Les StaRREs – Stations de récupération des ressources de l'eau – Défis de modélisation

29[iéme] Congrès de l'Est du Canada de Recherche sur la Qualité de l'Eau

École Polytechnique Montréal

17 octobre 2014

Peter VANROLLEGHEM

Chaire de recherche du Canada en modélisation de la qualité de l'eau

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100 years! That's enough!

Willy Verstraete, Lisbon, 25-Sep-2014
Chair IWA Resource Recovery Cluster

Davyhulme WWTP, Manchester, UK

WRRF's – Water Resource Recovery Facilities : Modelling Challenges

29th Eastern Canadian Symposium on Water Quality Research

École Polytechnique Montréal

October 17th 2014

Peter VANROLLEGHEM

Canada Research Chair in Water Quality Modelling

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Outline

- Water resources
- Water resource recovery
- Modelling challenges
- Take home

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Resources in Water & Sludge

- Water
- Energy
- Biofuels (butanol, ethanol, methanol, H_2)
- Nutrients (Mg,N,P – struvite, $(NH_4)_2CO_3$)
- Sulphur (S, H_2SO_4)
- Fibers (toilet paper)
- Bioplastics (PHA)
- Building blocks for bio-refineries (succinic acids, carotenoids, fatty acids, …)

Outline

- Water resources
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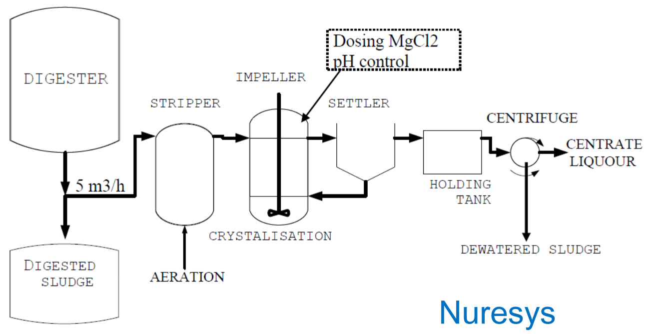
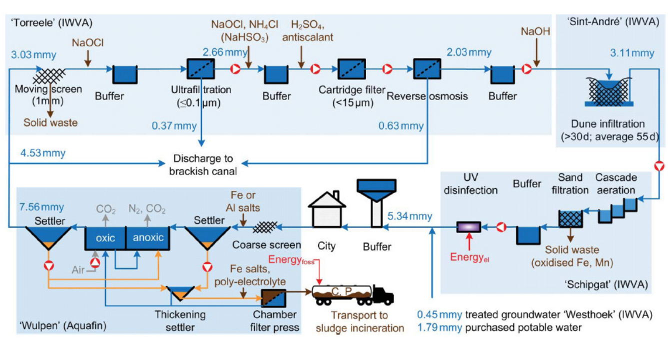
"Wurfs"

- Water resource recovery facility (WRRF)



"Wurfs"

- Water resource recovery facility (WRRF)

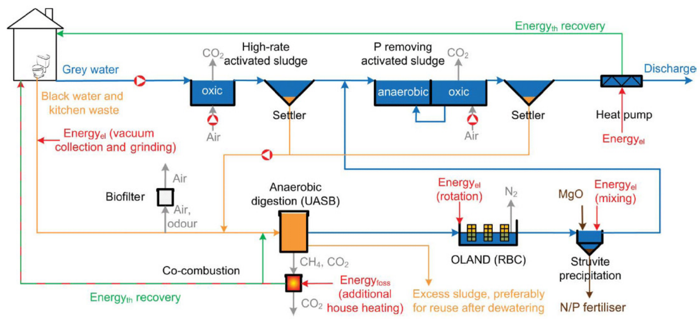


Scheme of wastewater reuse as practised in Koksijde (Belgium), with IWVA (Intercommunale Waterleidingsmaatschappij -Ambacht) responsible for drinking water production and distribution and Aquafin for sewage and wastewater treatment

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

"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.

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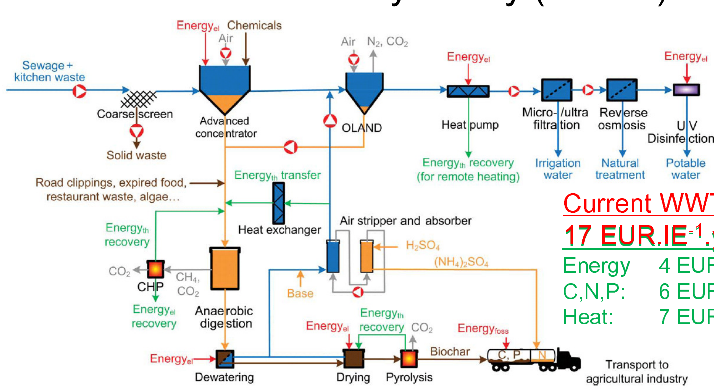
"Wurfs"

