Modelling in Sanitary Engineering

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Wastewater treatment plant – Part 1

University of Natural Resources and
Life Sciences, Vienna
Department of
Water, Atmosphere, and Environment

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Modelling of WWTPs

Content

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- Theory:
    - **Components of a WWTP model (Flow and transport models, Biokinetic models, Activated Sludge Models, Settler models)**
    - Control of AS plants (incl. sensor models)
    - Simulation studies (Unified Protocol data quality, calibration)
    - Simulation of constructed wetlands for wastewater treatment
- Modelling exercises:
    - **Development of a biokinetic model (nitrification)**
    - **Dynamic simulation of a AS plant**
    - Control of a AS plant
    - Calibration of a WWTP model

Components of a WWTP model

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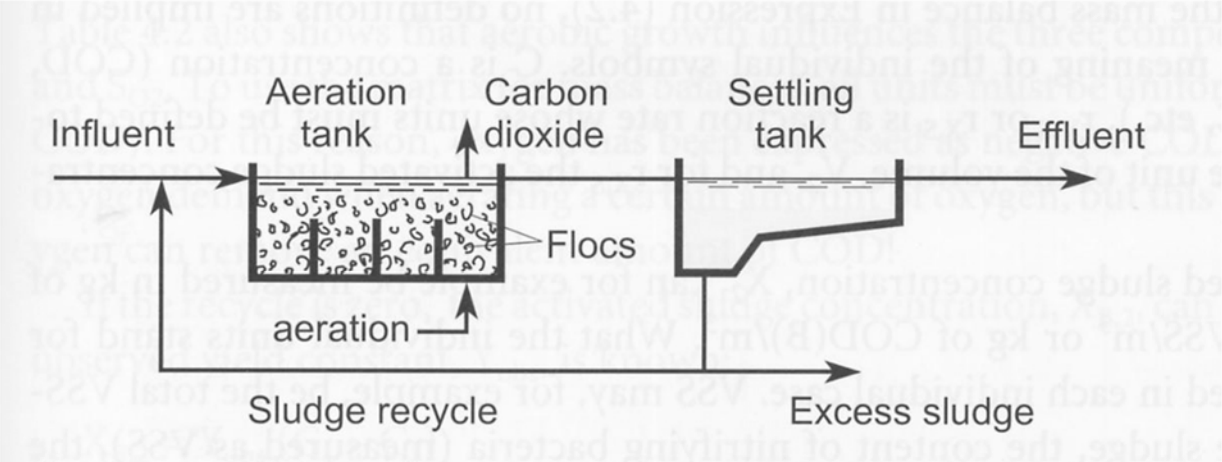
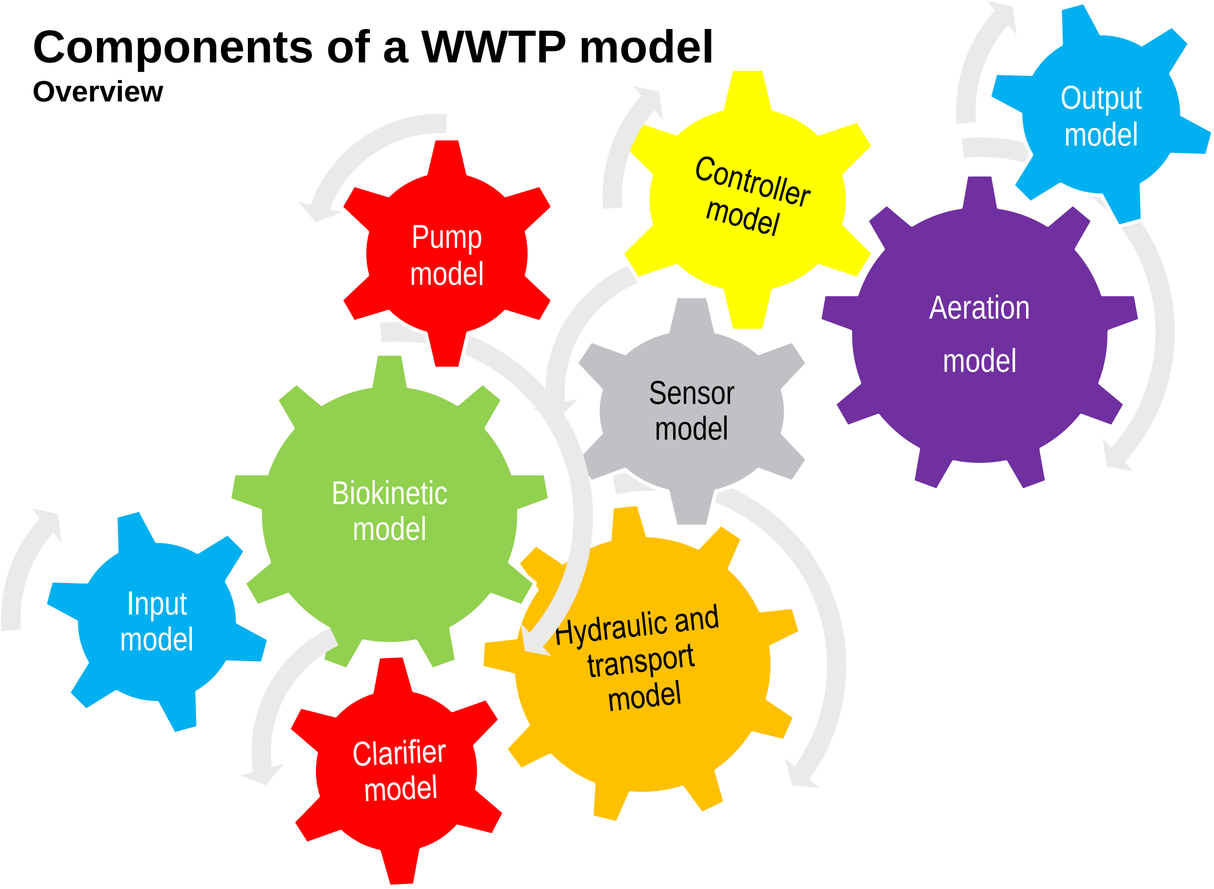


