Wastewater treatment models: Current developments & trends

Användergrupp modellering ARV

Linköping, Sweden

26 August 2014

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Canada Research Chair
in Water Quality Modelling

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Table of Contents

- Use of models in North-America
- New developments and trends
  - Micropollutants
  - Greenhouse gases
  - Suspended solids
  - Resource recovery (physicochemical models)

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Use of models in North-America

- History:
  - 70s: North-America led the development
  - 80s-90s: Europe moved into practical application
  - 00s: North-America moved further
  - 10s: Renewed interest in Europe
- Application:
  - Design
  - Upgrade
  - Process optimization – Control development
  - Operation support

Use of models in NA for design

- All larger consulting companies use it
- Check guideline-based steady state design
- Direct design (special configurations)
- Capacity evaluation:
  - Aeration capacity (blower size)
  - Wet weather impact evaluation (special operations)
- Commercial element: good practice

Use of models in NA for design

- Probabilistic design

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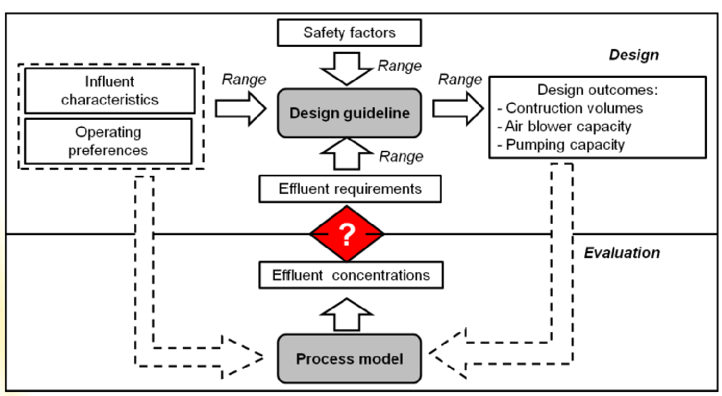
Use of models in NA for design

- Probabilistic versus traditional design



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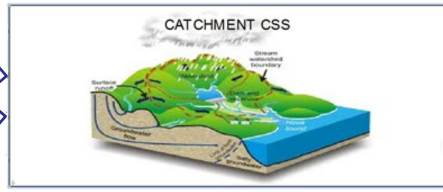
Probabilistic influent generator

Rainfall
(Markov chain exponential model)

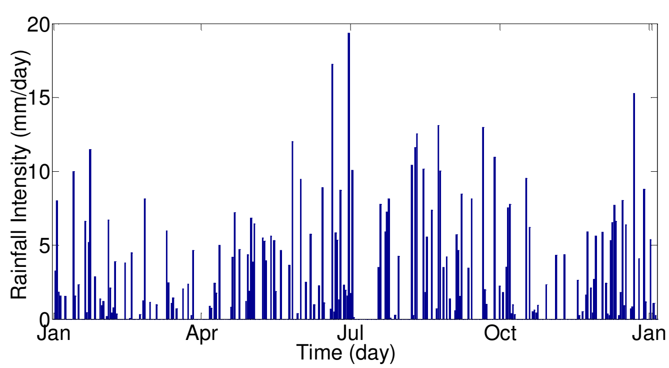


Influent
time series

DWF
(Multivariate AR model)

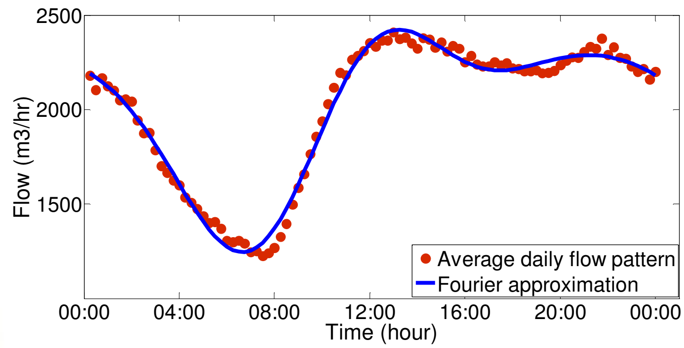
Probabilistic influent generator

- Daily rainfall series



Probabilistic influent generator

- Dry weather flow - average



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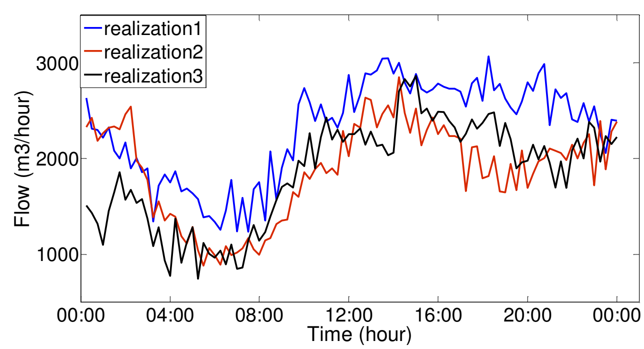
Probabilistic influent generator

- Dry weather flow - variability



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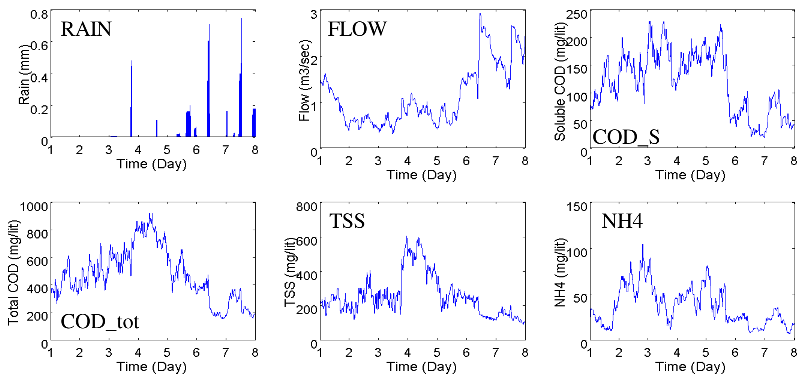
Probabilistic influent generator

- Time series of 1 week of generated data



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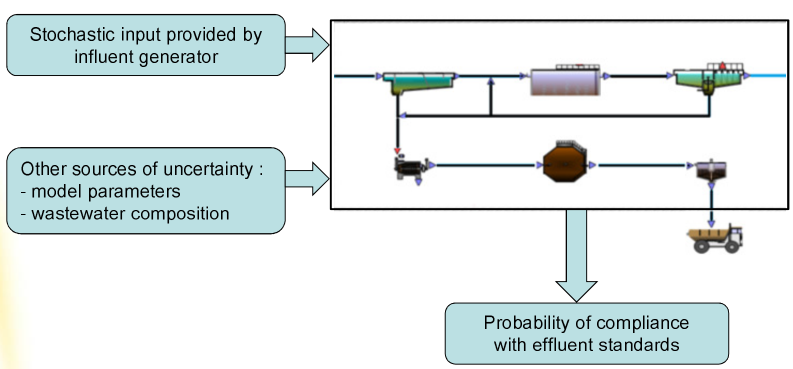
Probabilistic influent generator

- Use in probabilistic design



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Micropollutants

- Increased interest since 2000
  → Priority pollutants in EU WFD
- Challenges:
  - The analysis of low concentrations
  - The sheer number of chemicals
  - The diversity of impacts

Crossed beak in birds caused by chemicals

*US EPA

*Joanne Parrott

Feminization of male fish by endocrine disruptors

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Micropollutants

- Increased interest since 2000
  → priority pollutants in EU WFD
- Challenges:
  - The analysis of low concentrations
  - The sheer number of chemicals
  - The diversity of impacts
  - The diversity of processes affecting them
- Studies at level of WWTP, but also at level of integrated urban wastewater system (IUWS)

