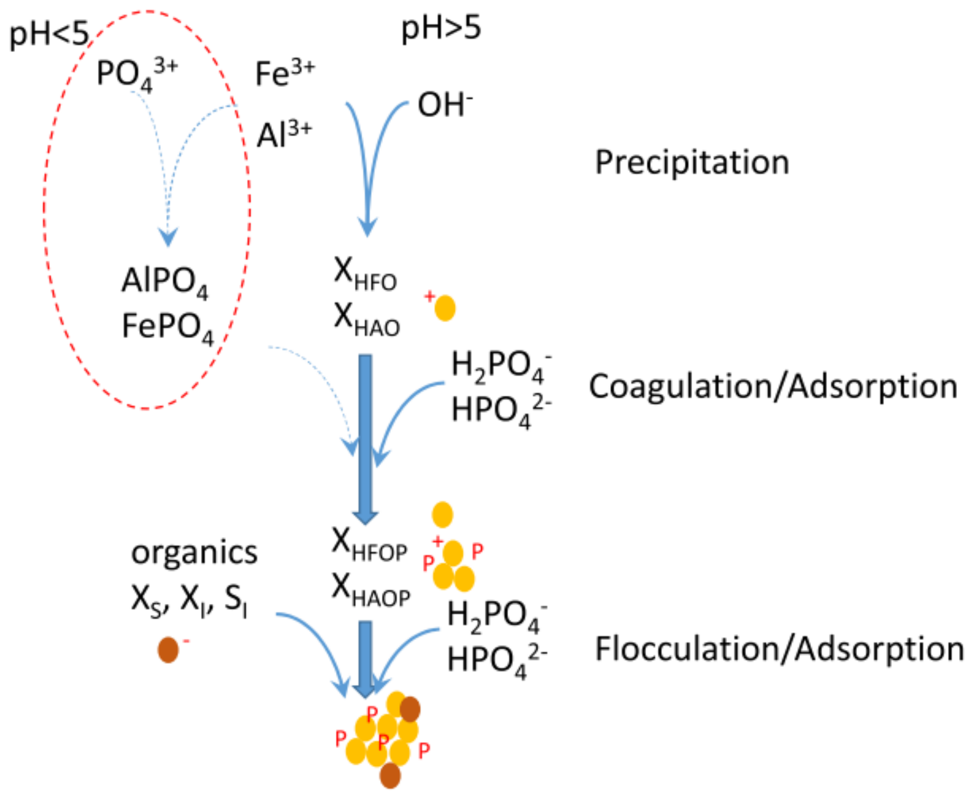
- Chemical phosphorus removal
  - Precipitation
  - Coagulation/Adsorption
  - Flocculation/Adsorption

$$\sigma = \left(\frac{(a_{Ca^{2+}})(a_{CO_3^{2-}})}{K_{sp,\,CaCO_3\,(s)}}\right)\text{-1}$$

$$R_{crys} = k_{crys} X_{crys} \sigma^{n}$$

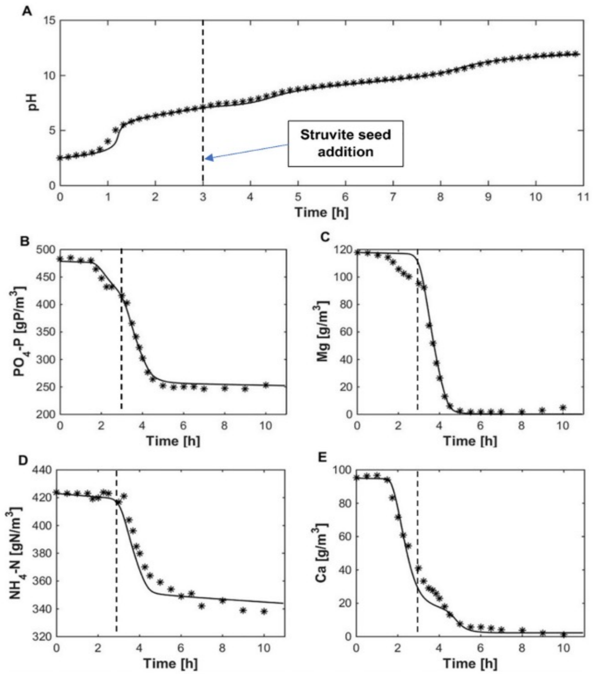
TYPES OF MINERALS IN WASTEWATER

- Iron and aluminum phosphates and sulfides



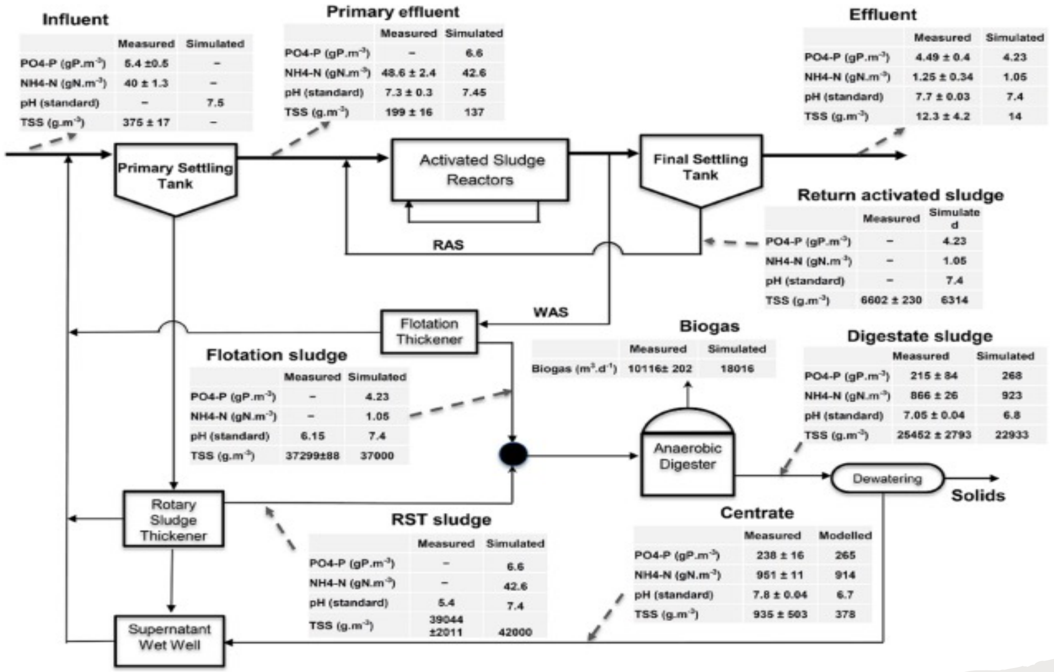
CASE STUDIES

- Case study 1: Ca–Mg–PO4
  - Model validation using titration
  - Increase in pH led formation of precipitates
  - Minerals: Struvite, DCPD, ACP
  - Nonlinear optimization technique to determine kinetic rates



CASE STUDIES

- Case study 2: application of the PCM to a full-scale municipal WWTP



CONCLUSION

- Precipitation has been investigated by multiple groups with focus on different mineral groups.
- Approach is consistent across conventional treatment units
- Largely equilibrium driven in terms of including a supersaturation driving force based on speciation in the aqueous liquid phase
- Model is identifiable: minimal number of parameters.
- Minerals could be classed as rapidly forming, moderately forming and slow forming.
- Nutrient and resource recovery is an emerging area of mineral precipitation modelling.

AGENDA AND HOUSEKEEPING

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Kimberly Solon (Ghent Uni., Belgium)

Speaker 2
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Speaker 3
Damien Batstone (Uni. Queensland, Australia)

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Speaker 5
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Q&A Session Moderator: *Damien Batstone (Uni. Queensland, Australia)*

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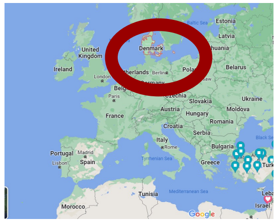
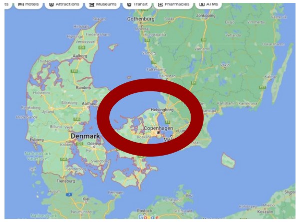
Application of the PCM1 to predict the perfomance of an industrial wastewater treatment plant

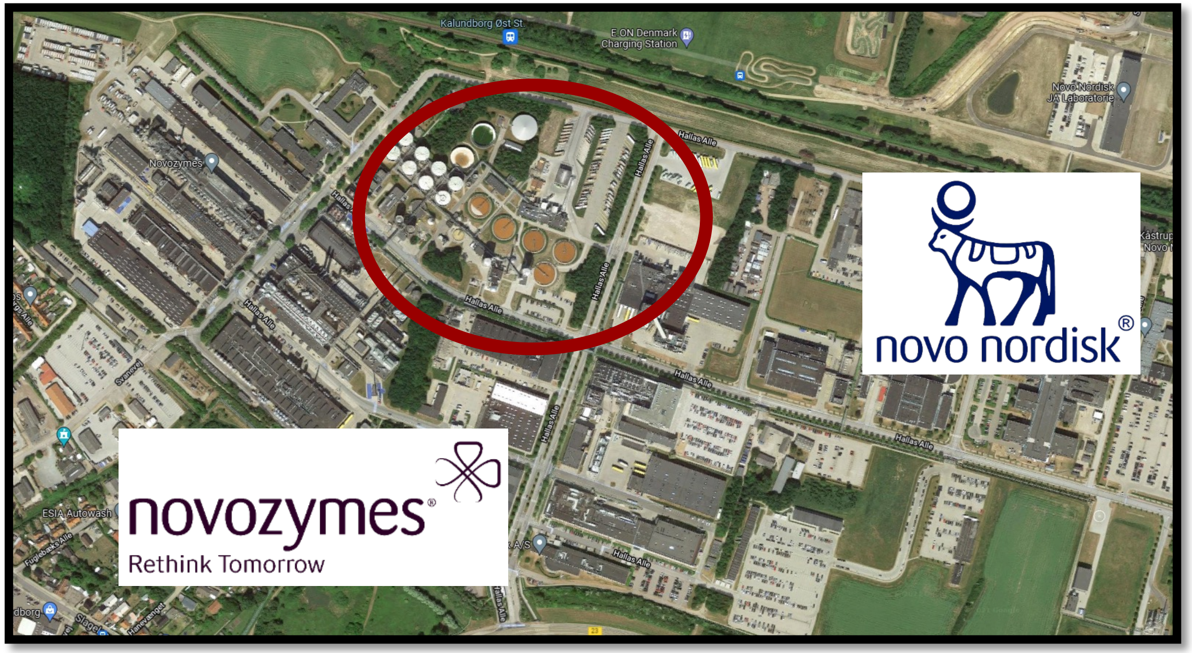
Xavier Flores-Alsina

Process and Systems Engineering Centre (PROSYS), Department of Chemical and Biochemical Engineering, Technical University of Denmark.