Figure 4.1. Definition of activated sludge process elements.

Components of a WWTP model

Overview



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Components of a WWTP model
Overview

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- Flow model (hydraulics)
- Model of transport processes
    - Settling: Primary and secondary clarifier
    - Activated sludge tank
    - Distribution and mixing devices
- Biokinetic model (model of the reactions)
- Operation parameters (control, sensors/actuators such as pumps and aeration)
- Input and output models

Components of a WWTP model

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Flow and transport models

- Ideal reactors
- Transport processes
- Tracer experiments

An accurate description of the flow and transport processes is at least as important as the biokinetic model

Components of a WWTP model
Flow and transport models

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Ideal reactors

- Completely stirred tank reactor – CSTR
- Cascade of CSTRs
- CSTR with variable volume
- Plug-flow reactor

Components of a WWTP model
Flow and transport models - Ideal reactors

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Completely stirred tank reactor – CSTR

Properties of a CSTR:

- Inflow = outflow
- Volume = constant
- Mixing homogeneous
- No concentration gradients
- Effluent concentration = concentration in the reactor
- Usually in steady-state

Mass balance: $V \cdot \frac{dC_A}{dt} = Q \cdot C_{A,in} - Q \cdot C_A + r_A \cdot V$

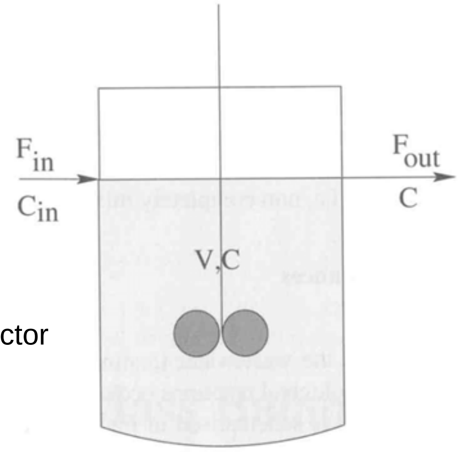
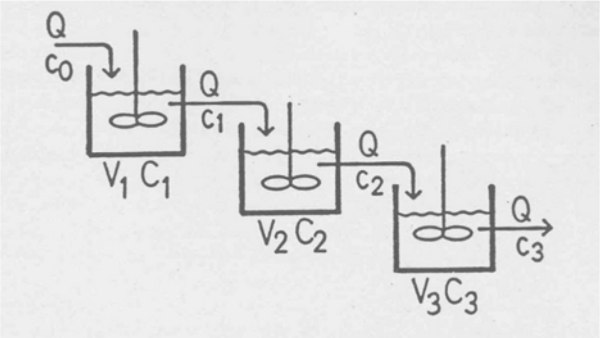


FIG. 2.1. Schematic view of a stirred tank reactor.

Components of a WWTP model

Flow and transport models - Ideal reactors

Cascade of CSTRs



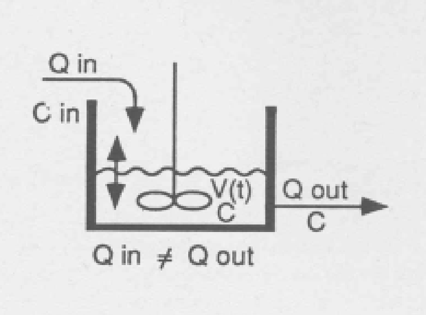
$$\frac{C_k}{C_{k-1}} = \frac{1}{1+K\cdot V_k/Q} \quad \text{with } r=-K\cdot C_k$$

$$\frac{C_k}{C_0} = \frac{1}{(1+\frac{K\cdot V_{ges}}{k\cdot Q})^k} \quad \text{with } V_{ges} = \sum_k V_k \text{ and } V_k = \frac{V_{ges}}{k}$$

Components of a WWTP model

Flow and transport models - Ideal reactors

CSTR with variable volume



Properties of CSTRs with variable volume:

- Inflow not equal outflow
- Volume variable
- Mixing homogeneous
- No concentration gradients
- Effluent concentration = concentration in the reactor
- Steady-state corresponds to CSTR
- Open system

$$\frac{dV}{dt} = Q_{in} - Q_{out}$$

$$\frac{d(V\cdot C_A)}{dt} = C_A\cdot\frac{dV}{dt} + V(t)\cdot\frac{dC_A}{dt} = Q_{in}\cdot C_{A,in} - Q_{out}\cdot C_A + r_A\cdot V(t)$$

$$\boxed{V(t)\cdot\frac{dC_A}{dt} = Q_{in}\cdot(C_{A,in}-C_A) + r_A\cdot V(t)}$$

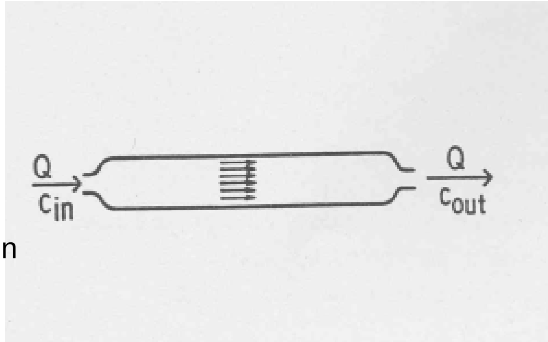
Components of a WWTP model

Flow and transport models - Ideal reactors

Plug-flow reactor

Properties of plug-flow reactors:

- Inflow = outflow
- Volume constant
- Homogeneous Mixing only in dx
- Concentration gradients along flow direction
- Steady-state is interesting



$$\frac{\partial C_A}{\partial t} = -\frac{Q}{F}\cdot\frac{\partial C_A}{\partial x} + r_A$$

Components of a WWTP model

Flow and transport models

Transport processes

- Convection (advection or turbulence)
- Molecular diffusion
- Sedimentation / Floatation
- Dispersion

Components of a WWTP model

Flow and transport models - Transport processes

Convection

- used synonymously with advection
- transport of migrants due to bulk flow of a fluid mixed phase
- $j_A = v \, . \, C_A$ (mass flux density)
- v ... flow velocity (vector)

- in turbulent water no analytical description is possible

Components of a WWTP model

Flow and transport models - Transport processes

Molecular diffusion

- Primarily due to Brownian motion in solids, liquids, and gases
- Transport von molecules driven by concentration gradients (in the direction from higher concentrations to lower concentrations)
- Fick‘s 1st law
- $j_{A,x} = - D_A \, . \, dC_A/dx$ (1D mass flux density)
- D_A ... diffusions coefficient of migrant A in liquid phase

Components of a WWTP model

Flow and transport models - Transport processes

Sedimentation / Flotation

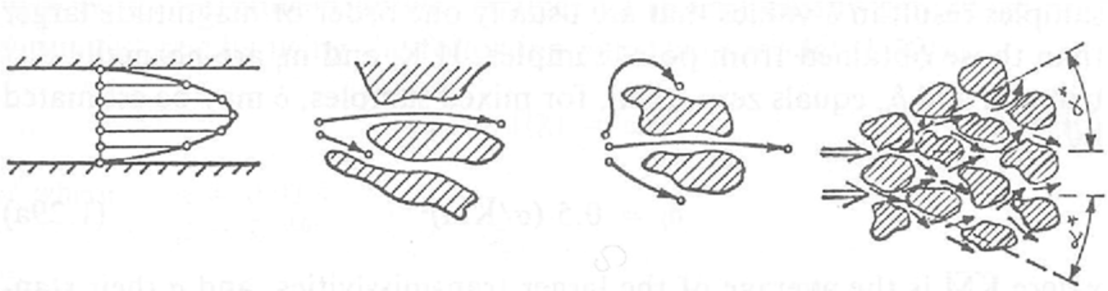
- Transport due to gravity
- $j_A = v_S \cdot C_A$ (mass flux density)
- v_S ... sedimentation velocity
- Flotation: opposite direction

Components of a WWTP model

Flow and transport models - Transport processes

Hydrodynamic dispersion

- Motion of migrants relative to the convective motion (bulk flow)
- Mathematically described as diffusion



Components of a WWTP model

Flow and transport models - Tracer experiments

Tracer experiments

- To measure the HRT of systems

Properties of tracer substances

- the same transport properties as water (similar molecular diffusion, no sedimentation)
- no influence on mixing and flow (temperature, density)
- no reaction and no adsorption
- cheap, high solubility in water, and easy to analyse
- background concentration low and/or constant

Components of a WWTP model

Flow and transport models - Tracer experiments

Possible tracers

- Salts
  - NaCl und KCl can be measured with the electrical conductivity
  - Li^+ can be measured with atomic adsorption
  - Br^- low background concentration
- fluorescent tracers
- radioactive tracers
  - very accurate, but radioactive (usually special permission needed)

Components of a WWTP model

Biokinetic models

describe

- **Degradation of organic matter**
  - Oxygen consumption and sludge production
- **Nutrient elimination**
  - Nitrogen (Nitrification/Denitrification)
  - Phosphorus (Bio-P, Precipitation)