ScorePP

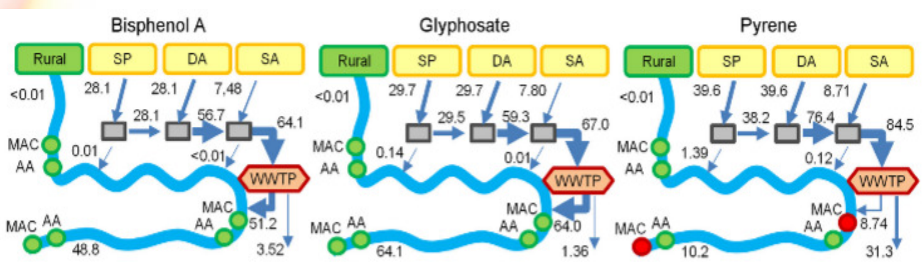
Unit model Processes	Sewer	Stormwater unit (water)	Stormwater unit (sediments)	Primary settling	Activated sludge tank	Secondary settling	Sludge thickener	Sludge anaerobic digester	Sludge dewatering	River (water)	River (sediments)
Physical processes											
Sedimentation	+	+		+		+	+			+	
Resuspension	+		+								+
Volatilization	+	+		+	+	+	+	+	+	+	
Sediment-water exchange										+	+
physicochemical											
Adsorption-desorption	+	+	+	+	+	+	+	+		+	+
Hydrolysis	+	+	+	+	+	+	+			+	
Photolysis		+								+	
Biological											
Aerobic biodegradation	+	+	+	+	+	+	+			+	+
Anoxic biodegradation	+	+	+	+	+	+	+	+		+	+

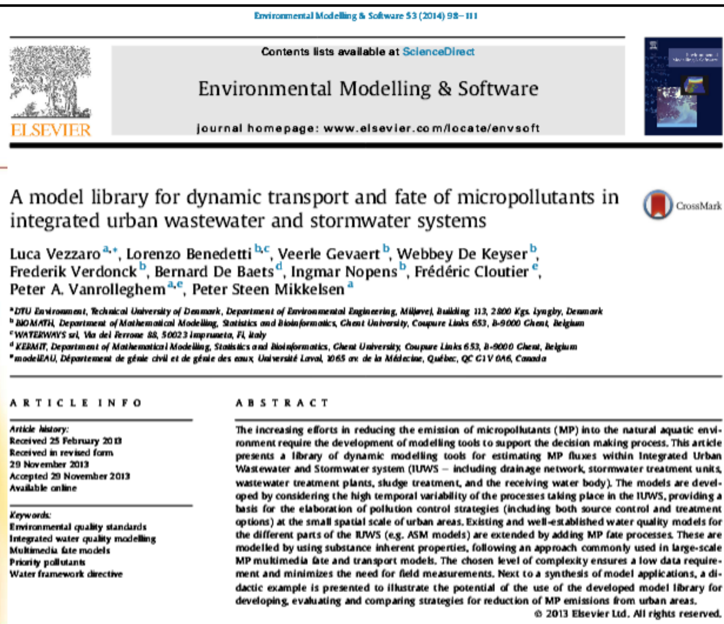
ScorePP

Process	MP properties	Other relevant parameters
Physical processes		
Sedimentation and resuspension	-	Water depth, bottom shear stress, critical shear stress, erodibility constant
Volatilization	Henry's law constant, molecular weight	Water depth, wind speed, water currents and temperature
Sediment-water exchange	Molecular weight	Sediment porosity
Physicochemical		
Adsorption-desorption	Partition coefficient (k_d or k_{OC})	TSS concentration, organic fraction
Hydrolysis	First-order degradation rate (or half life)	pH, temperature
Photolysis	Half-life	Light intensity, water depth, water pollution
Biological		
Aerobic biodegradation	Half-life	Oxygen concentration, temperature
Anoxic biodegradation	Half-life	Oxygen/nitrate concentration, temperature

Micropollutants: A case study

- Substance flow analysis (g/d)





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A model library for dynamic transport and fate of micropollutants in integrated urban wastewater and stormwater systems

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ABSTRACT

The increasing efforts in reducing the emission of micropollutants (MP) into the natural aquatic environment require the development of modelling tools to support the decision making process. This article presents a library of dynamic modelling tools for estimating MP fluxes within Integrated Urban Wastewater and Stormwater system (IUWS – including drainage network, stormwater treatment units, wastewater treatment plants, sludge treatment, and the receiving water body). The models are developed by considering the high temporal variability of the processes taking place in the IUWS, providing a basis for the elaboration of pollution control strategies (including both source control and treatment options) at the small spatial scale of urban areas. Existing and well-established water quality models for the different parts of the IUWS (e.g. ASM models) are extended by adding MP fate processes. These are modelled by using substance inherent properties, following an approach commonly used in large-scale MP multimedia fate and transport models. The chosen level of complexity ensures a low data requirement and minimizes the need for field measurements. Next to a synthesis of model applications, a didactic example is presented to illustrate the potential of the use of the developed model library for developing, evaluating and comparing strategies for reduction of MP emissions from urban areas.

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Vezzaro et al. (2014)
Environ. Modelling & Software 53, 98-111

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Wastewater utility GHG

- Greenhouse gases in wastewater systems:
  - CO_2 (Biodeg., energy, chemicals) 1 CO_{2eq}
  - CH_4 (Anaerobic digestion) 18 CO_{2eq}
  - N_2O (Nitrogen removal) 300 CO_{2eq}

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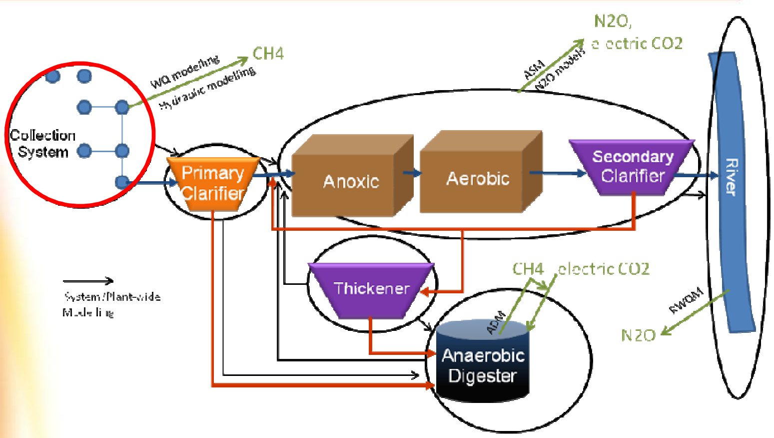
Wastewater utility GHG



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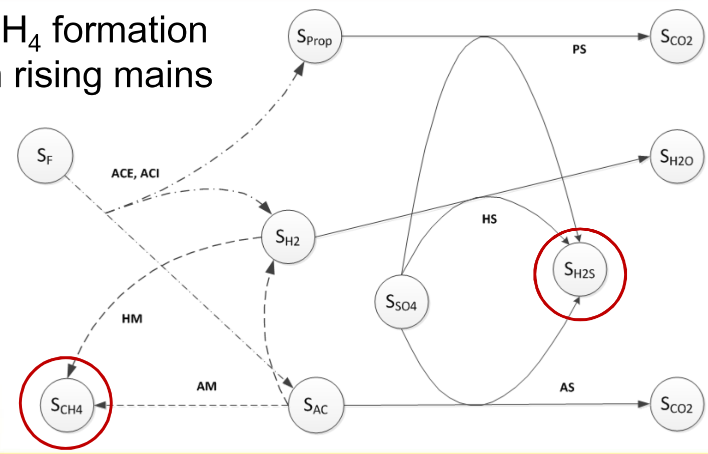
GHG from sewer systems