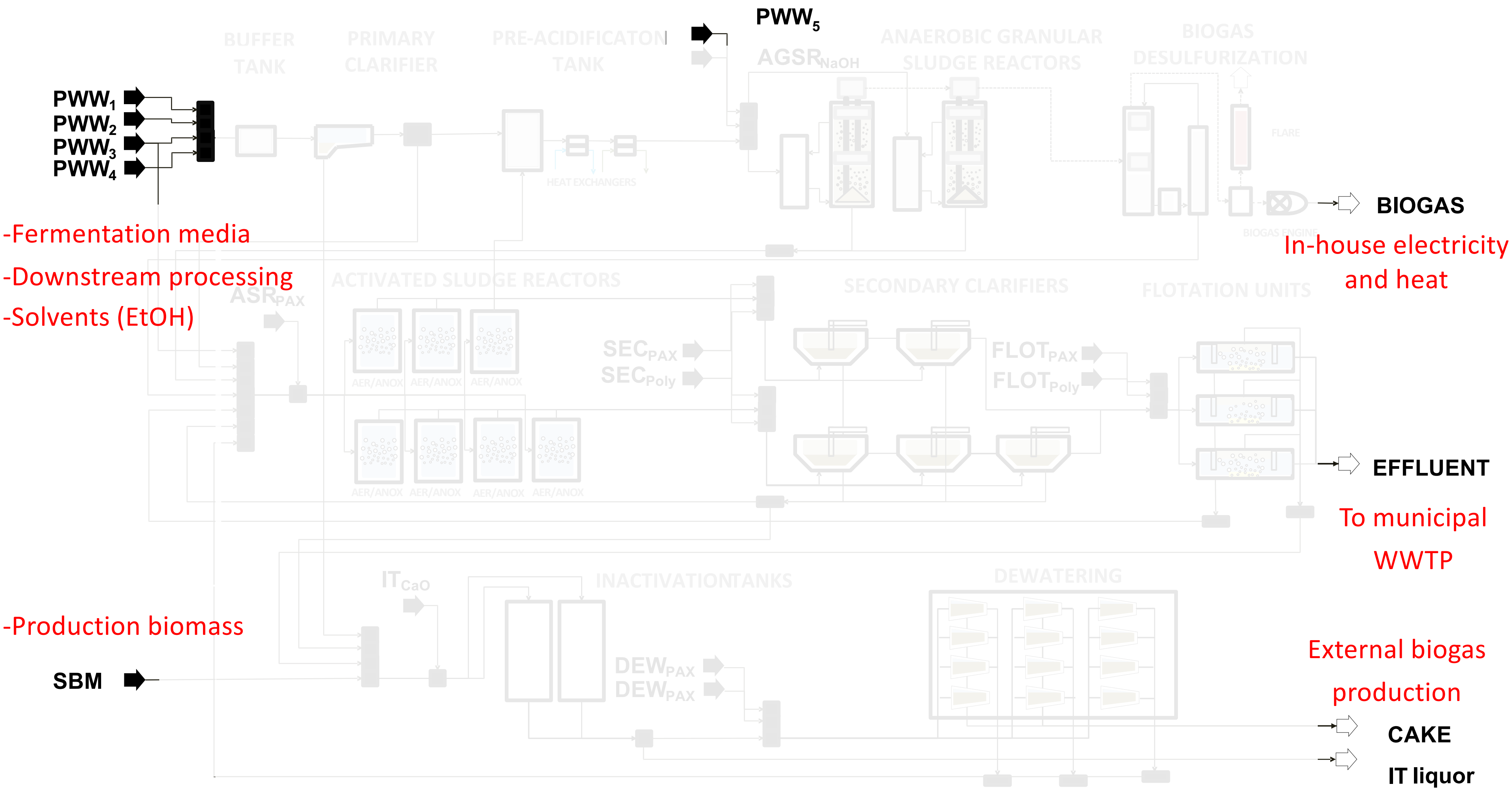
INTRODUCTION TO A MODELLING CASE STUDY



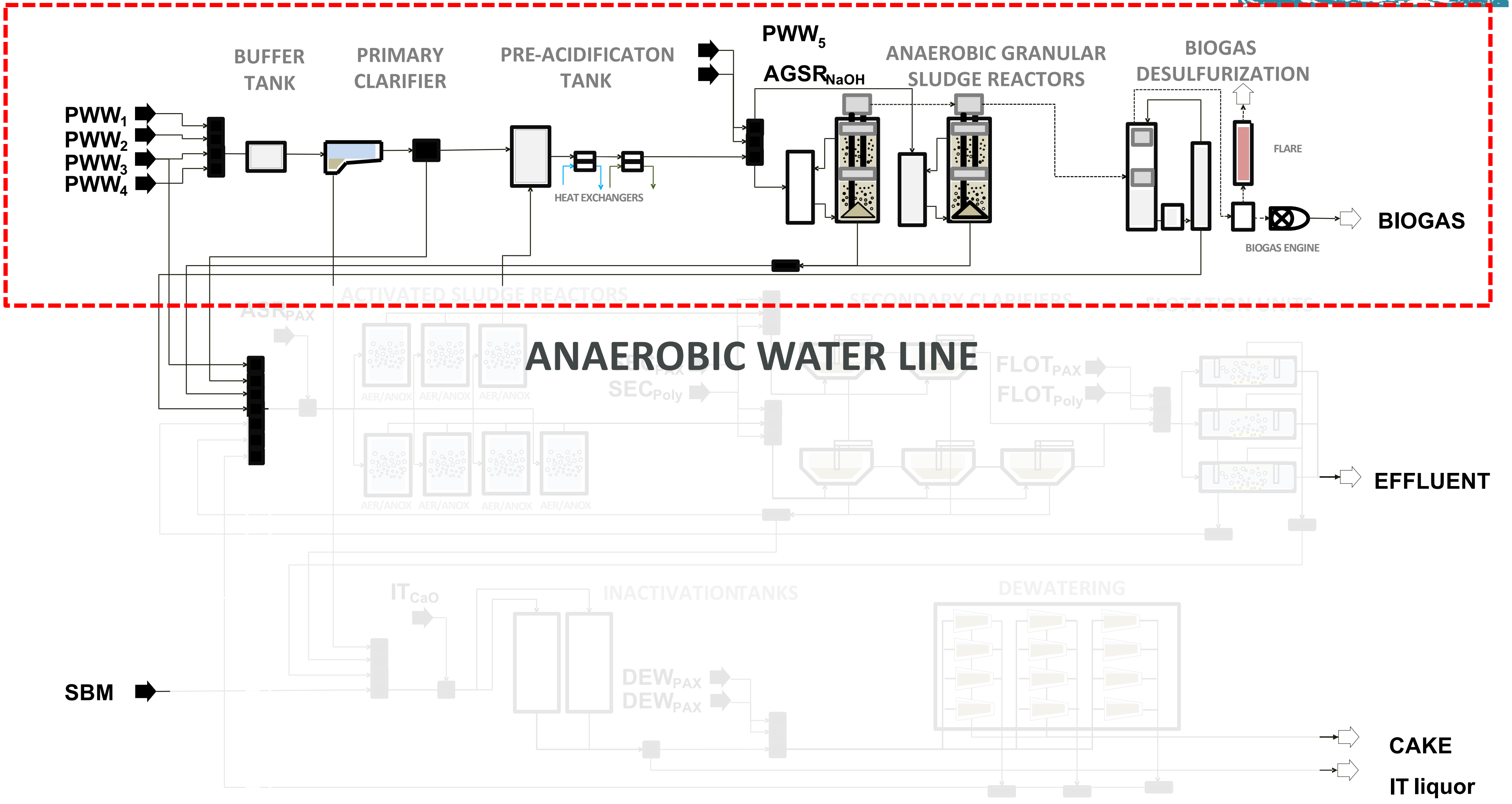




- Largest industrial wastewater treatment plant of Northern Europe
- **2.5 mill PE (in load) in 10,000 m^3/d**
- Sustained increase in capacity demand
- Integrated in Kalundborg’s industrial cluster



PWW5
BUFFER TANK
PRIMARY CLARIFIER
PRE-ACIDIFICATON TANK
AGSR NaOH
ANAEROBIC GRANULAR SLUDGE REACTORS
BIOGAS DESULFURIZATION
PWW1
PWW2
PWW3
PWW4
HEAT EXCHANGERS
FLARE
BIOGAS ENGINE
BIOGAS
-Fermentation media
-Downstream processing
-Solvents (EtOH)
In-house electricity and heat
ASR PAX
ACTIVATED SLUDGE REACTORS
SECONDARY CLARIFIERS
FLOTATION UNITS
SEC PAX
SEC Poly
FLOT PAX
FLOT Poly
AER/ANOX
EFFLUENT
To municipal WWTP
IT CaO
INACTIVATIONTANKS
DEWATERING
DEW PAX
DEW PAX
-Production biomass
SBM
External biogas production
CAKE
IT liquor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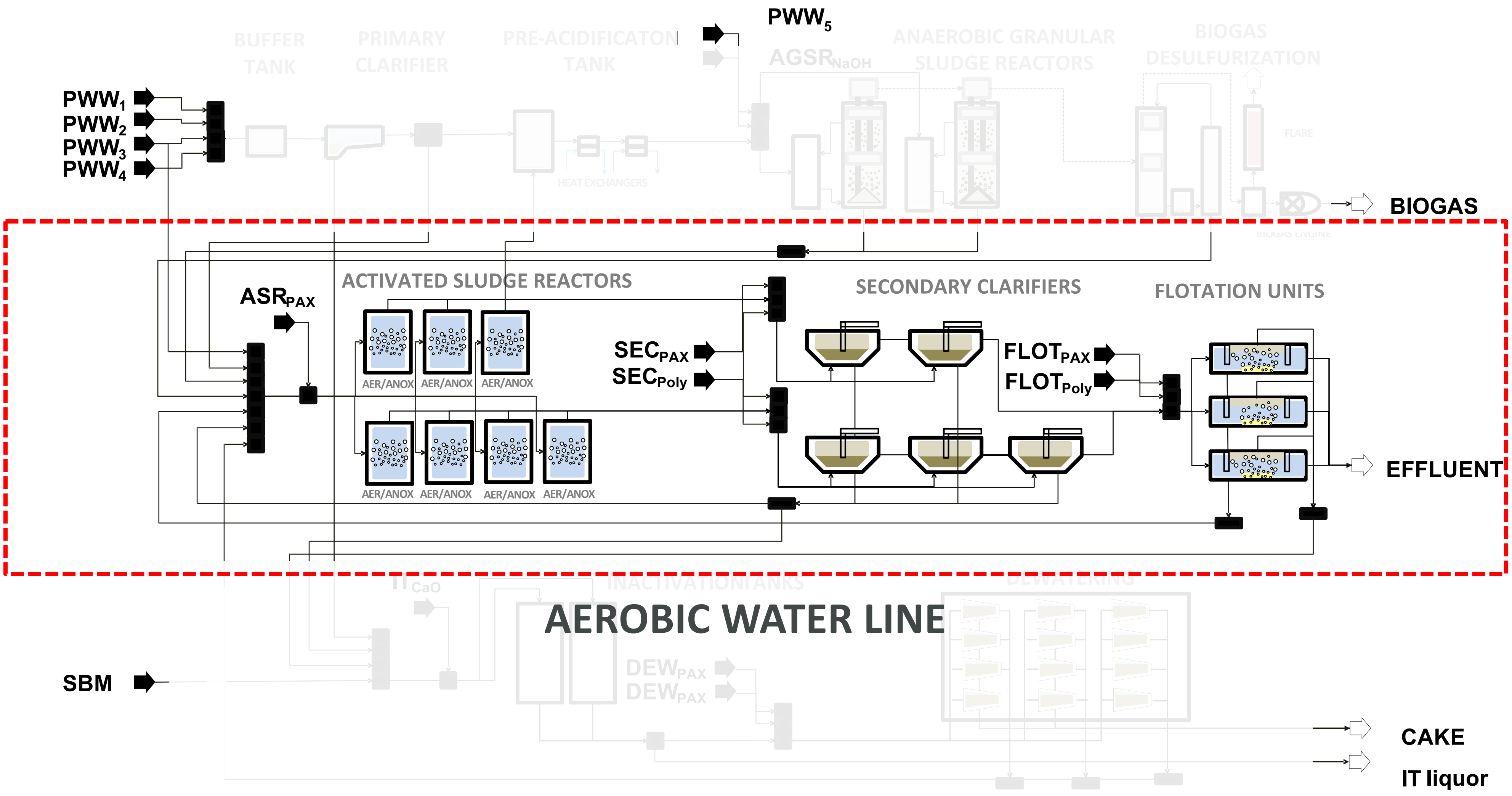
BIOGAS
BIOGAS ENGINE
ANAEROBIC WATER LINE
EFFLUENT
SBM
CAKE
IT liquor