Components of a WWTP model

Biokinetic models

Development of a biokinetic model for nitrification

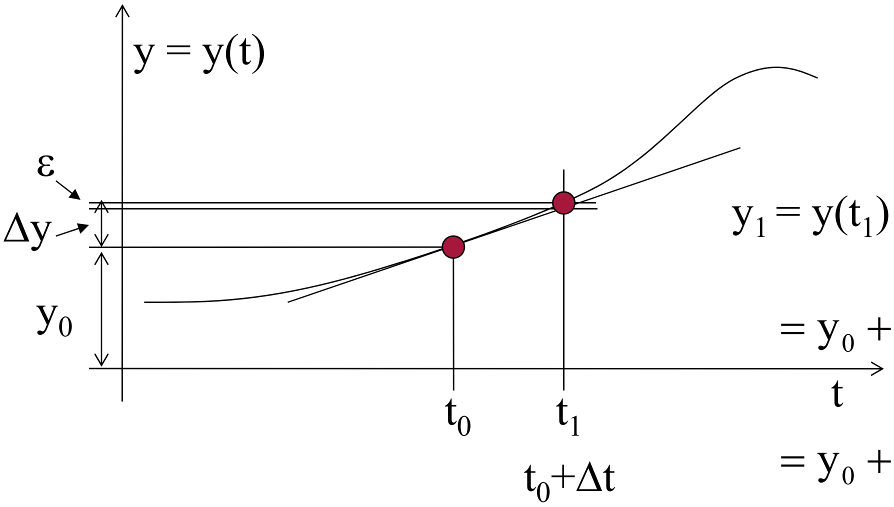
Nitrification

$NH_4^+ + 2\ O_2 \rightarrow NO_3^- + H_2O + 2\ H^+$
14 g NH_4-N require 64 g O2
- 4,57 g O_2/g NH_4-N and +1 g NO_3-N/g NH_4-N

2-stage process:
$NH_4^+ \rightarrow NO_2^-$ (*Nitrosomonas spec.*) $\rightarrow NO_3^-$ (*Nitrobakter spec.*)

In reality much more complicated.

Numerical integration



$$y_1 = y(t_1) \quad = y_0 + \Delta y + \varepsilon$$

$$= y_0 + \dot{y}(t_0) \cdot \Delta t + \varepsilon$$

$$= y_0 + \frac{\Delta y(t_0)}{\Delta t} \cdot \Delta t + \varepsilon$$

Components of a WWTP model

Development of a biokinetic model for nitrification

Model 1 - Reaction with zero-order kinetics

Reaction rate: r = k0

1 g NH_4-N result in 1 g NO_3-N
100 mg XAUT/l
k_0 = 11 g_N / h

Excel-File: Nitrification.xls[Model 1]

Components of a WWTP model
Development of a biokinetic model for nitrification

Model 2 - Reaction with first-order kinetics

Reaction rate: $r = k_1 \cdot C_{SNH4}$
$k1 = 0.15\ g_N / (g_N \cdot h)$

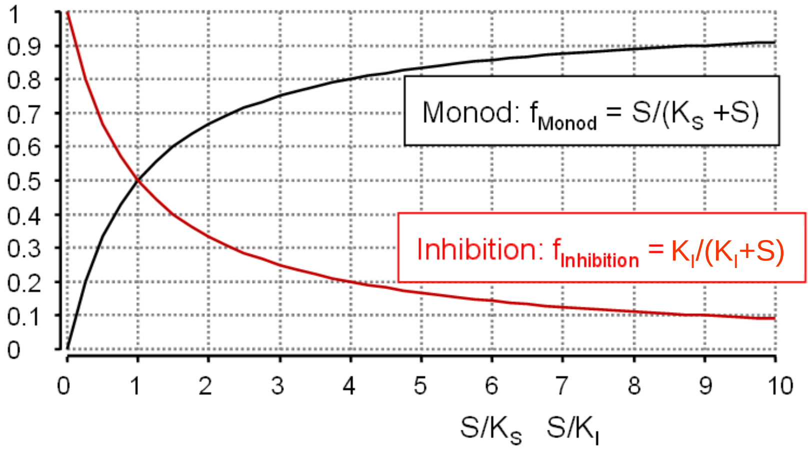
Components of a WWTP model
Development of a biokinetic model for nitrification

Model 3 - Reaction with Monod kinetics

Growth rate $\mu = \mu_{max} * f_{Monod}$
Reaction rate $r = \mu \cdot X$

Stoichiometric matrix related to biomass

$\mu_m = 0.15\ g_{NO3\text{-}N}/(g_{COD,BM} \cdot h)$
$k_S = 0.20\ mg_{NH4\text{-}N}/l$



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Components of a WWTP model

Development of a biokinetic model for nitrification

Model 4 - including bacterial growth

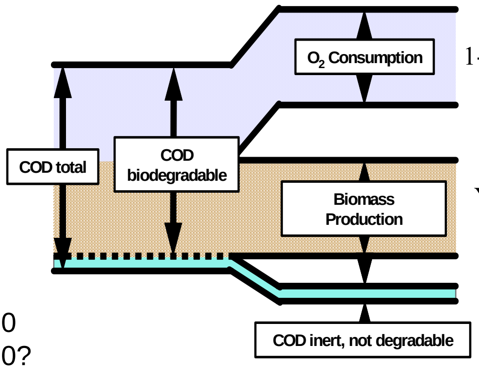
Autotrophic yield

- $Y_{AUT} = 0.24\ g_{COD,BM}/g_N$

Yield for different biological systems

Heterotrophic bacteria	0.67
Fish (1 yr, 0.5 kg)	0.45
Hen	0.32
Pig (to 65 kg)	0.23
Human (0-16 yrs)	0.010
Human (from 16 yrs)	0.000?