- CH_4 formation in rising mains



Guisasola et al. (2009)
Water Res. 43: 2874-2884

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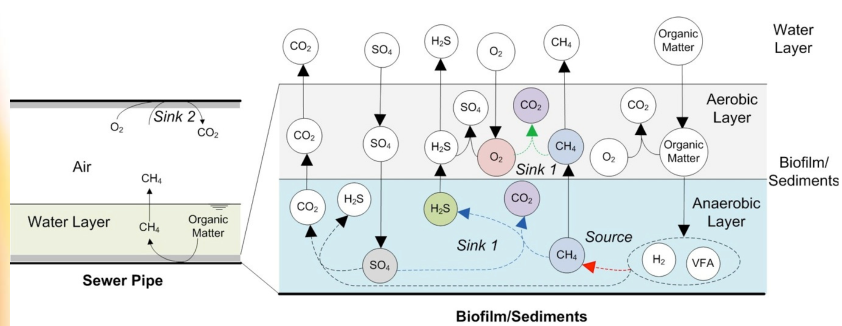
GHG in sewer systems

- CH_4 formation in gravity sewers (with O_2 transfer)



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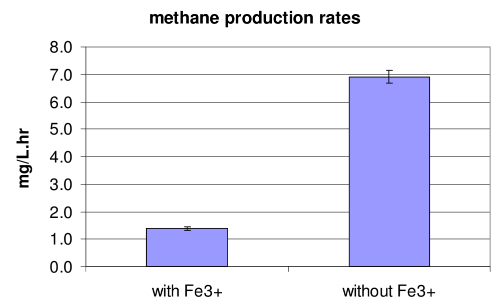
What can we do? Add chemicals!

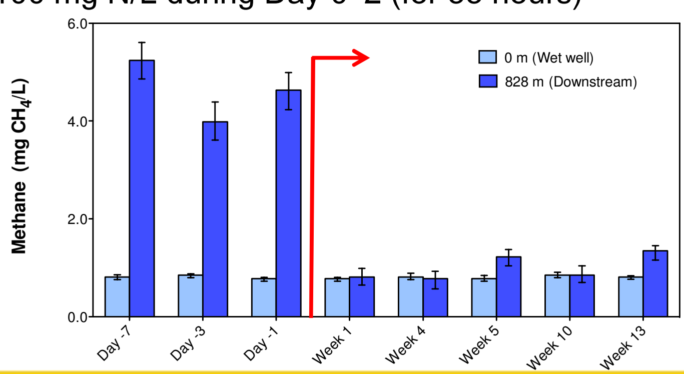
- Chemicals used for sulfide control
  (Brisbane: 6 M$/yr repair → 1 M$/yr chemical addition)
  also reduce methane formation



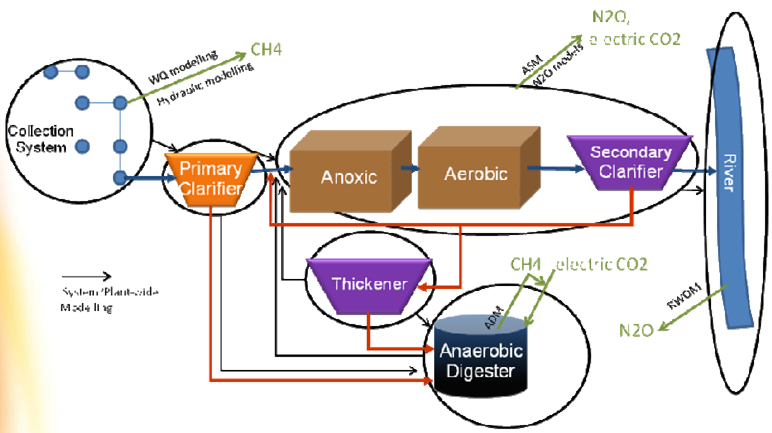
Zhang et al. (2009)
Water Res 43(17), 4123

What can we do? Add chemicals!

Acidified nitrite was added in the sewer intermittently at 100 mg N/L during Day 0–2 (for 33 hours)



Wastewater utility GHG



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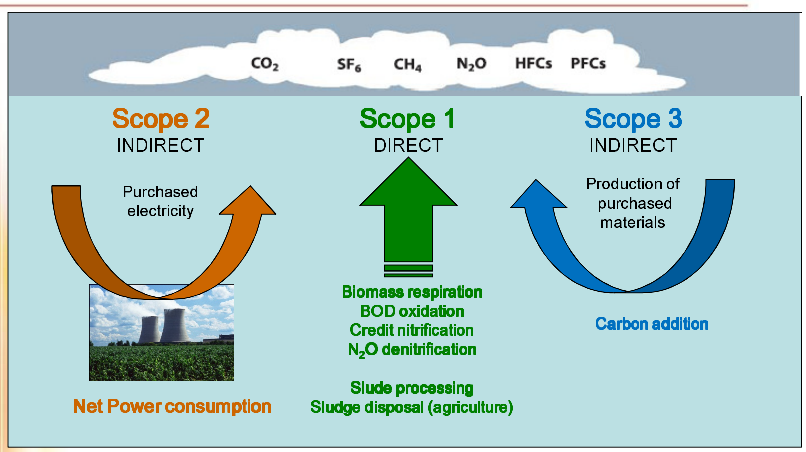
GHG emissions from WWTP



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Evaluation of GHG emissions

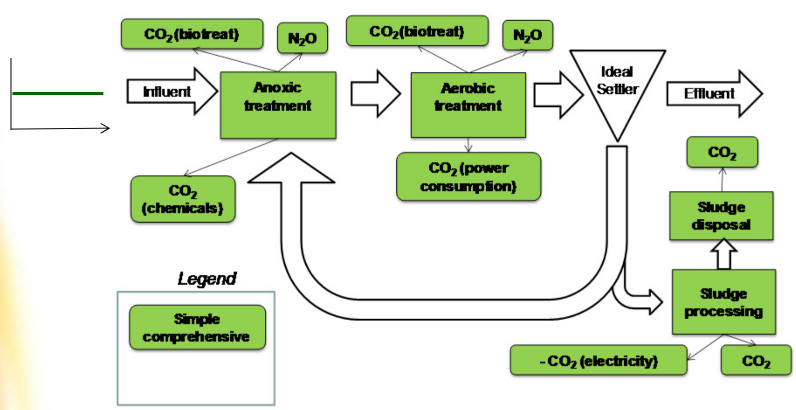
- Different approaches to estimate GHG emissions:
  - Empirical factors:
    - e.g. IPCC, 2006; LGO, 2008; NGER, 2008
  - Simple comprehensive models:
    - e.g. Cakir and Stenstrom, 2005; Monteith *et al.*, 2005; Bridle *et al.*, 2008; Foley *et al.*, 2009
  - Dynamic deterministic models:
    - ASMG1 (Guo & Vanrolleghem, 2014) → N_2O
    - ADM1 (Batstone et al., 2002) → CH_4

+ complexity

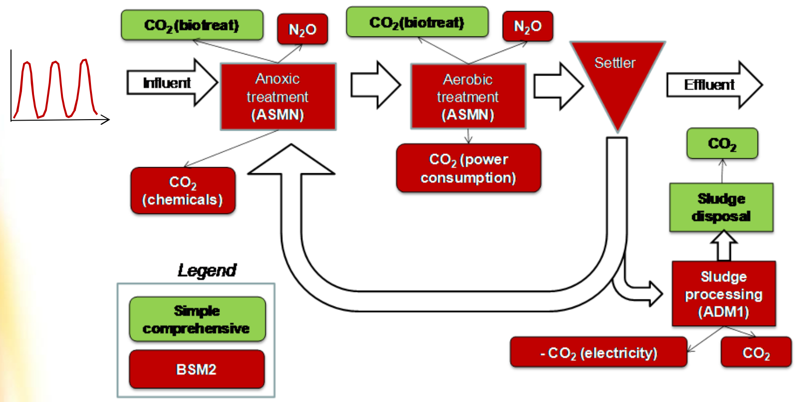
BSM2G benchmarking platform

Guo & Vanrolleghem (2014)
Bioprocess Biosyst. Eng., 37, 151-163.