PWW$_5$
AGSR$_{NaOH}$
BUFFER TANK
PRIMARY CLARIFIER
PRE-ACIDIFICATON TANK
ANAEROBIC GRANULAR SLUDGE REACTORS
BIOGAS DESULFURIZATION
PWW$_1$
PWW$_2$
PWW$_3$
PWW$_4$
HEAT EXCHANGERS
FLARE
BIOGAS
ASR$_{PAX}$
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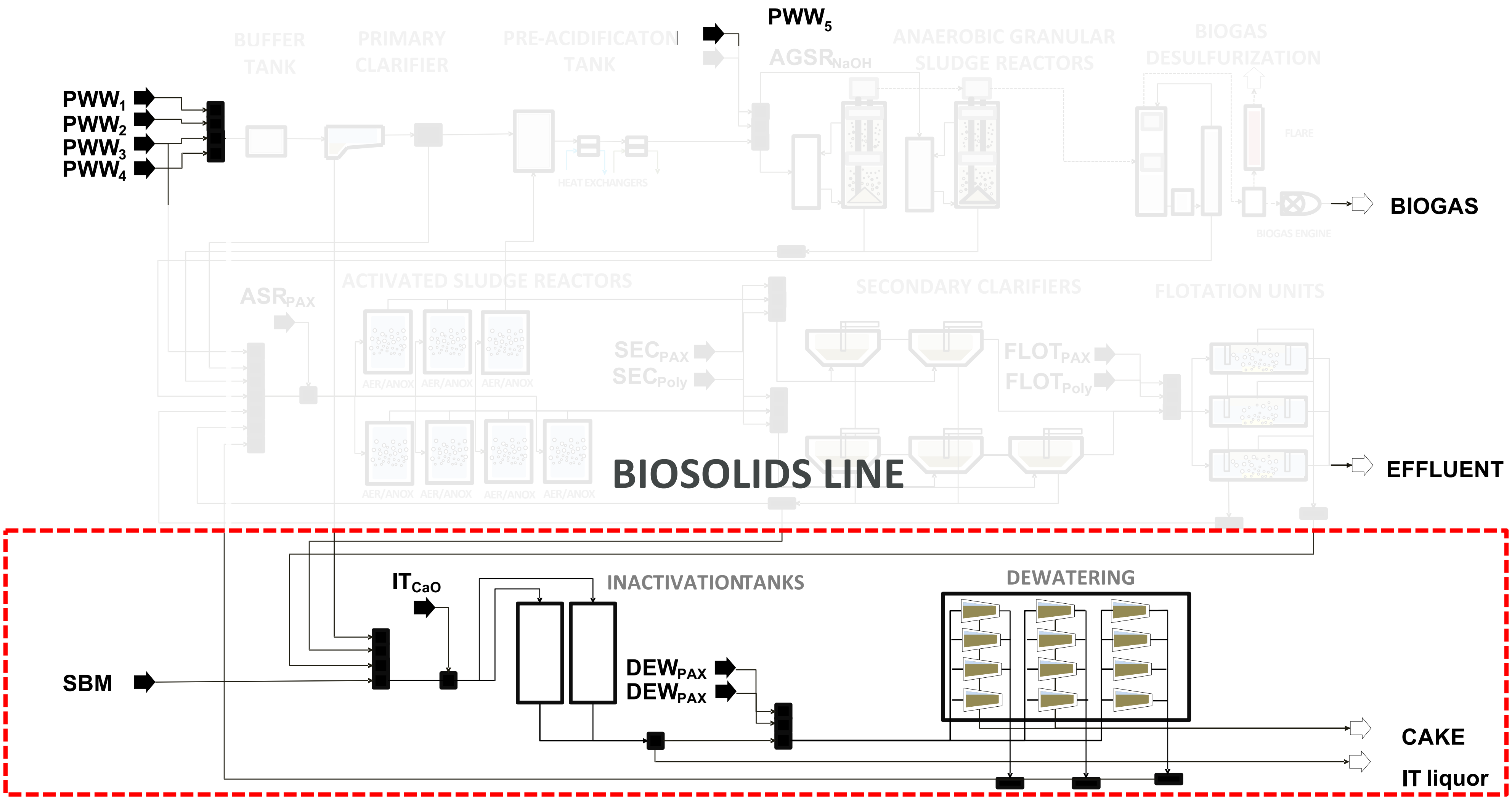
IT liquor


PWW1
PWW2
PWW3
PWW4
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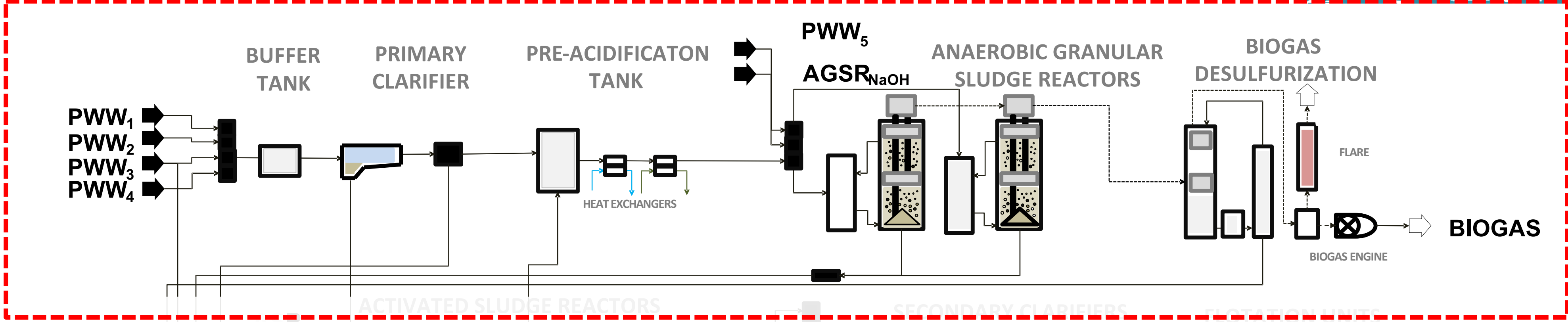
https://www.sciencedirect.com/science/article/pii/S1385894722022690



ANAEROBIC WATER LINE

BUFFER TANK

- pH prediction
- Ion speciation
- Ca-P precipitation

PAT

- pH prediction
- Ion speciation
- G-L transfer (H_2, N_2, CO_2)

AnGSR

- pH prediction
- Ion speciation
- G-L transfer (H_2, CH_4, CO_2 and H_2S)
- $CaCO_3$ precipitation