(in kg body weight produced per kg food consumed, Henze et al., 2002)



$$1\text{-Yield} \Rightarrow \frac{1\text{-Yield}}{\text{Yield}} = 1 - \frac{1}{\text{Yield}}$$

$$\text{Yield} \Rightarrow \frac{\text{Yield}}{\text{Yield}} = 1$$

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Components of a WWTP model

Development of a biokinetic model for nitrification

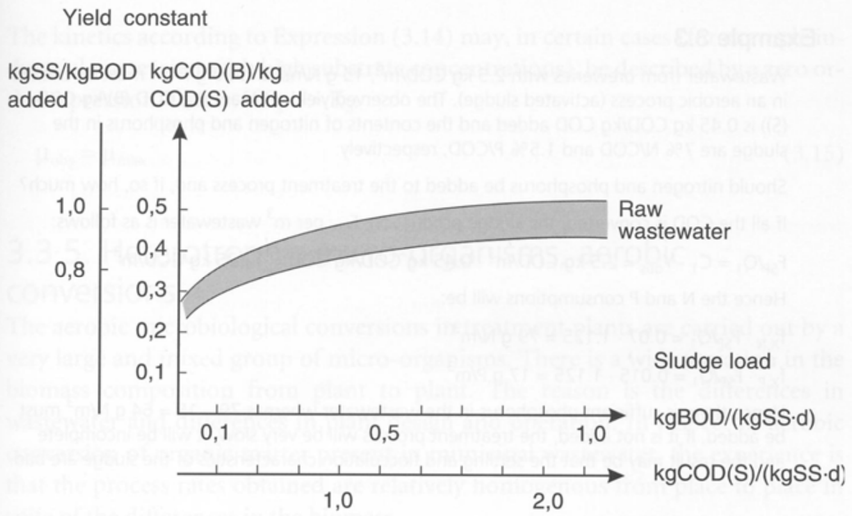

Figure 3.5. Observed yield constant as a function of the sludge load in activated sludge plants.

Components of a WWTP model

Development of a biokinetic model for nitrification

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Model 4a - including N incorporation (organic N of biomass)

$i_N = 0.08\ g_N\ /\ g_{COD,BM}$

Components of a WWTP model

Development of a biokinetic model for nitrification

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Model 5 - including microbial decay (lysis)

Concepts to describe the energy balance of micro-organisms

- Endogenous respiration
  - direct respiration (oxygen demand) of micro-organisms (O_2 or NO_3^- required)
- Death-regeneration (lysis)
  - Death ➔ degradation ➔ new substrate is generated that is available for other micro-organisms [biomass ➔ substrate (COD) + nutrients (N + P)]
  - Results in indirect oxygen demand

$r = b\ .\ X$
$b = 0.025\ g_{COD}\ /\ (g_{COD,BM}.h)$

Components of a WWTP model

Development of a biokinetic model for nitrification

Model 6 - including oxygen consumption

+ 1 g_{O2} / $g_{COD,BM}$ and - 4.57 g_{O2} / $g_{NH4\text{-}N}$

4.57 / 0.24

(g_{O2} / $g_{NH4\text{-}N}$) / ($g_{COD,BM}$ / $g_{NH4\text{-}N}$)

Stoichiometric factor $1-\frac{4{,}57}{Y_{AUT}}=-\frac{4{,}57-Y_{AUT}}{Y_{AUT}}$

Growth rate $\mu=\mu_{\max}\cdot\frac{C_{SNH4}}{K_{S,NH4}+C_{SNH4}}\cdot\frac{C_{SO2}}{K_{S,O2}+C_{SO2}}$

$K_{S,O2}$ = 1 mg_{O2}/l

Components of a WWTP model

Development of a biokinetic model for nitrification

Model 7 - including aeration

$$\frac{dC_{SO2}}{dt}=kLa\cdot(C_{SO2,sat}-C_{SO2})$$

k_{La} = 0.1 h-1
$C_{SO2,sat}$ (20°C) = 9.08 mg_{O2}/l

Components of a WWTP model

Development of a biokinetic model for activated sludge plants

describing

- **Degradation of organic matter**
    - Oxygen consumption and sludge production
- **Nutrient elimination**
    - Nitrogen (Nitrification/Denitrification)
    - Phosphorus (Bio-P, Precipitation)

Components of a WWTP model

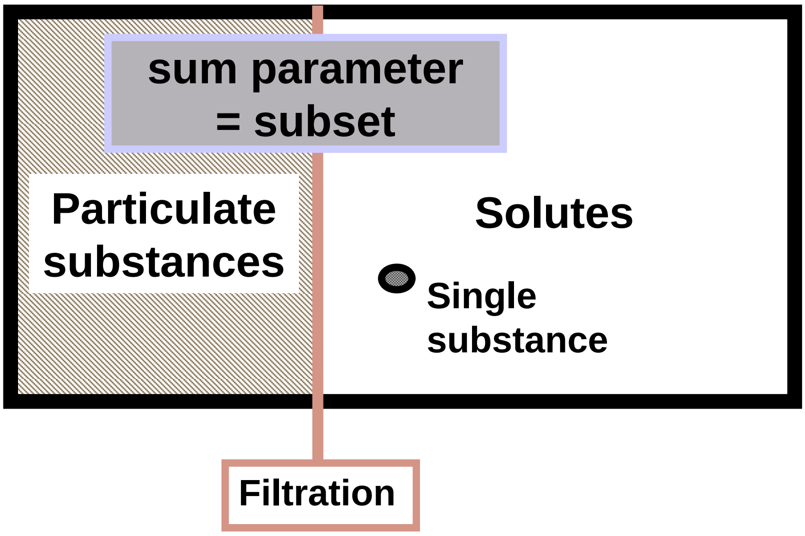
Development of a biokinetic model for AS plants