Evaluation of GHG emissions



Evaluation of GHG emissions



Corominas et al. (2012)
Biotechnol. Bioeng., 109, 2854-2863

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Benchmarking control strategies

- Comparison of ***no control*** and ***yes control*** (DO control in aerobic reactors, DO = 2mg·L^{-1})

Breakdown of GHG emissions (kg CO_2e·m^{-3})	**No control**	**Yes control**	**%**
Bio-treatment GHG emissions	**0.451**	**0.376**	**-17**
Biomass respiration	0.179	0.178	-1
BOD oxidation	0.212	0.212	0
Credit nitrification	-0.168	-0.167	-1
N_2O emissions	0.228	0.152	-33
Sludge processing GHG emissions	**0.231**	**0.231**	**0**
Net power GHG emissions	**0.000**	**-0.038**	-
Power	0.311	0.272	-13
Credit power GHG emissions	-0.311	-0.310	0
Embedded GHG emissions from chemical use	**0.099**	**0.099**	**0**
Sludge disposal and reuse GHG emissions	**0.193**	**0.193**	**0**

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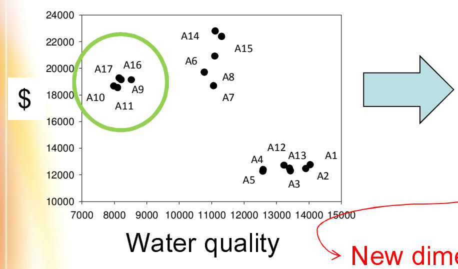
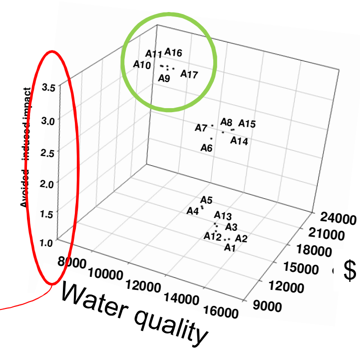
Benchmarking control strategies

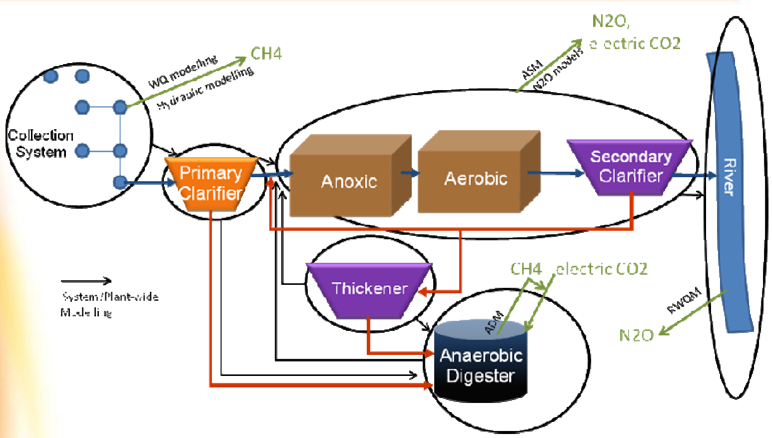
- Overall result of our studies so far:
- Compromise between:
  - Effluent quality
  - Treatment costs
  - GHG emissions



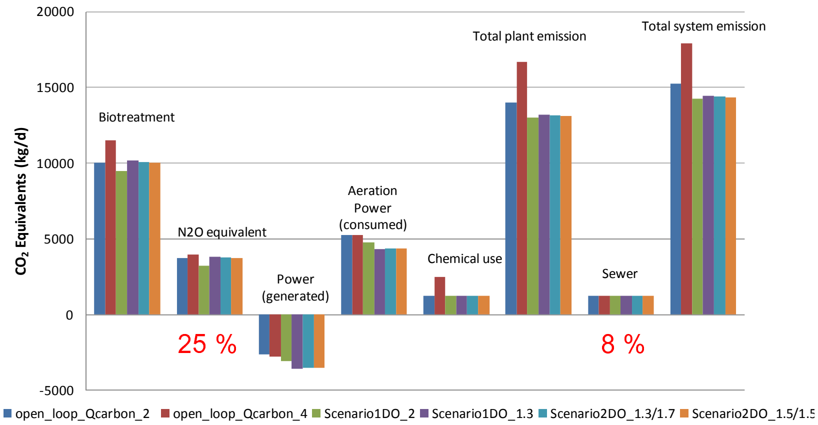


New dimension: Greenhouse gases

Wastewater utility GHG



GHG emissions from WW utility



Guo et al. (2012) Towards …
Wat. Sci. Tech., 66(11), 2483-2495.

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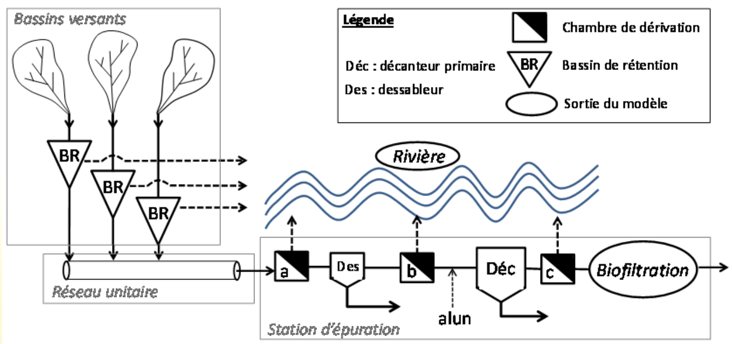
Suspended solids – the source

- Households + run-off from catchment
  + resuspension from sewer sediments



Tik et al. (2014)
Proc. Internat. Conf. Urban Drainage (ICUD2014)

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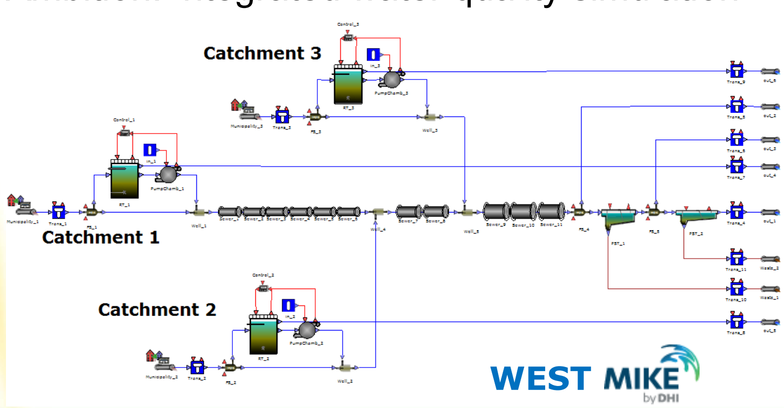
Suspended solids – the source

- Ambition: Integrated water quality simulation



Tik et al. (2014)
Proc. Internat. Conf. Urban Drainage (ICUD2014)