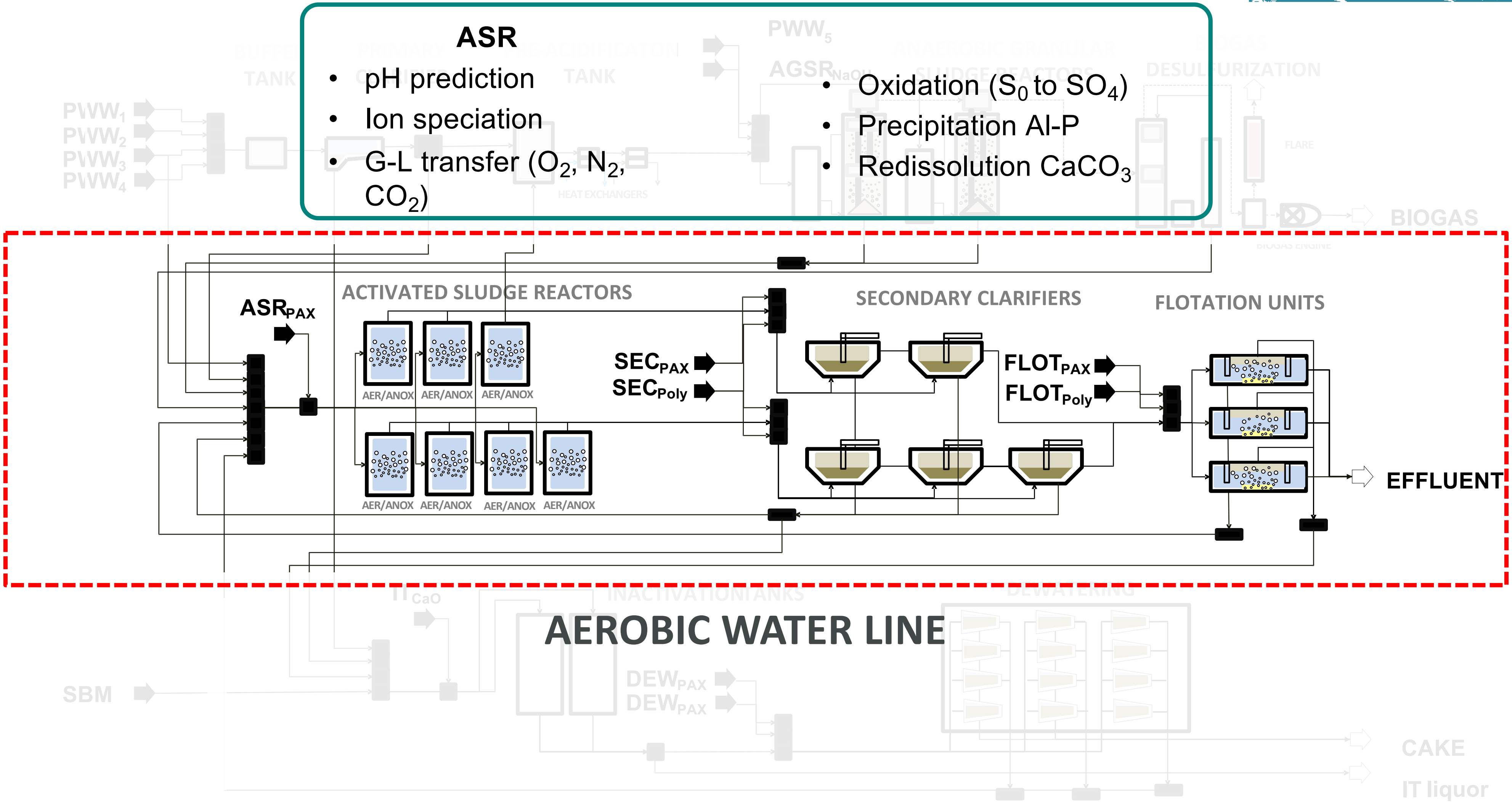
BDT

- pH prediction
- Ion speciation
- G-L transfer (H_2S absorption on NaOH)
- Oxidation (H_2S conversion to S_0)

ASR

- pH prediction
- Ion speciation
- G-L transfer (O_2, N_2, CO_2)

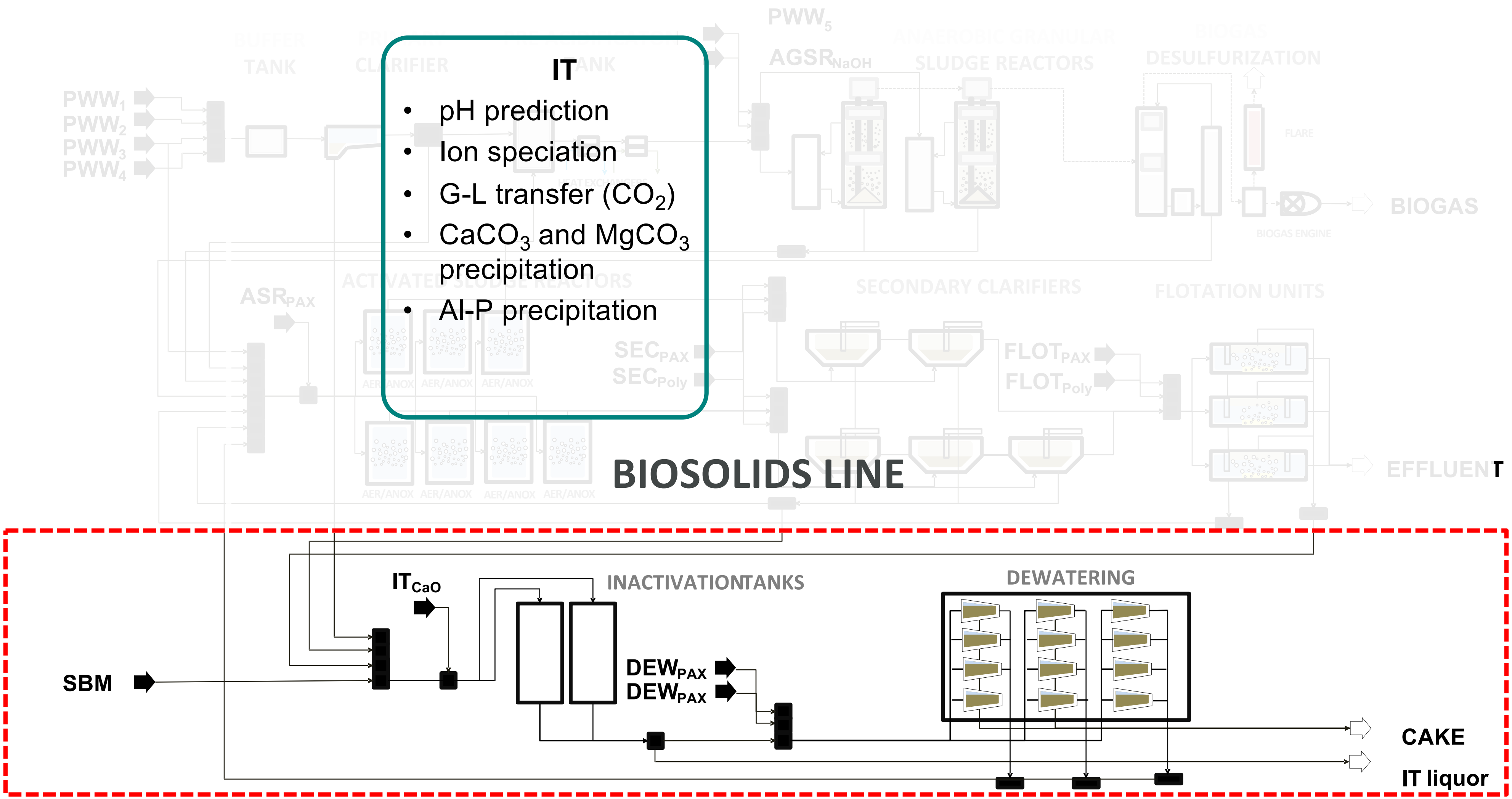
- Oxidation (S_0 to SO_4)
- Precipitation Al-P
- Redissolution $CaCO_3$



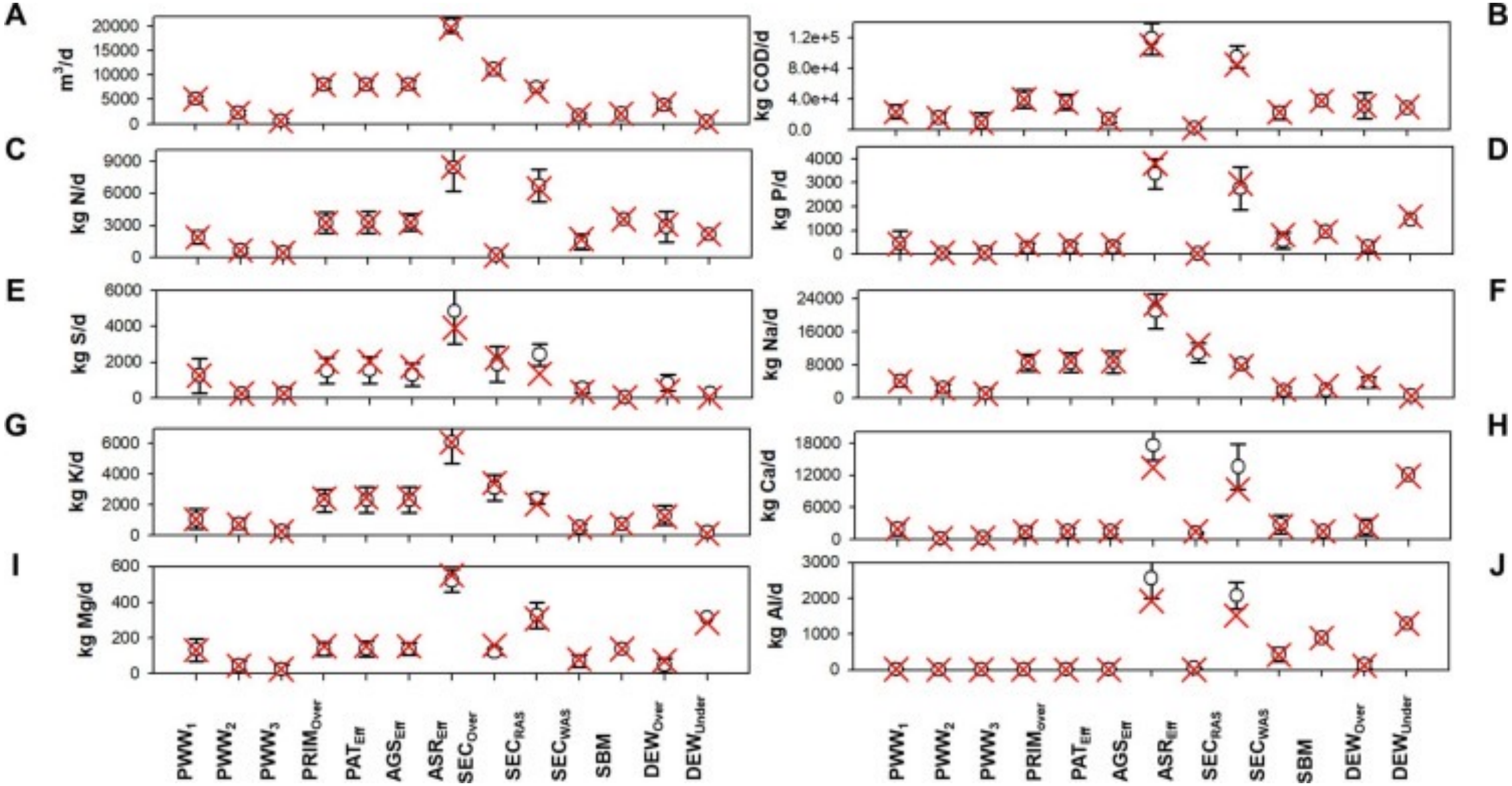
IT

- pH prediction
- Ion speciation
- G-L transfer (CO_2)
- $CaCO_3$ and $MgCO_3$ precipitation
- Al-P precipitation