The concept of sum parameters

- Wastewater is a „raw product“ with unknown composition
- Numerous organic substances ➔ not detectable as single substances
- Behaviour of sum parameters is described with models
- Behaviour of single substances (e.g. ammonia is a special case)

Components of a WWTP model

Development of a biokinetic model for AS plants



sum parameter = subset

Particulate substances

Solutes

Single substance

Filtration

Components of a WWTP model

Development of a biokinetic model for AS plants

Example: Aerobic degradation of glucose (1)

in mol:

$$C_6H_{12}O_6 + 2.45\ O_2 + 0.71\ NH_3 \rightarrow 0.71\ C_5H_7NO_2 + 2.45\ CO_2 + 4.58\ H_2O$$

in mass units :

$$180g\ C_6H_{12}O_6 + 2.45 \cdot 32g\ O_2 + 0.71 \cdot 17g\ NH_3 \rightarrow$$

$$0.71 \cdot 113g\ C5H7NO_2 + 2.45 \cdot 44g\ CO_2 + 4.58 \cdot 18g\ H_2O$$

Components of a WWTP model

Development of a biokinetic model for AS plants

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Example: Aerobic degradation of glucose (2)

Stoichiometric factors n based on biomass:

reactants:	products:
- 2.24 $g_{C6H12O6}$ / g_{BM}	+ 1 $g_{C5H7NO2}$ / g_{BM}
- 0.98 g_{O2}/ g_{BM}	+ 1.34 g_{CO2}/ g_{BM}
- 0.15 g_{NH3} /g_{BM}	+ 1.03 g_{H2O} /g_{BM}

Growth rate ρ = 1500 g_{BM}/d

Reaction rates: $r(C_6H_{12}O_6)$ = - 2.24 . 1500 g/d

$r(CO_2)$ = + 1.34 . 1500 g/d

Components of a WWTP model

Development of a biokinetic model for AS plants

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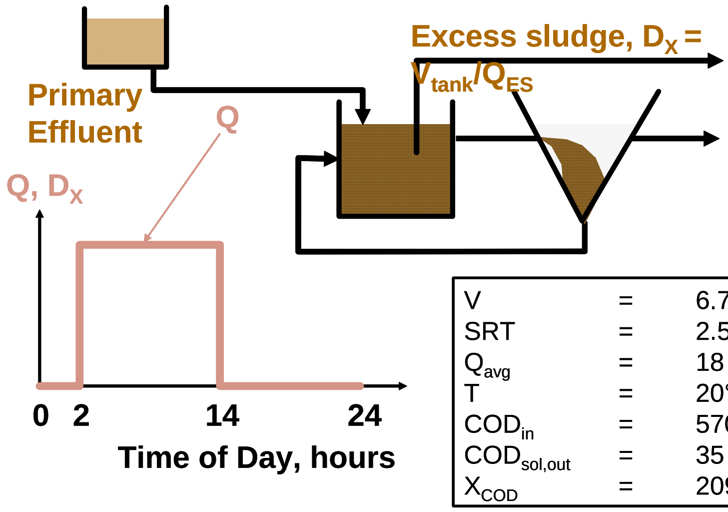
Pilot plant – characteristics (Ekama and Marais, 1978)

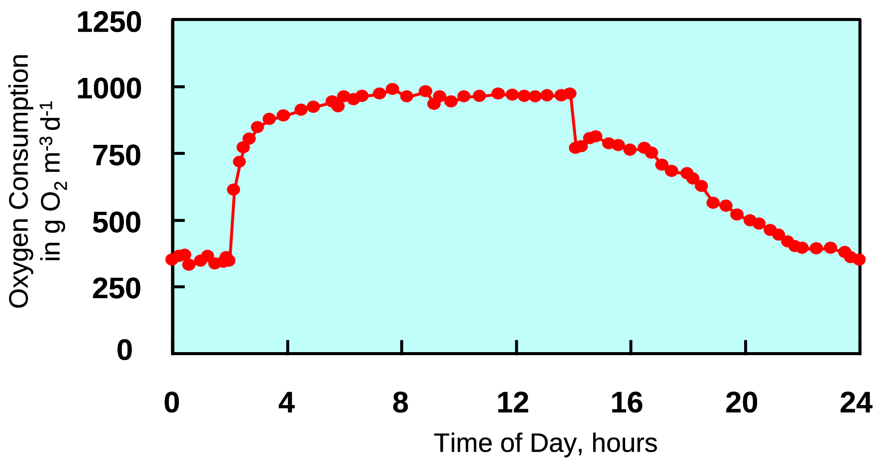


V = 6.7 l
SRT = 2.5 d
Q_{avg} = 18 l d^{-1}
T = 20°C
COD_{in} = 570 g m^{-3}
$COD_{sol,out}$ = 35 g m^{-3}
X_{COD} = 2090 g m^{-3}