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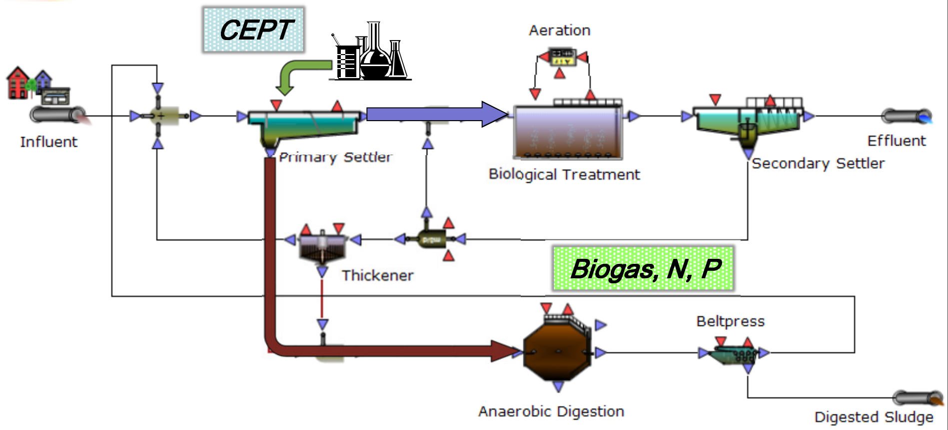
The future WWTP → WRRF



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Bachis et al. (2014)
Proceedings WWTmod2014

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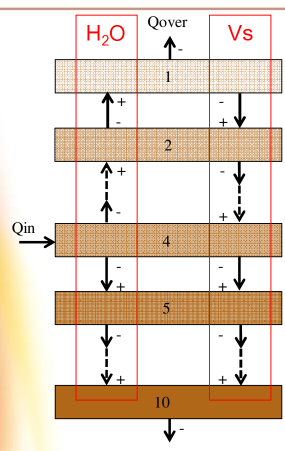
Primary clarifier model



- 'PSVD' model
  - Particle Settling Velocity Distribution
  - No size, density, size !
  - Developed for storm tanks
- Adaptation of model of Bachis *et al.* (2012) incorporating 5 particle classes
- 10 layers
- Calibrated with field data

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Bachis et al. (2012)
IWA Particle Separation Conference

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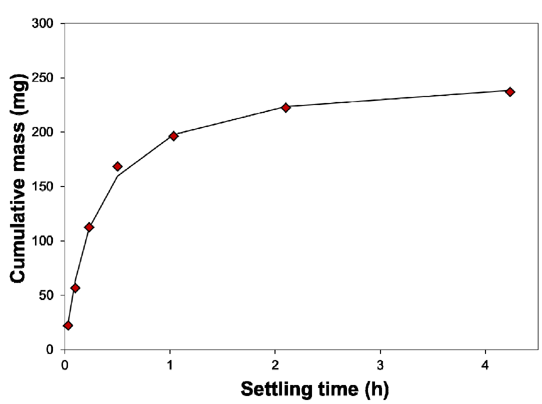
PSVD model – ViCAs methodology

ViCAs (*Settling Velocity in Sanitation*), Chebbo&Gromaire, 2009

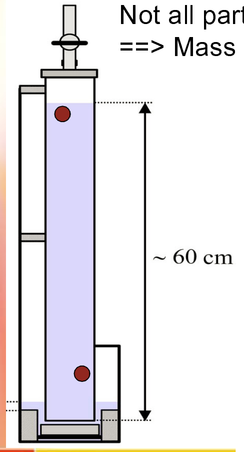
PSVD model – ViCAs methodology

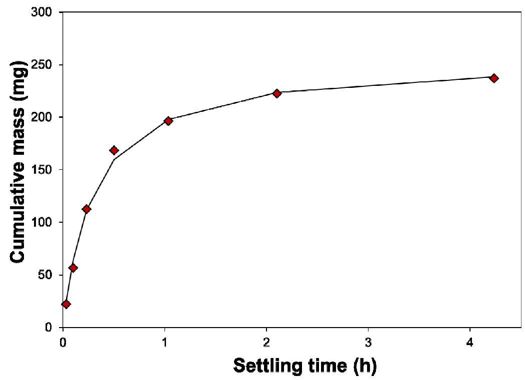
ViCAs (*Settling Velocity in Sanitation*), Chebbo&Gromaire, 2009



PSVD model – ViCAs methodology

Not all particles settle over the same column height
==> Mass not directly associated to a class of velocity





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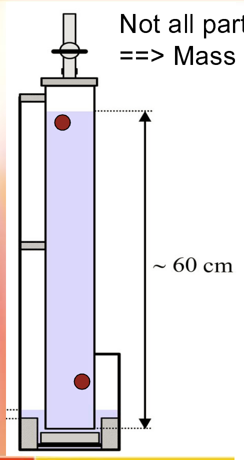
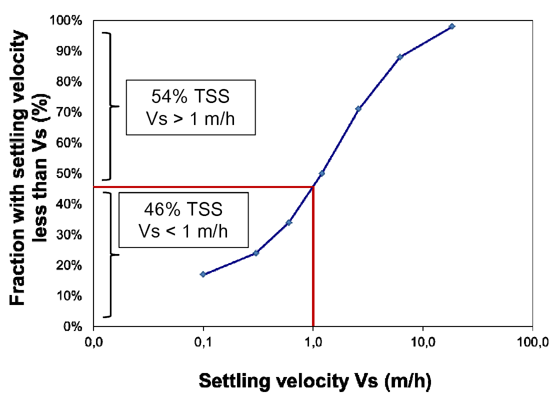
PSVD model – ViCAs methodology

Not all particles settle over the same column height
==> Mass not directly associated to a class of velocity





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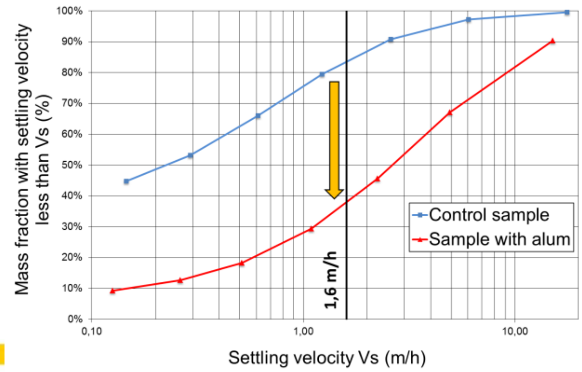
PSVD model – ViCAs methodology

- ViCAs allows modelling chemically enhanced primary treatment (CEPT)



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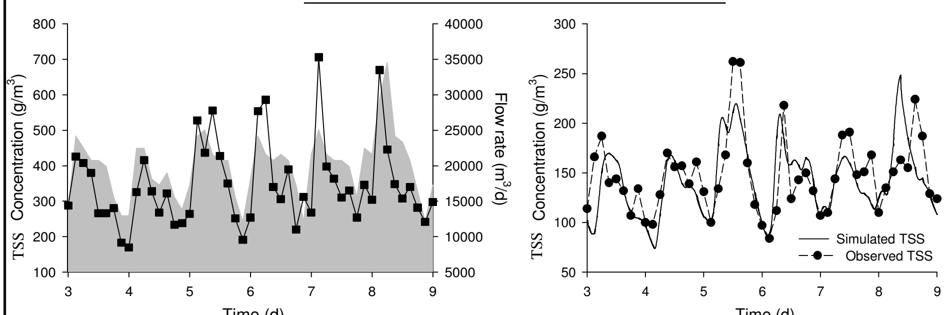
Primary clarifier: Calibration

Norwich WWTP, England	
Flow rate (1,000 m^3/d)	10 - 35
Overflow rate range (m/h)	0.6 – 2
Shape	Circular