- Water resource recovery facility (WRRF)



Current WWT cost

17 EUR.IE^{-1}.yr^{-1}

Energy 4 EUR.IE^{-1}.yr^{-1}
C,N,P: 6 EUR.IE^{-1}.yr^{-1}
Heat: 7 EUR.IE^{-1}.yr^{-1}

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

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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

Outline

- Water resources
- Water resource recovery
- Modelling challenges
- Take home

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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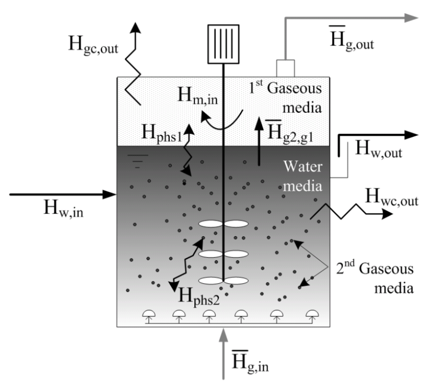
Modelling physicochemical processes

- We have to do it differently:

  <u>Temperature:</u>



Fernandez T., Grau P., Beltran S., Ayesa E. (CEIT)

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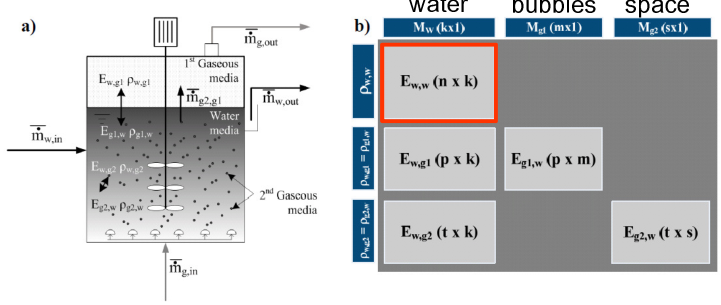
Modelling physicochemical processes

- We have to do it differently:

Gas exchange:



Fernandez T., Grau P., Beltran S., Ayesa E. (CEIT)

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Modelling physicochemical processes

- We have to do it differently:

Precipitation:

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

Towards a generalized physicochemical framework

Damien J. Batstone, Youri Amerlinck, George E
Paloma Grau, Bruce Johnson, Ishin Kaya, Jean-
Stephan Tait, Imre Takács, Peter A. Vanrollegh
Christopher J. Brouckaert and Eveline Volcke

ABSTRACT

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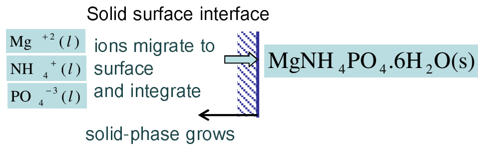
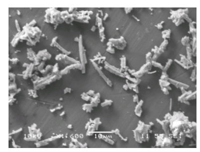
Modelling physicochemical processes

- We have to do it differently:

Precipitation:





Modelling physicochemical processes

- We have to do it differently:

Precipitation:

It gets a little crowded in wastewater

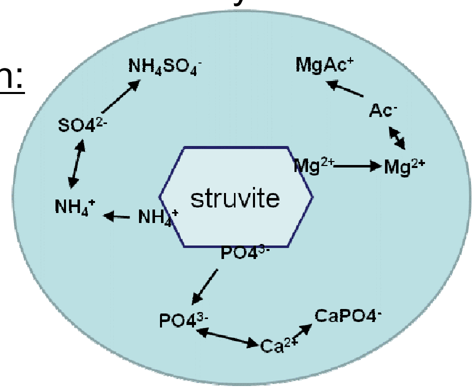
Mg^{2+} HCO^{3-} $CaOH^{+}$ $NaHPO_4^{-}$ Ca^{2+} $MgHCO_3^{+}$,$CaHPO_4$ (aq) $MgH_2PO_4^{+}$ $CaAc^{+}$ Na^{+} Cl^{-} $CaHCO_3^{+}$ Mg^{2+} $NaHCO_3$ (aq) $SO4^{2-}$ $NaCO_3^{-}$ $NaSO_4^{-}$ $HPO4^{2-}$ $MgSO_4$ (aq) $CaSO_4$ (aq) K^{+} $CO3^{2-}$ Na^{+} NaAc (aq) $CaCO_3$ (aq)

Modelling physicochemical processes

- We have to do it differently:

Precipitation:

Ion pairs increase solubility



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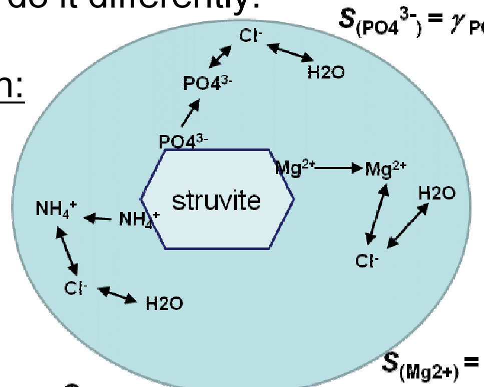
Modelling physicochemical processes

- We have to do it differently:

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

Precipitation:

Ionic strength increases solubility



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

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

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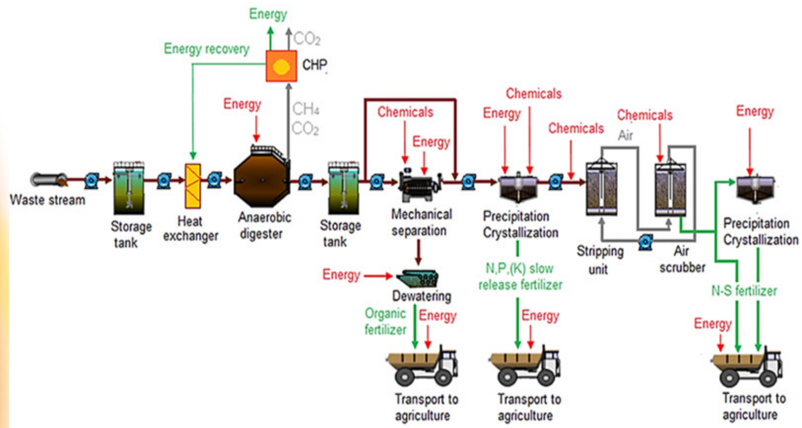
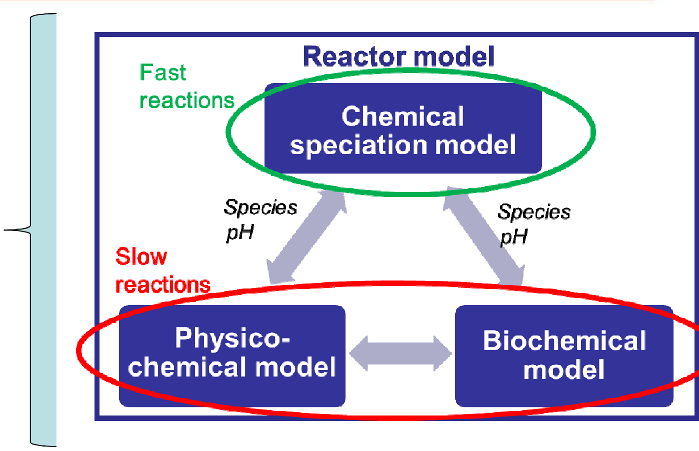
Modelling physicochemical processes in WRRFs



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

Modelling physicochemical processes

Model stiffness !



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 ↕ > 3000 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

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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