Components of a WWTP model

Development of a biokinetic model for AS plants

Pilot plant – Experimental results: (Ekama and Marais, 1978)



Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model 0 - Growth of heterotrophic organisms

Component	SO2	SI	SS	XH	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1	$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot X_H$

Y_H = 0.67 g COD(BM) / g COD(SS) ... Heterotrophic yield factor

μ_H = 4.0 d^{-1} ... max. heterotrophic growth rate

$K_{H,O2}$ = 0.2 g O_2/L ... Half-saturation coefficient for O2

$K_{H,SS}$ = 5.0 g COD(SS)/L ... Half-saturation coefficient for substrate

Influent: COD = 570 mg/L ➔ SS = 540 mg/L; SI = 30 mg/L

Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model 0 - Growth of heterotrophic organisms

Component	SO2	SI	SS	XH	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1	$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$

$$\frac{d\,SO2}{dt} = (1-\frac{1}{Y_H}) \cdot \mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$$

$$\frac{d\,SS}{dt} = (-\frac{1}{Y_H}) \cdot \mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$$

$$\frac{d\,XH}{dt} = (1) \cdot \mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$$

Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model 0 - Growth of heterotrophic organisms

Components

1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. Heterotrophic biomass XH

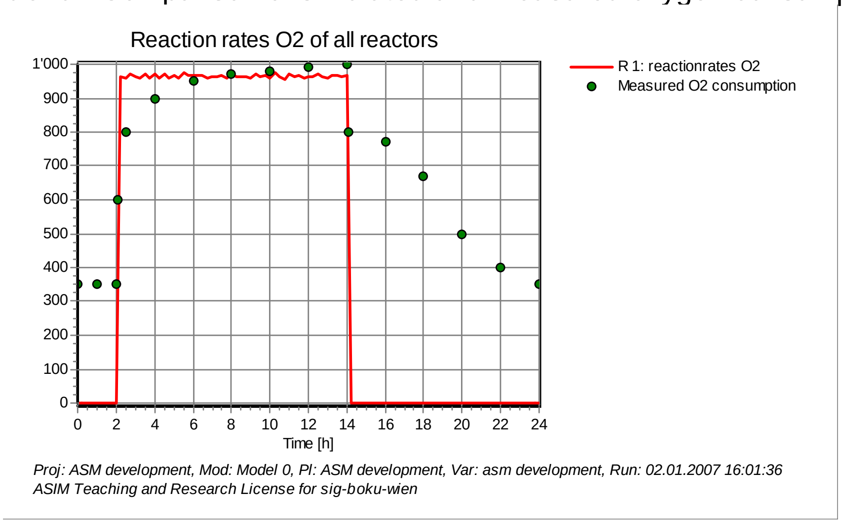
Processes

1. Aerobic growths of heterotrophic organisms

Components of a WWTP model

Development of a biokinetic model for AS plants

Model 0 - Comparison of simulated and measured oxygen consumption



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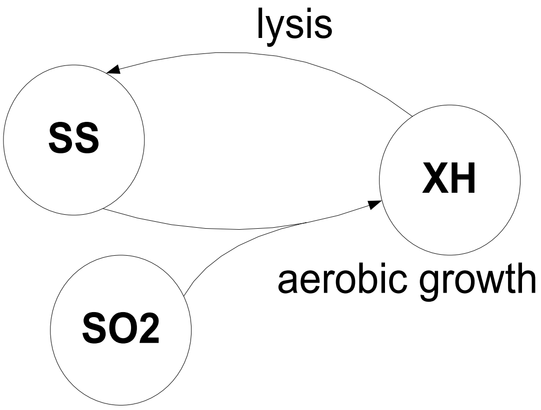
Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model A - Growth and Lysis of heterotrophic organisms



Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model A - Growth and Lysis of heterotrophic organisms

Components

1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. Heterotrophic biomass XH

Processes

1. Aerobic growths of heterotrophic organisms
2. **Lysis of heterotrophic organisms**

Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model A - Growth and Lysis of heterotrophic organisms

Component	SO2	SI	SS	XH	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1	$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$
Lysis			**+1**	**-1**	$b_H \cdot XH$

Y_H = 0.67 g COD(BM) / g COD(SS) ... Heterotrophic yield factor
μ_H = 2.5 d^{-1} ... max. heterotrophic growth rate
$K_{H,O2}$ = 0.2 g O_2/L ... Half-saturation coefficient for O2
$K_{H,SS}$ = 5.0 g COD(SS)/L ... Half-saturation coefficient for substrate
b_H = 0.4 d^{-1} ... Heterotrophic decay constant
Influent: COD = 570 mg/L ➔ SS = 540 mg/L; SI = 30 mg/L

Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model A - Growth and Lysis of heterotrophic organisms