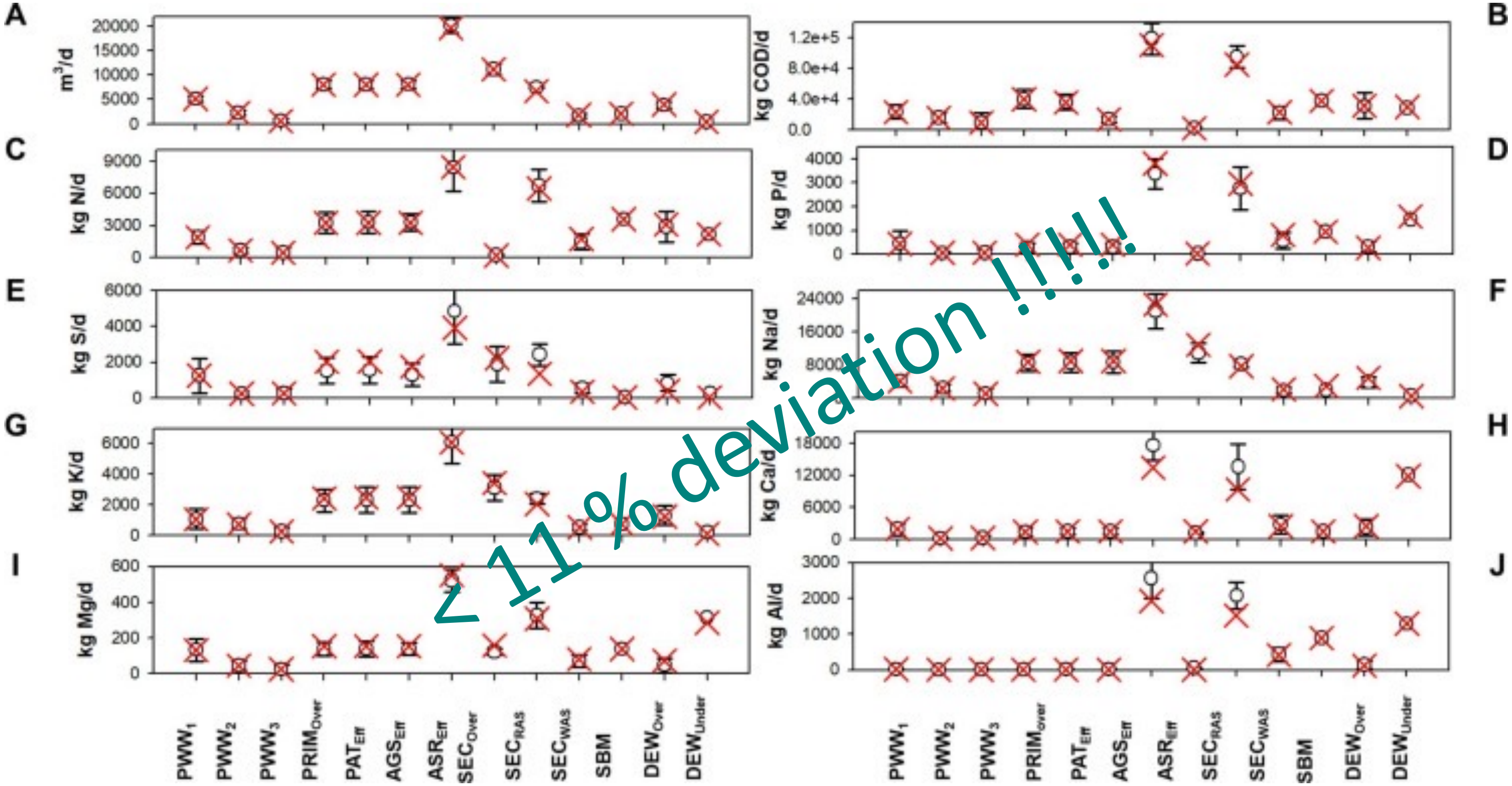
BIOSOLIDS LINE



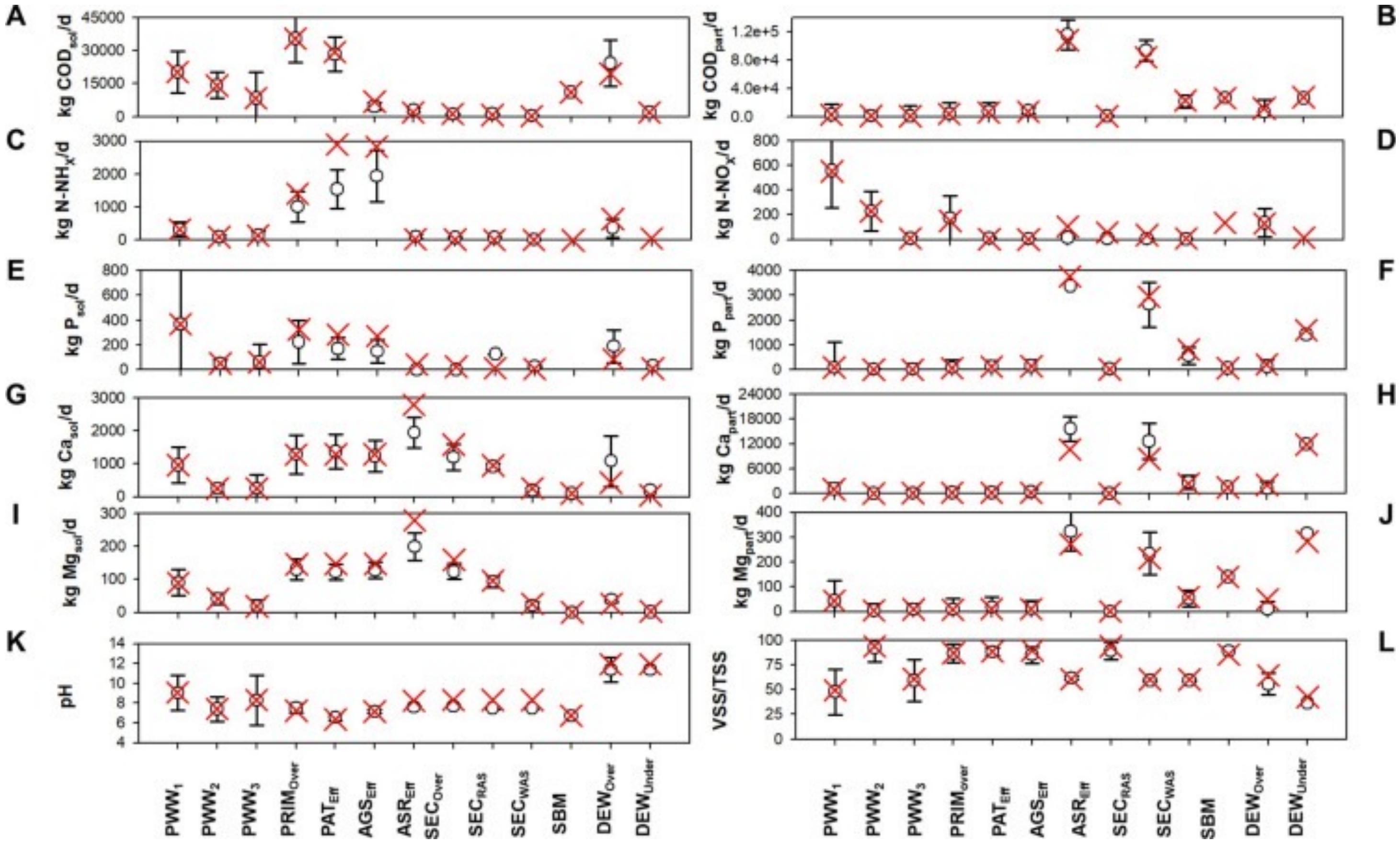
Steady state results: prediction of total loads



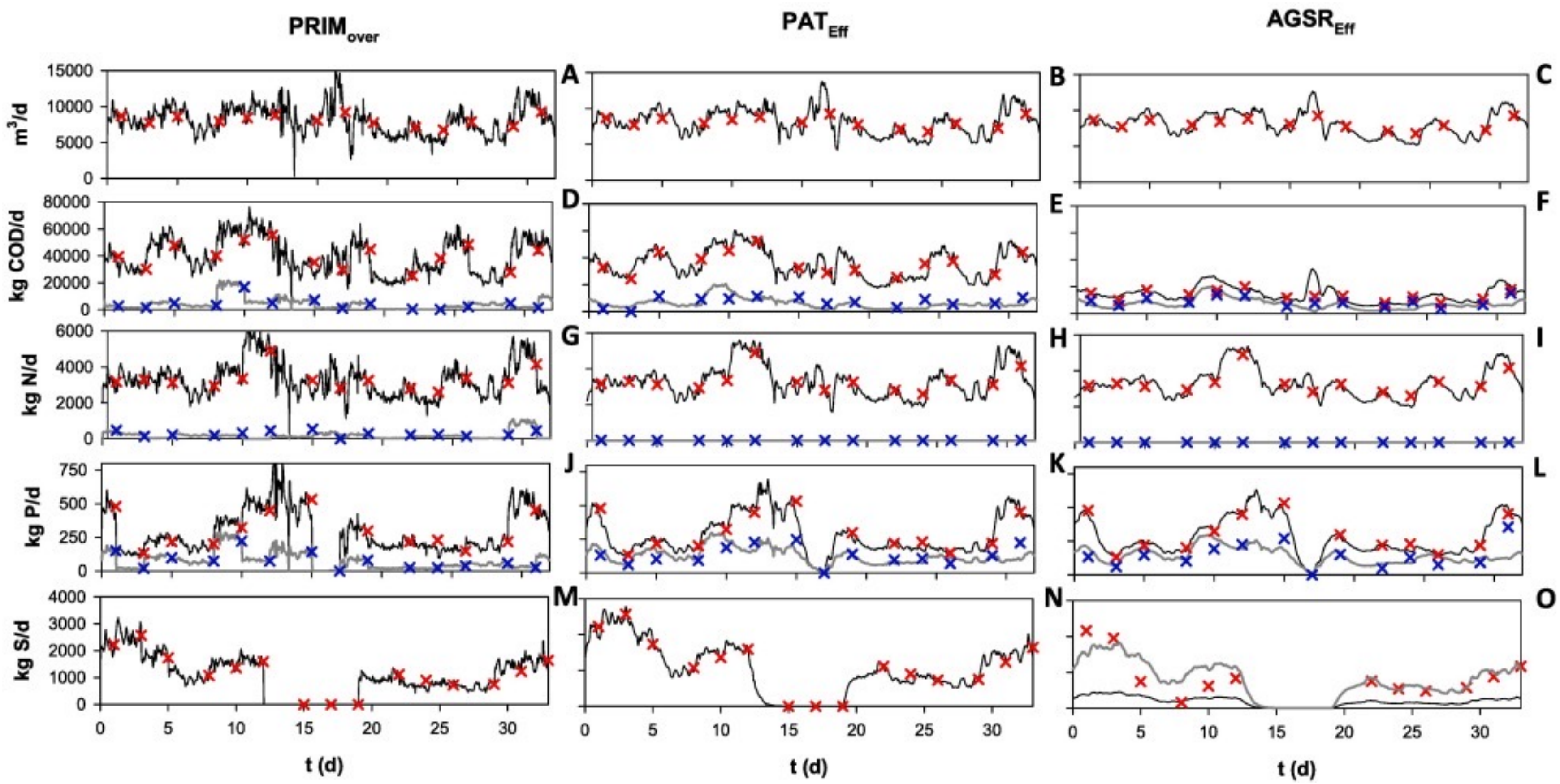
Steady state results: prediction of total loads