Lessard & Beck (1988)
Journal of Environmental Engineering

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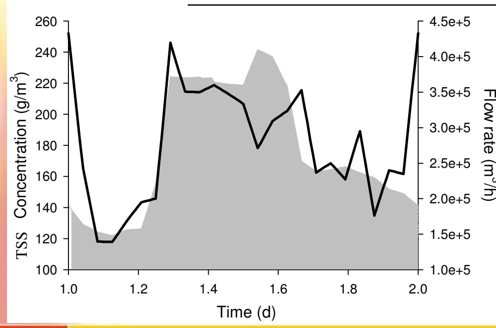
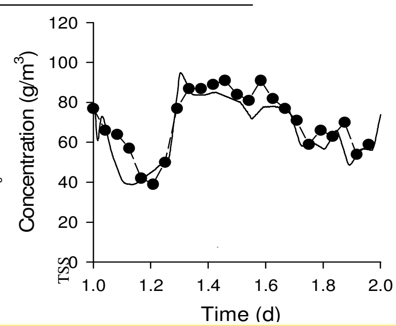
Primary clarifier: Calibration

April 9th 2010

Eastern Quebec WWTP, Canada	
Flow rate range (1,000 m³/d)	120 - 470
Overflow rate range (m/h)	1 – 3.7
Shape	Rectangular





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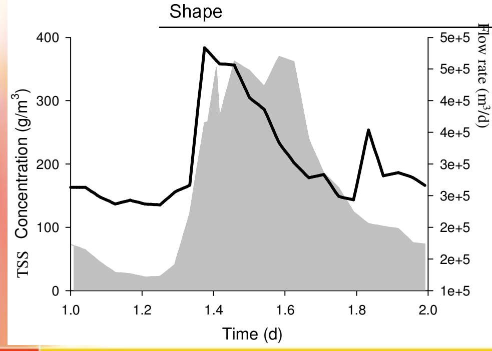
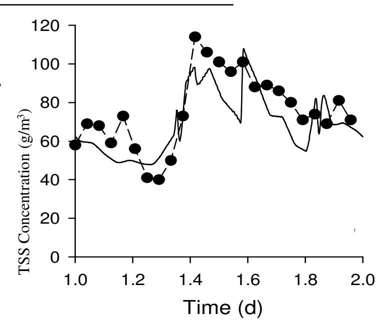
Primary clarifier: Validation

April 17th 2010

Eastern Quebec WWTP, Canada	
Flow rate range (1,000 m³/d)	120 - 470
Overflow rate range (m/h)	1 – 3.7
Shape	Rectangular





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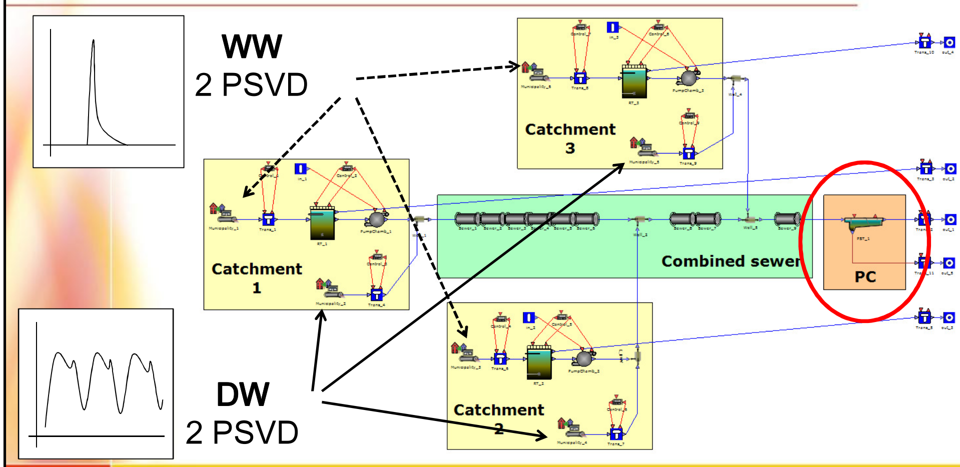
Integrated system evaluation
Inputs



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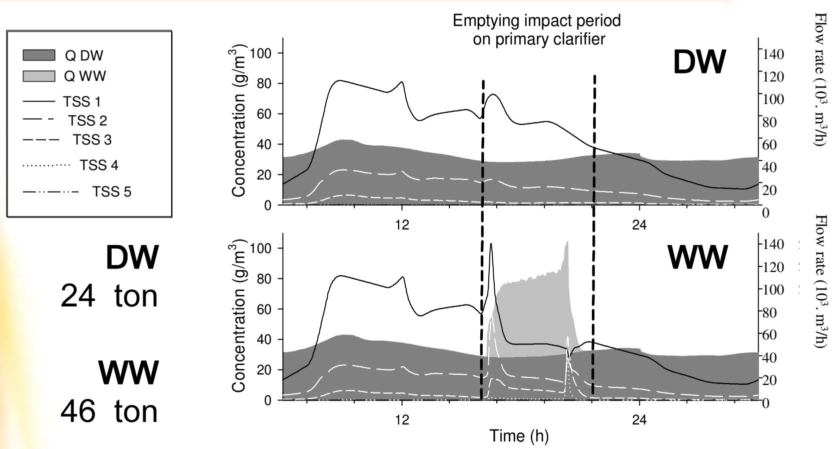
Integrated system evaluation
Primary clarifier effluent composition



DW
24 ton

WW
46 ton

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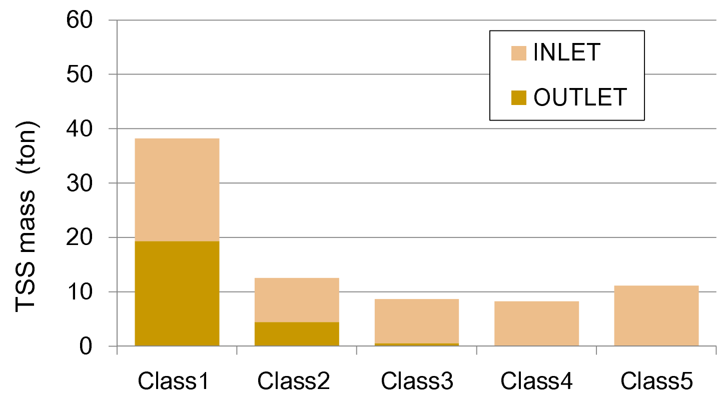
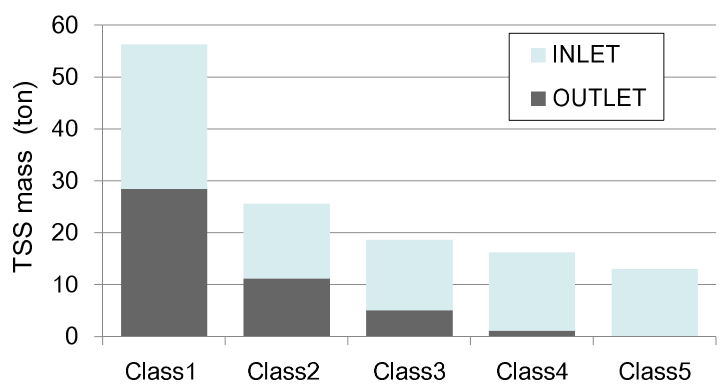
Integrated system evaluation

Primary clarifier effluent (Dry Weather)



Integrated system evaluation

Primary clarifier effluent (Wet Weather)



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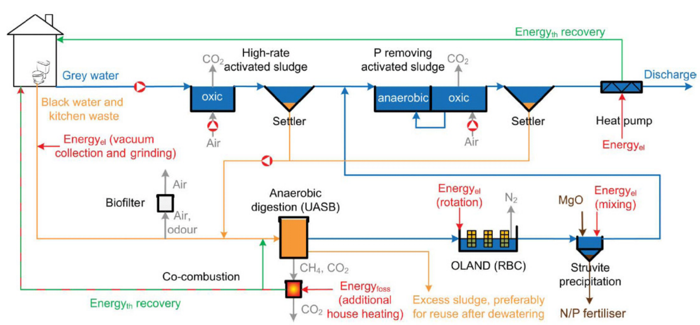
"Wurfs"

- Water resource recovery facility (WRRF)



Scheme of source-separated sanitation implementing energy and nutrient recovery as practised for 32 houses in Sneek

Verstraete & Vlaeminck (2011)
Int. J. Sust. Dev. World Ecol., 18, 253-264.