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

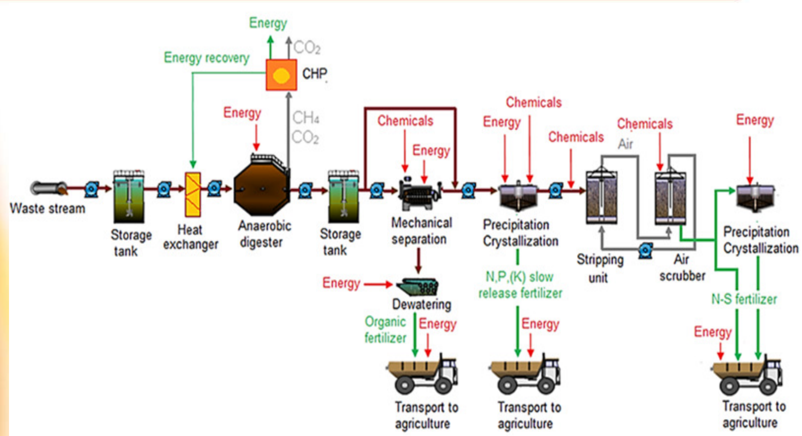
ADM1 Extension 2: Hydrolysis

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

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

Model-based optimization of resource recovery trains in WRRFs



Outline

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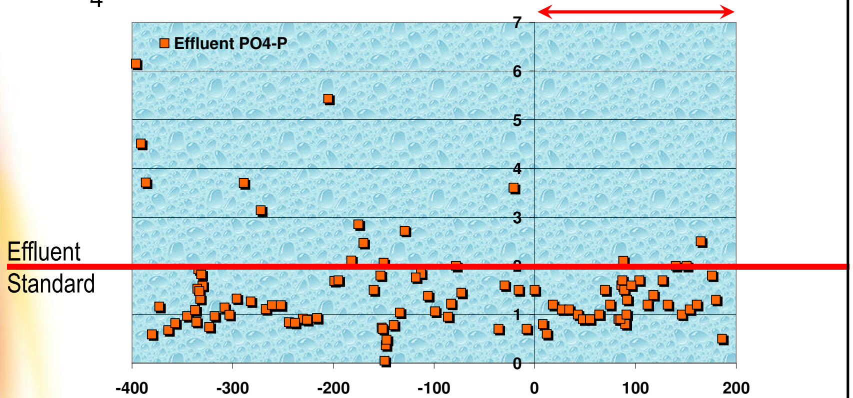
- Modelling challenges
- Control challenges
- Take home

Successful control in WWTP

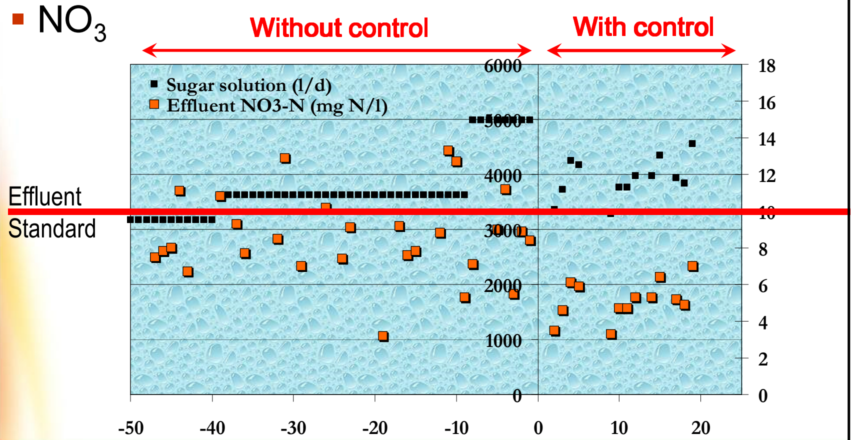
- PO_4

Fe dosage control



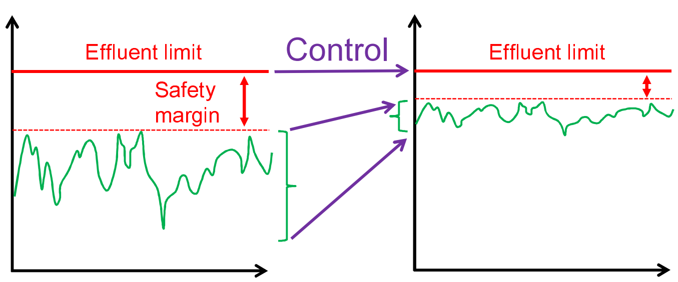
Successful control in WWTP

- NO_3



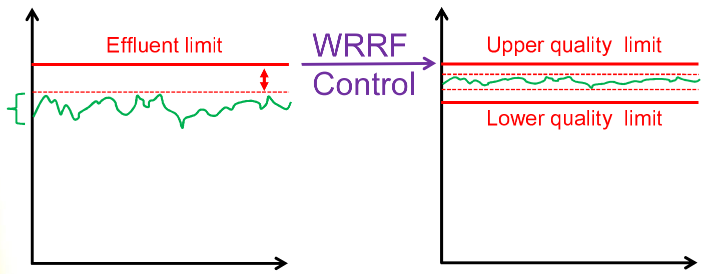
Control challenges

- Paradigm shift:



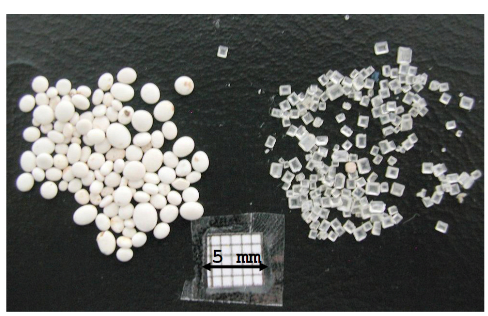
Control challenges

- Paradigm shift:



Control challenges

- Much stricter product specifications!



Control challenges

- No more forgiving client

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Control challenges

- No selection of raw materials

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Outline

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Take home messages

- WWTPs/STEPs → WRRFs/StaRREs !
- Physicochemical processes !
- Modelling challenges are non-trivial
- Resource recovery products must compete with existing products
- Product specifications are strict
- Control is much more strict (no more forgiveness!)

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Acknowledgements

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