Steady state results: S, X, pH and VSS/TSS ratio

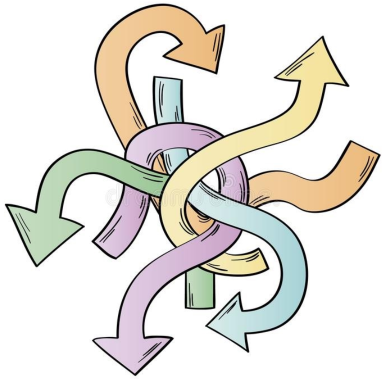


Dynamic state results



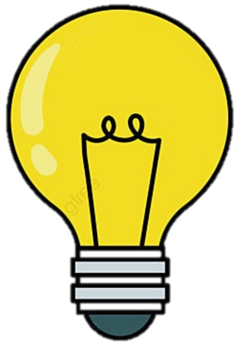
Optimization scenarios

Refluxing

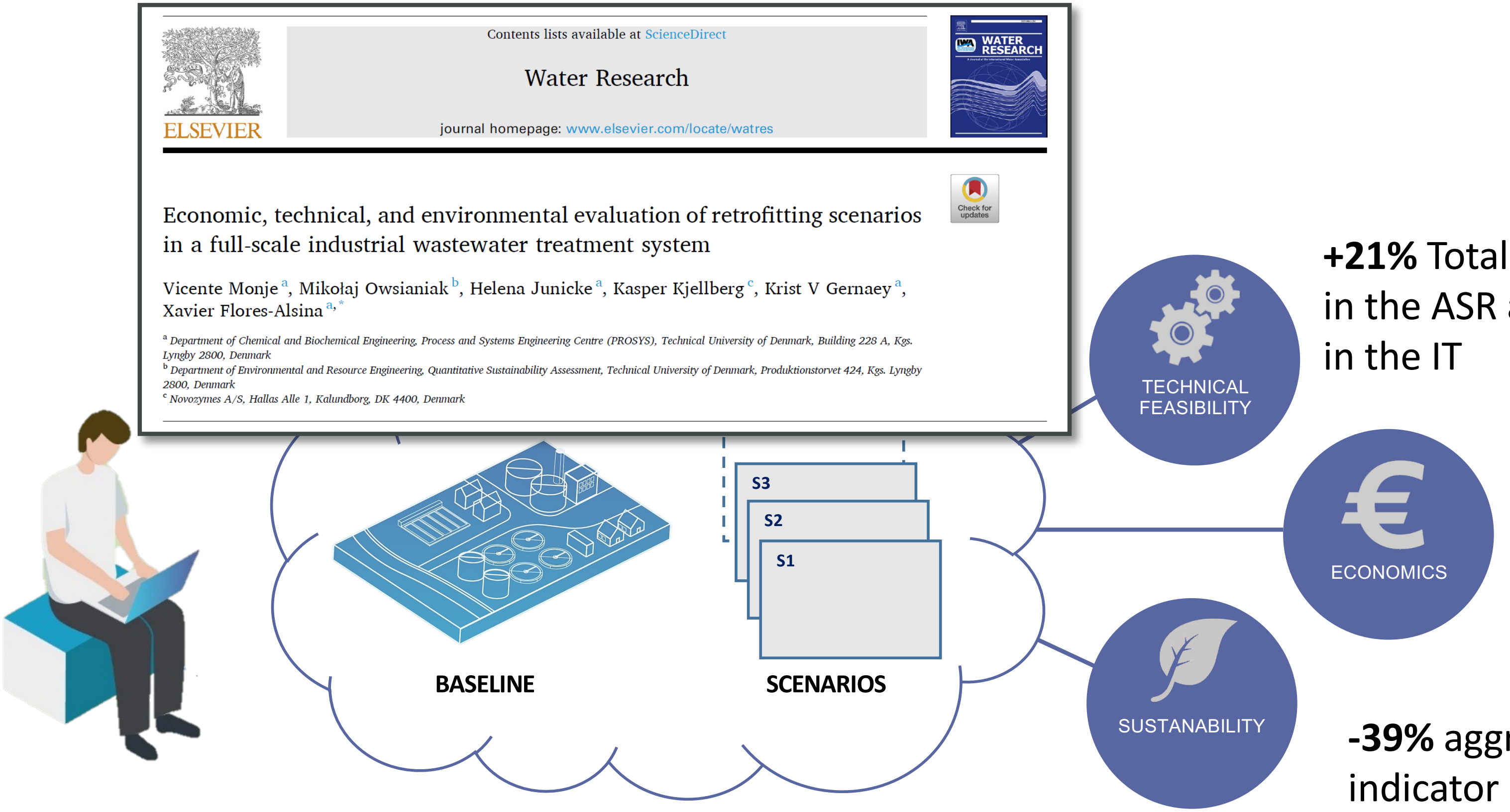


Operation Conditions

New Technology



Why modeling?



+21% Total Capacity in the ASR and **50 %** in the IT

-47% OPEX

-39% aggregated indicator used in LCA

CONCLUSIONS

- Key aspect → Commitment from academia and indus
  - ✓ Man power
  - ✓ Budget
  - ✓ Availability
- Measuring campaign was crucial (flow proportional s
  soluble inorganics)
- Traditional WWTP models are based on biology (but PCM is important too)
- Most of the economic related criteria were quantified using the PCM1 (energy recovery, energy consumption, use of chemicals….)
- Plant-wide models open the door for predicting mass and energy fluxes
  - ✓ Capacity
  - ✓ OPEX
  - ✓ Sustainability


Senior researcher
Xavier Flores Alsina


Professor
Krist V. Gernaey


Professor
Damien Batstone


Sr. Technology Manager
Dr. Kasper Kjellberg


Process. Engineer
Per Nobel

DTU CHEMICAL ENGINEERING
PROSYS Centre

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Linkedin:
Vicente Monje López

FBM grant number: NNF17SA0031362

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MODEL-BASED OPTIMISATION OF P MANAGEMENT STRATEGIES IN A REAL WWTP

Tamara Fernández-Arévalo

tfernandez@ceit.es

Researcher at ceit MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

LA SUR WWPT

OBJECTIVE OF THE STUDY:

Model-based scenario analysis to assess the maximum amount of struvite that can be recovered in a real WWTP + analysis of the benefits on plant operation.

- The SUR WWTP is the **largest** WWTP in Spain.
- **3 million PE** (load) for a flow of **518,400 m3/d**.
- **COD and P removal** (AO configuration)

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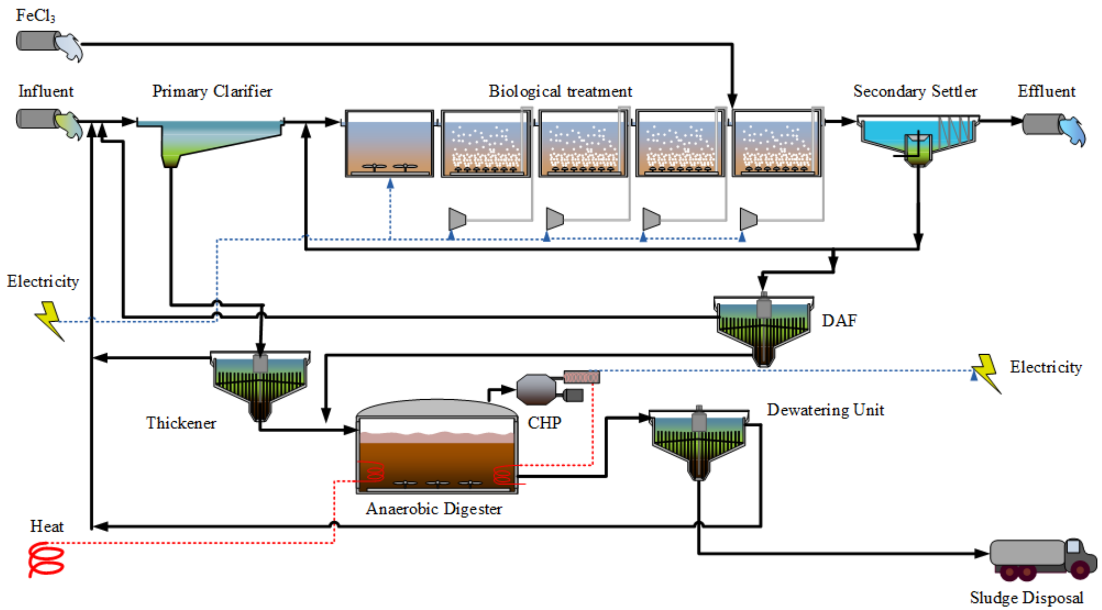
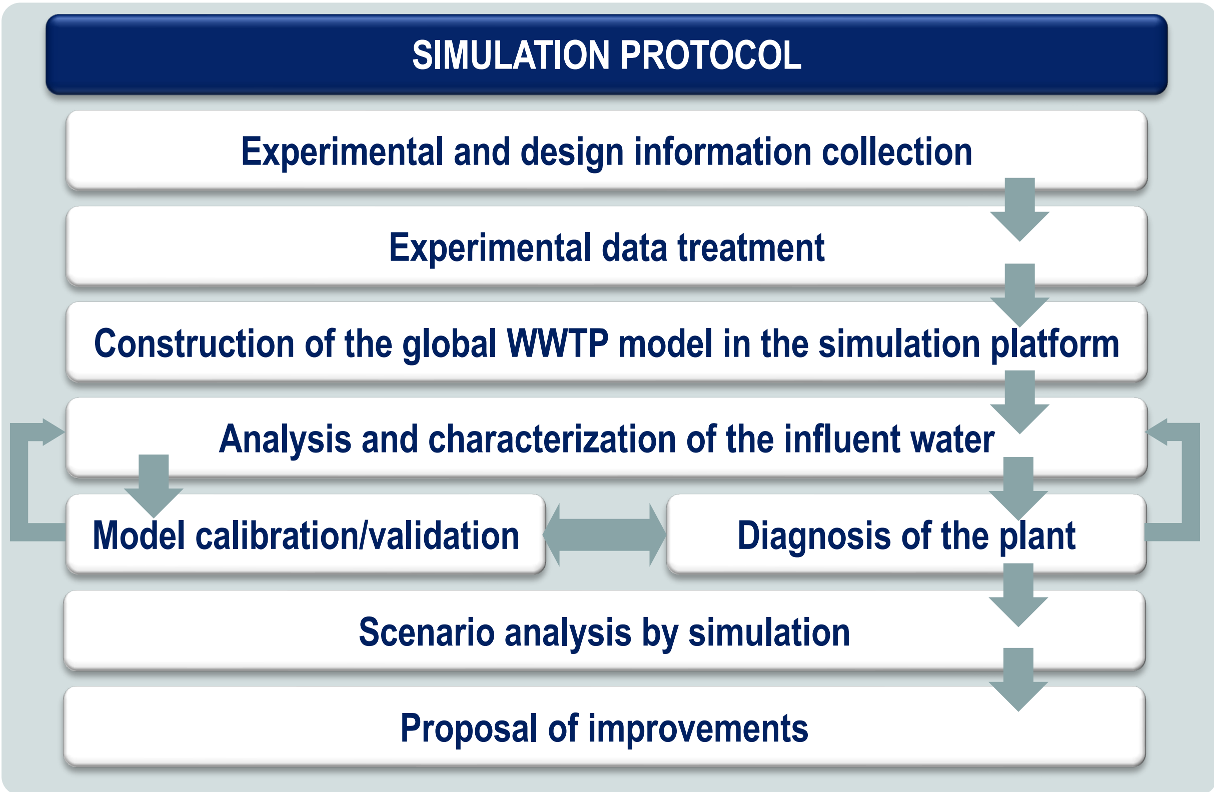