Resource recovery processes

- Stripping (NH_3, fatty acids)
- Precipitation (struvite)
- Filtering (paper fibers)
- Extraction (PHA)
- Ion exchange (NH_4^+)
- Reverse osmosis (H_2O)
- Phase separation (butanol)
- Pyrolysis, gasification, incineration (energy)
- Chemically enhanced primary treatment (COD)

All physico-chemical unit processes

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Modelling physicochemical processes

- We've done it simply:
  - Aeration: Kla (C_{sat}-C)
  - pH: f(pKa, TAN, Alk, …)
  - Precipitation: MeOH/MeP
  - Membrane: J = TMP/μ.(R_m+R_f+R_c)

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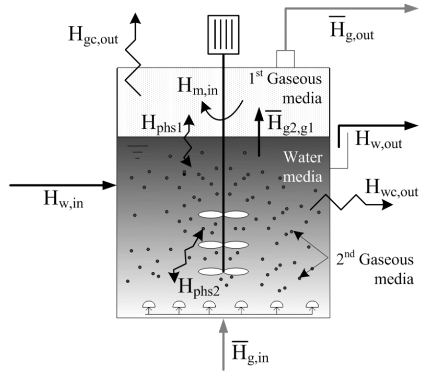
Modelling physicochemical processes

- We have to do it differently:

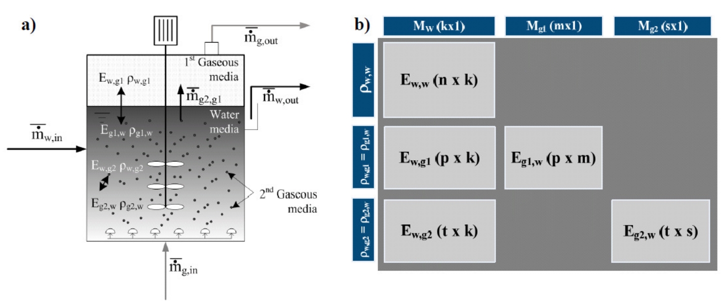
<u>Temperature:</u>



Modelling physicochemical processes

- We have to do it differently:

<u>Gas exchange:</u>



Modelling physicochemical processes

- We have to do it differently:

Precipitation:

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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

ABSTRACT

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Modelling physicochemical processes

- We have to do it differently:

Precipitation:

It gets a little crowded in wastewater

Mg^{2+} $HCO3^{-}$ $CaOH^{+}$
$NaHPO_4^{-}$ Ca^{2+}
$MgHCO_3^{+}$,$CaHPO_4$ (aq)
Na^{+} $MgH_2PO_4^{+}$ $CaAc^{+}$
Cl^{-} $CaHCO_3^{+}$ Mg^{2+}
$SO4^{2-}$ $NaCO_3^{-}$ $NaHCO_3$ (aq)
$NaSO_4^{-}$ $HPO4^{2-}$ $MgSO_4$ (aq)
$CaSO_4$ (aq) K^{+} $CO3^{2-}$
Na^{+} NaAc (aq)
$CaCO_3$ (aq)

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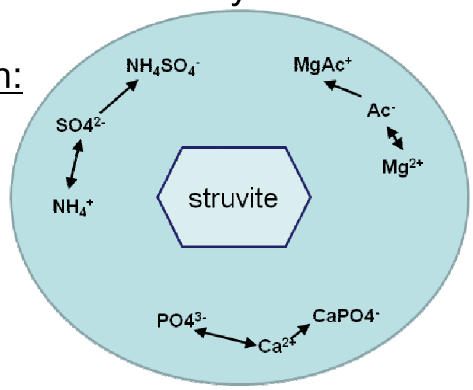
Modelling physicochemical processes

- We have to do it differently:

Precipitation:

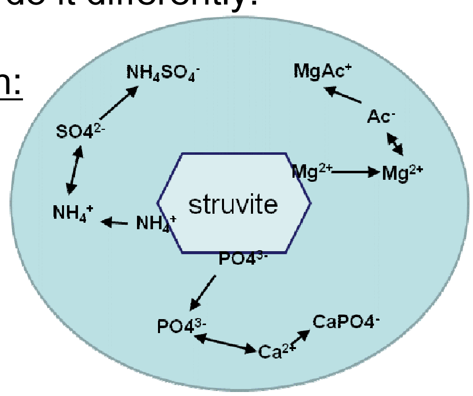


Modelling physicochemical processes

- We have to do it differently:

Precipitation:

Ion pairs increase solubility



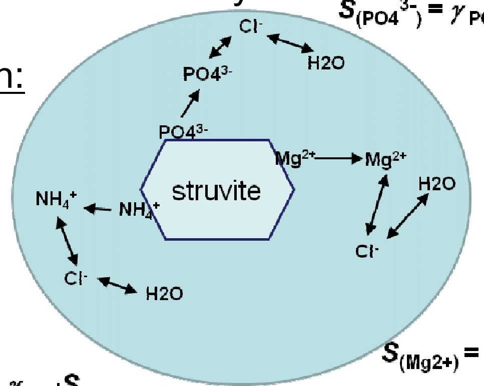
Modelling physicochemical processes

- We have to do it differently:

$S_{(PO4^{3-})} = \gamma_{PO4} \cdot S_{[PO4^{3-}]}$

Precipitation:

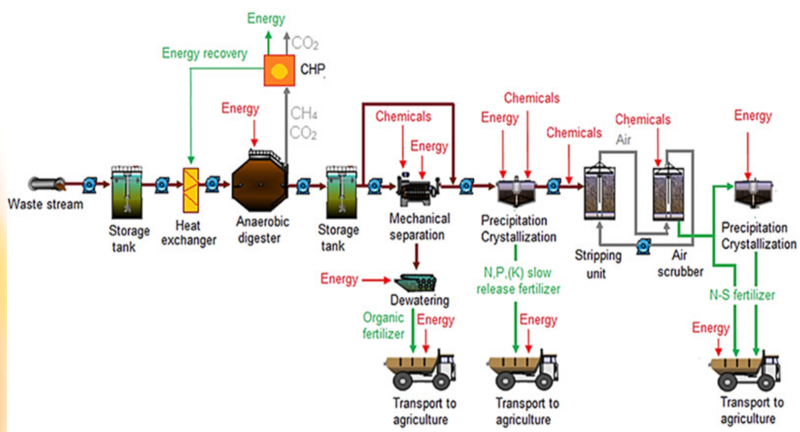
Ionic strength increases solubility



$S_{(Mg2+)} = \gamma_{Mg} \cdot S_{[Mg2+]}$

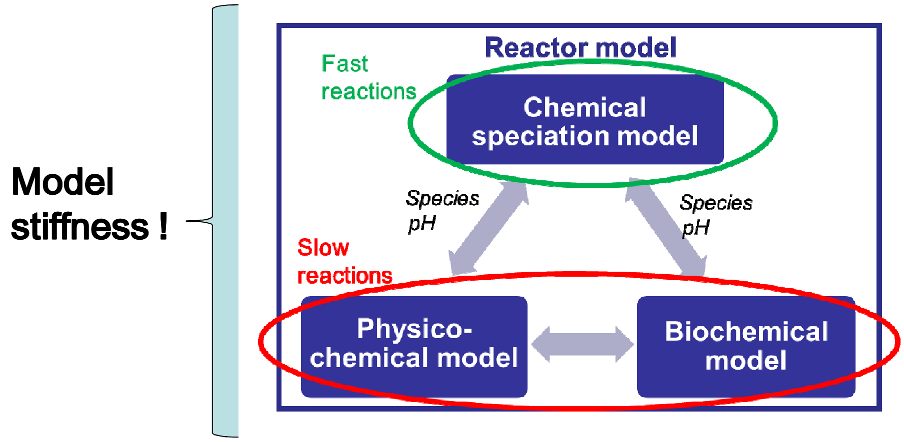
$S_{(NH4+)} = \gamma_{NH4} \cdot S_{[NH4+]}$

Modelling physicochemical processes in WRRFs



Céline Vaneeckhaute (2014)
PhD thesis, Université Laval, in preparation

Modelling physicochemical processes



Modelling physicochemical processes

- Two options to solve dynamic models:

1: ODE	2: DAE	
All reactions: Ordinary differential equations (ODE)	Slow reactions: differential equations (ODE)	Fast reactions: algebraic equations calculated at each iteration step
		Tailored code to solve water chemistry / External software tool (PHREEQC)

Setting up a reduced PCM model

I. Physicochemical component selection

II. Speciation calculation

III+IV. Selection of species/reactions ⟹ reduced model

SO_4 NH_4 H PO_4
Na K Ca Mg CO_3
Fe Cl Al N_2 HS
Ac Pr Bu Va

→ PHREEQC/ MINTEQC

Corrections:
- *Ion activity*
- *Temperature*

→ 73 species ↕ ± 253 species

→ 12 acid-base reactions
43 ion-pairing reactions
22 precipitation reactions
7 gas-liquid reactions

Modelling WRRFs – ADM1.5

- To properly model P in WRRFs,
  we need to extend ADM1 (only COD & N):
  - Consider Fe and its interaction with Sulphide (FeS!)
  - Phosphate fate, including PAO's
  - P-release from organics

ADM1 Extension 1: Sulfurgenesis

- Model of Knobel & Lewis (2002)

Components → Transformations ↓		S_{hbu} gCOD	S_{hpro} gCOD	S_{hac} gCOD	S_{h2} gCOD	S_{co2} molC	S_{so4} molS	S_{h2s} molS	X_{SRB_bu} gCOD	X_{SRB_pro} gCOD	X_{SRB_ac} gCOD	X_{SRB_h} gCOD
1	Butirate sulphate reduction	-1				$f_{co2,bu}$	$-f_{s,bu}$	$f_{s,bu}$	Y_{SRB_bu}			
2	Propionate sulphate reduction		-1			$f_{co2,pro}$	$-f_{s,pro}$	$f_{s,pro}$		Y_{SRB_pro}		
3	Acetate sulphate reduction			-1		$f_{co2,ac}$	$-f_{s,ac}$	$f_{s,ac}$			Y_{SRB_ac}	
4	Hydrogen sulphate reduction				-1	$-f_{co2,h}$	$-f_{s,h}$	$f_{s,h}$				Y_{SRB_h}

$$\rho_1 = \mu_{SRB\_bu} \cdot \frac{S_{bu}}{K_{s,SRBbu} + S_{bu}} \cdot \frac{S_{so4}}{K_{SO4\_bu} + S_{so4}} \cdot I_{pH,SRB} \cdot I_{H2S\_SRBbu} \cdot X_{SRB\_bu}$$

$$\rho_2 = \mu_{SRB\_pro} \cdot \frac{S_{pro}}{K_{S,SRBpro} + S_{pro}} \cdot \frac{S_{so4}}{K_{SO4\_pro} + S_{so4}} \cdot I_{pH,SRB} \cdot I_{H2S\_SRBpro} \cdot X_{SRB\_pro}$$

$$\rho_3 = \mu_{SRB\_ac} \cdot \frac{S_{ac}}{K_{S,SRBac} + S_{ac}} \cdot \frac{S_{so4}}{K_{SO4\_ac} + S_{so4}} \cdot I_{pH,SRB} \cdot I_{H2S\_SRBac} \cdot X_{SRB\_ac}$$

$$\rho_4 = \mu_{SRB\_h2} \cdot \frac{S_{h2}}{K_{S,SRBh2} + S_{h2}} \cdot \frac{S_{so4}}{K_{SO4,h2} + S_{so4}} \cdot I_{pH,SRB} \cdot I_{H2S\_SRBh2} \cdot X_{SRB\_h2}$$

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Knobel & Lewis (2002)
Water Research, 36(1), 257-265.

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ADM1 Extension 1: Sulfurgenesis

- Model of Knobel & Lewis (2002)
  - 4 Types of bacteria
  - Electron acceptor: SO_4^{2-}
  - Electron donor & carbon source for growth:
    - Pro, Bu, Ac
    - Donor = H_2 and carbon source = CO_2
  - Inhibition factor H_2S included

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Knobel & Lewis (2002)
Water Research, 36(1), 257-265.

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ADM1 Extension 2: Hydrolysis

- Incorporation in disintegration/hydrolysis: release of P, K and S, based on the composition of bacterial cells

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ADM1 Extension 3: EBPR

- PAO's (heterotrophs with anaerobic metabolism)
- Poly-P accumulation in cells (1-2%P → 5-7%P)
- Reactions in AD (Ikumi, 2011):
  - Release of polyphosphate (PP) (+ release of K, Ca and Mg) with uptake of acetate by PAOs while they are still alive
  - Maintenance by hydrolysis of PP (Last supper ;-)
  - Decay of PAOs
  - Hydrolysis of poly-hydroxy-alkanoate (PHA) when PAOs die

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Ikumi (2011)
PhD thesis, University of Cape Town.

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Current state of PCM of WRRFs

√ *PhreeqC*
Fast reactions:
- Selective model code
- Reduced data base

√ *Modelica*
Physico-chemical slow transfer

√ *Modelica*
Biochemical slow transfer (ADM 1)

Tornado

Alternative simulation results (PhreeqC)

Check √

Simulation results

On-going

Experimental data

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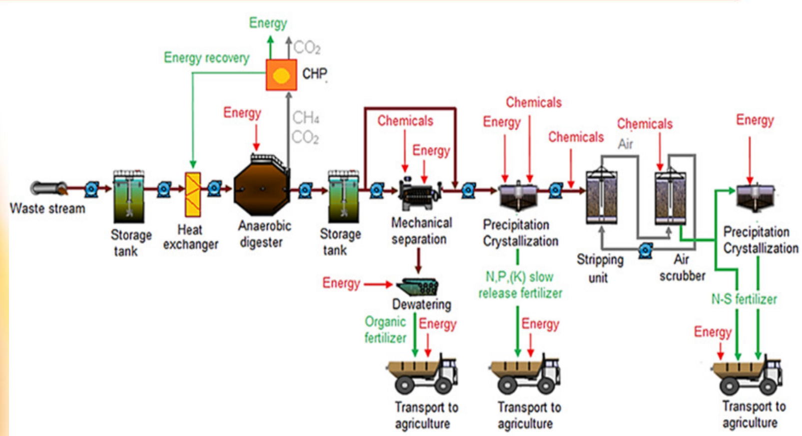
Model-based optimization of resource recovery trains in WRRFs



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Acknowledgements

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CRSNG NSERC

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MIKE by DHI

Otto Mønsted

Waterschap De Dommel

VILLE DE QUÉBEC

Primodal

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