* Configuration of the year 2016

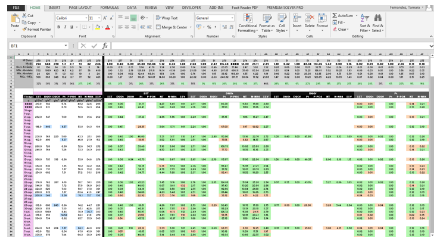
- The SUR WWTP is the **largest** WWTP in Spain.
- **3 million PE** (load) for a flow of **518,400 m3/d**.
- **COD and P removal** (AO configuration) **+ AD** *

SIMULATION PROTOCOL

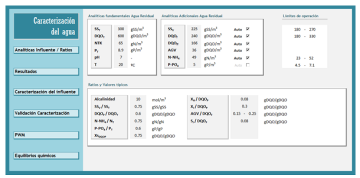
The key to carry out a correct simulation study is to follow simulation guidelines based on a high **methodological rigor** and an **appropriate modelling tools.**



Tools for detecting inconsistent data



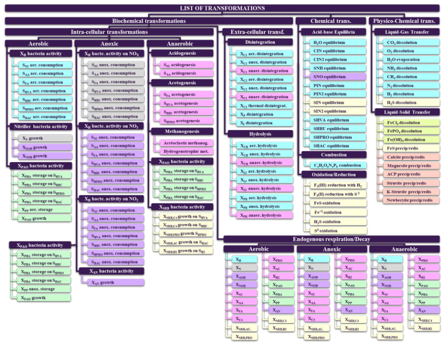
Influent characterization tools and tools for complete influent measures



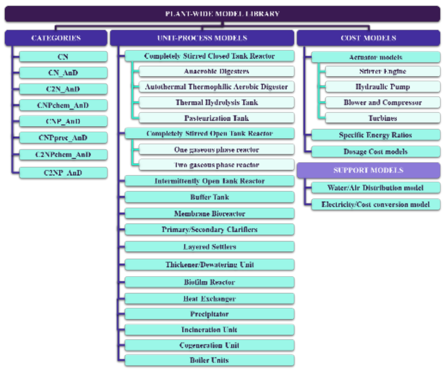
PLANT MODEL

The model used is based on the **Plant-Wide Modelling (PWM)** methodology proposed by Ceit (Grau *et al.,* 2007; Fernández-Arévalo *et al.,* 2014; Lizarralde *et al.,* 2015).

LIST OF TRANSFORMATIONS



UNIT-PROCESS MODELS



BIOCHEMICAL REACTIONS

Biological **organic matter, P and N removal transformations** under different environmental conditions (**aerobic, anoxic and anaerobic**).

PHYSICOCHEMICAL TRANSFORMATIONS

CHEMICAL TRANSFORMATIONS

Weak acid-base and complex ion-pairing equilibrium reactions between VFAs, inorganic C, N, P, Ca, Mg, K, Fe3+, Fe2+, Na and Cl.

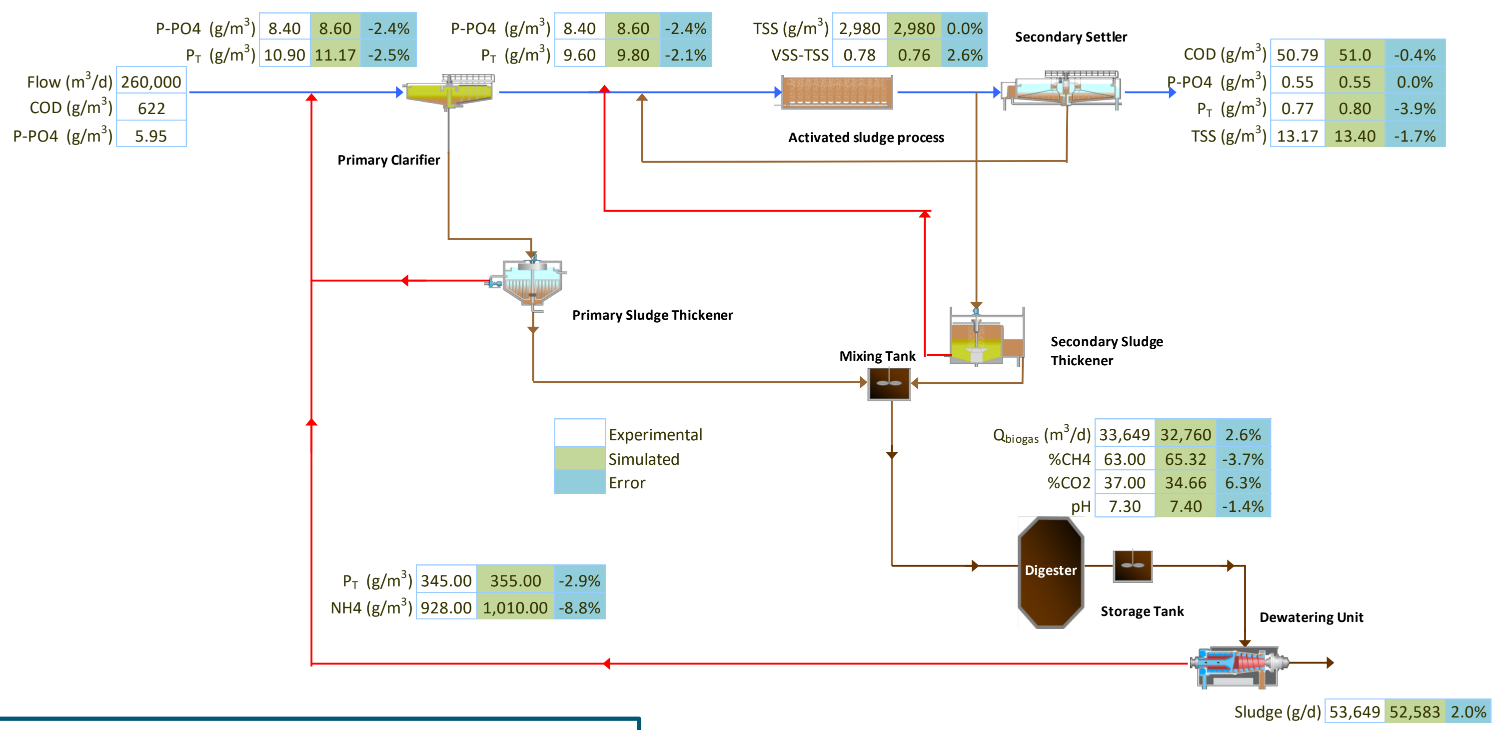
LIQUID-GAS PROCESSES

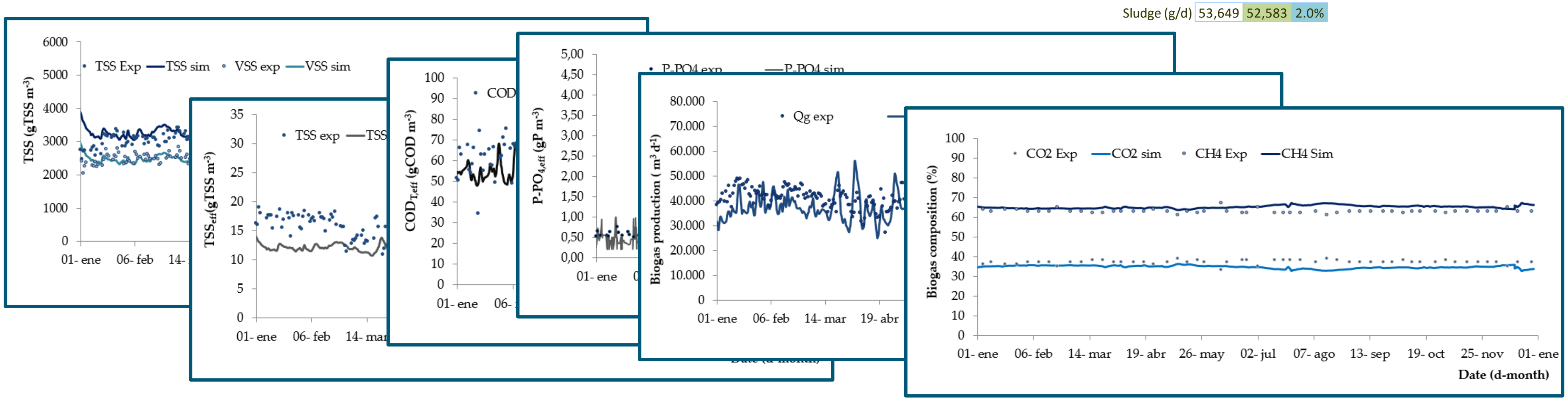
Mass exchange between gaseous and aqueous phases: H_2O, O_2, CO_2, NH_3, H_2 and CH_4.

PRECIPITATION-REDISSOLUTION REACTIONS

The most relevant sparingly soluble salts proposed by Musvoto *et al.* (2000) and their precipitation according to the equation proposed by Lizarralde *et al.* (2015) were considered, i.e. $CaCO_3$, $MgCO_3$, $Ca_3(PO_4)_2$, struvite, kstruvite and Newberyite, the chemical P removal reactions ($FePO_4$ and $Fe(OH)_3$).

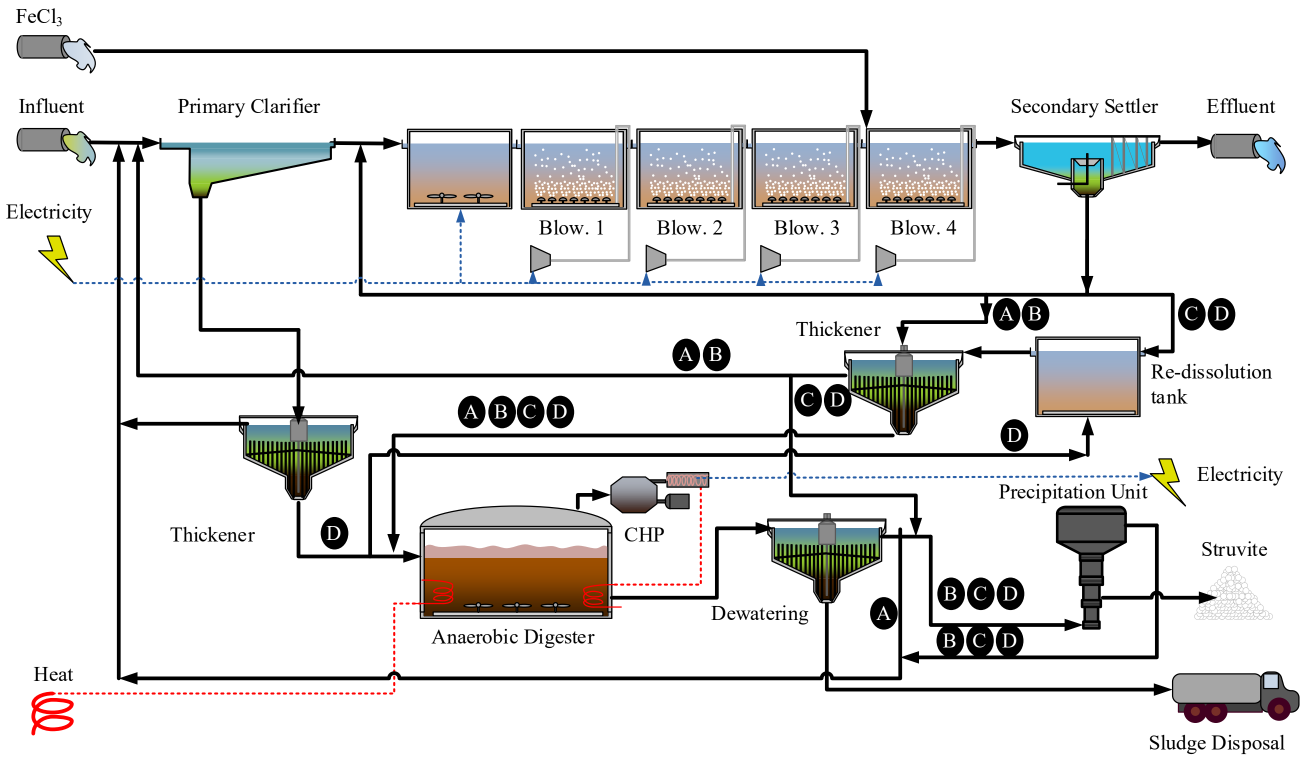
CALIBRATION





SCENARIO ANALYSIS

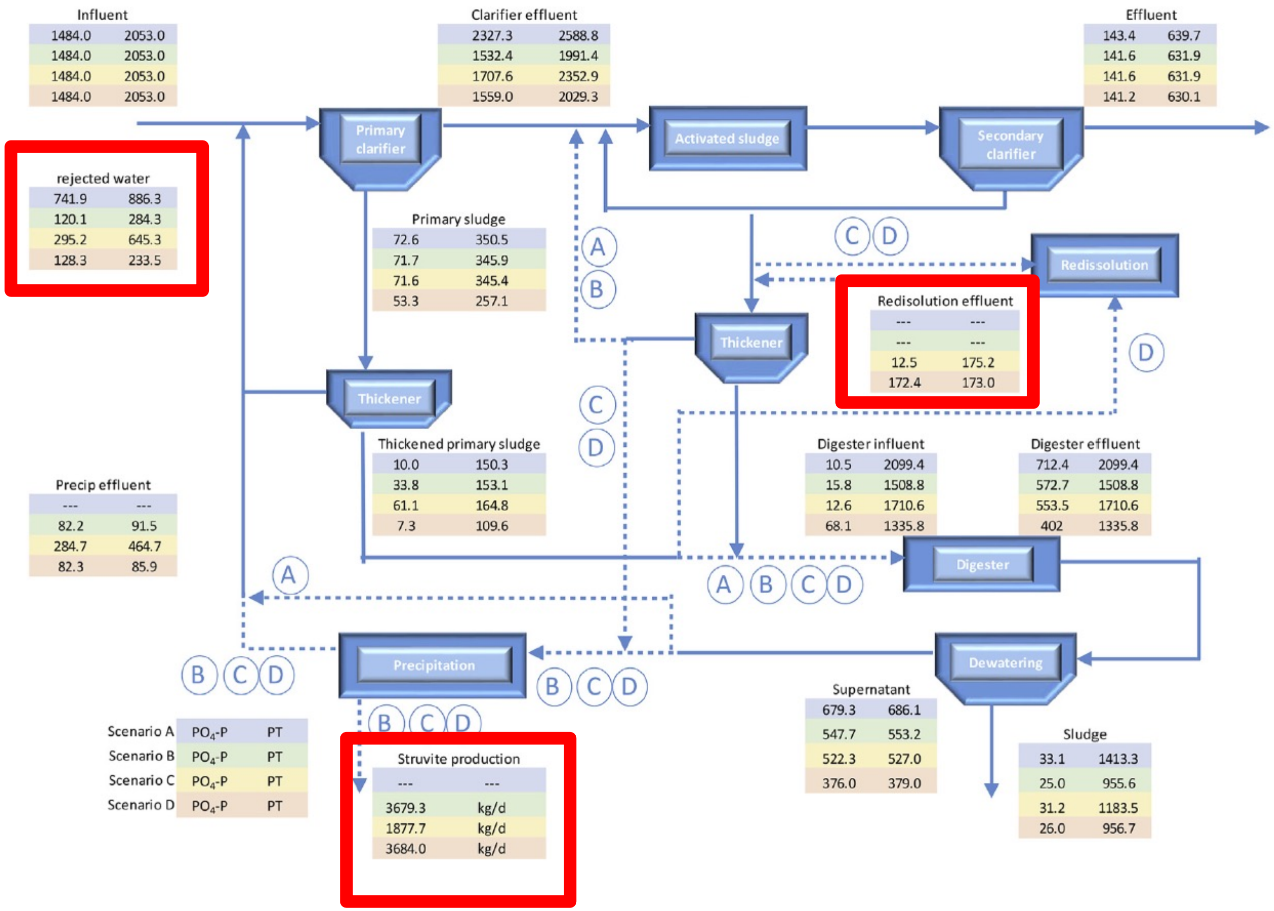
Objective of the study: Model-based scenario analysis to assess the maximum amount of struvite that can be recovered in a real WWTP.



- A: **A/O Configuration**
- B: **A/O + Stru**
- C: **A/O + Stru + ReDisso**
- D: **A/O + Stru + Enhanced ReDisso**

SCENARIO ANALYSIS

Objective of the study: Model-based scenario analysis to assess the maximum amount of struvite that can be recovered in a real WWTP.



A A/O Configuration

B A/O + Stru

C A/O + Stru + ReDisso

D A/O + Stru + Enhanced ReDisso

SCENARIO ANALYSIS

Objective of the study: Model-based scenario analysis to assess the maximum amount of struvite that can be recovered in a real WWTP.

Variable	Scenario A	Scenario B	Scenario C	Scenario D
Struvite production (Tn/year)	---	1343	685	1345
$MgCl_2$ dosage (Tn/year)	---	684	250	691
NaOH dosage (Tn/year)	---	403	26	444
Uncontrolled struvite precipitation (Tn/year)	126	95	119	38
Sludge production (Tn/year)	19070	17809	18821	17829
$FeCl_3$ dosage (Tn/year)	4979	2490	4914	2733

- **A** **A/O Configuration**
- **B** **A/O + Stru**
- **C** **A/O + Stru + ReDisso**
- **D** **A/O + Stru + Enhanced ReDisso**

REFLECTIONS & CONCLUSIONS

MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

1 **PLANT-WIDE MODELLING**

To perform a plant optimisation study or a feasibility analysis of incorporating a new technology, it is important that the model of the entire plant includes the liquid line, the sludge line and the interactions between them.

2 **PH MODELING ESPECIALLY IN THE SLUDGE LINE**

The degree of struvite precipitation is a function of Mg^{2+}, $NH4^{+}$, and PO_4^{3-} concentrations, but is strongly conditioned by the temperature and pH of the sludge.

3 **ELEMENTAL MASS CONTINUITY**

Especially COD, Mg^{2+}, K^{+}, N, and P continuity.

REAL PLANT

En 2016, Canal de Isabel II pone en marcha la primera planta de recuperación de fósforo en forma de estruvita a escala industrial en España en la EDAR Sur (Madrid). La planta, suministrada y montada llave en mano por la filial Española de Veolia Water Technologies, está dimensionada para tratar hasta 260 kg de fósforo al día procedente de dos corrientes de retorno de la depuradora. La formación controlada de estruvita se produce en un reactor de lecho fluidificado de flujo ascendente. Esta iniciativa ha supuesto para Canal de Isabel II una inversión de 2,3 M€, en línea con la apuesta de la Compañía por la economía circular, el cuidado del medio ambiente, la gestión sostenible y la inversión en I+D+i.

In 2016, Canal de Isabel II commissioned Spain's first industrial scale plant for the recovery of phosphorus in the form of struvite at the Sur WWTP (Madrid). The plant was supplied and assembled on a turnkey basis by the Spanish subsidiary of Veolia Water Technologies. It is sized to treat up to 260 kg of phosphorus per day from the WWTP's two return streams. The controlled formation of struvite is carried out in an upflow fluidised bed reactor. Canal de Isabel II has invested €2.3 million in this initiative, which is in line with the company's commitment to the circular economy, environmental care, sustainable management and investment in R&D&i.

MODEL-BASED OPTIMISATION OF P MANAGEMENT STRATEGIES IN A REAL WWTP

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Xavier Flores-Alsina (Tech. Uni. of Denmark)

Speaker 5
Tamara Fernández-Arévalo (CEIT, Spain)

Q&A Session Moderator: *Damien Batstone (Uni. Queensland, Australia)*

- This session is being recorded;
- Microphones and cameras have been disabled due to the large number of attendees;
- The normal chat function is disabled;
- Please put any questions and comments you may have in the Q&A (icon to the low right in Zoom) and we will do our best to answer them during the session (in writing or orally).

CLOSING REMARKS

Great thanks to all presenters for a wonderful show!

MIA will return with more webinars after the Summer, e.g.:

“Integrated Modelling”, “Digital Twins”, “CFD Modelling”

“Hybrid Modelling for Resource Recovery”

If you have ideas for your own future webinar then contact MIA MC and we will help you make it happen!

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