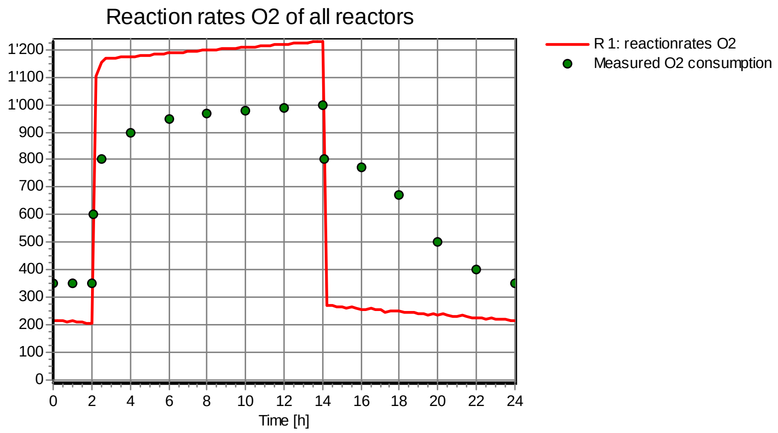
Component	SO2	SI	SS	XH	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1	$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$
Lysis			+1	-1	$b_H \cdot XH$

$$\frac{d\,SS}{dt} = (-\frac{1}{Y_H}) \cdot \mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH \quad \underline{+1 \cdot b_H \cdot XH}$$

Components of a WWTP model

Development of a biokinetic model for AS plants

Model A - Comparison of simulated and measured oxygen consumption



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Components of a WWTP model

Development of a biokinetic model for AS plants

Aerobic degradation of soluble organic C

Model A - Growth and Lysis of heterotrophic organisms

Simulation results

- too rapid increase and decrease of oxygen consumption

Extension

- higher molecular particulate organic substances XS that are transformed to low molecular solute organic substances SS due to hydrolysis

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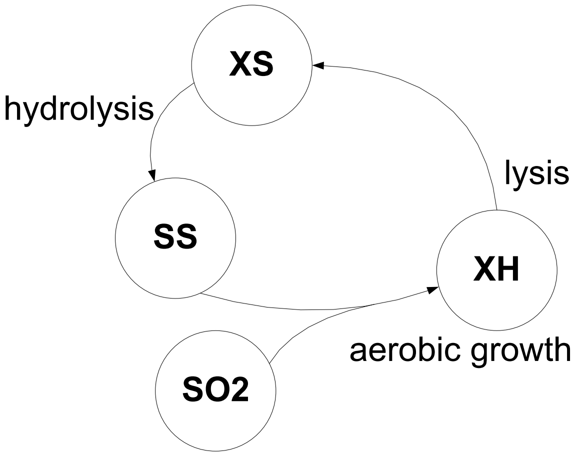
Components of a WWTP model

Development of a biokinetic model for AS plants

Model B - Aerobic degradation of soluble and particulate organic C



Components of a WWTP model

Development of a biokinetic model for AS plants

Model B - Aerobic degradation of soluble and particulate organic C

Components

1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. Heterotrophic biomass XH
5. **Slowly biodegradable particulate organic matter XS**

Processes

1. Aerobic growths of heterotrophic organisms
2. Lysis of heterotrophic organisms
3. **(Aerobic) Hydrolysis (transformation of XS to SS)**

Components of a WWTP model

Development of a biokinetic model for AS plants

Model B - Aerobic degradation of soluble and particulate organic C

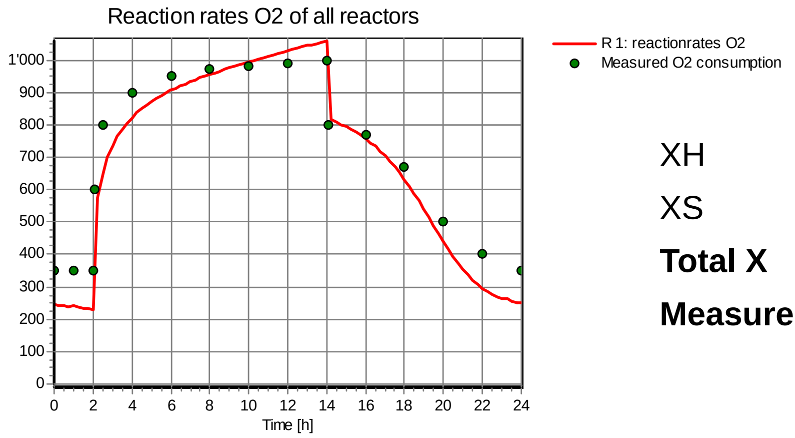
Component	SO2	SI	SS	XH	XS	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1		$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$
Lysis				-1	**+1**	$b_H \cdot X_H$
Hydrolysis			**+1**		**-1**	$k_H \cdot \frac{XS/XH}{K_X+XS/XH} \cdot \frac{SO2}{K_{Hyd,O2}+SO2} \cdot XH$

k_H = 1.6 g COD(SS) / g COD(XS) ... Hydrolysis constant
K_X = 0.04 g COD(SS) / g COD(BM) ... Saturation coefficient for adsorption
$K_{H,O2}$ = 0.1 g O_2 / L ... Saturation coefficient for O2
Influent: COD = 570 mg/L ➔ XS = 430 mg/L; SS = 110 mg/L; SI = 30 mg/L

Components of a WWTP model

Development of a biokinetic model for AS plants

Model B - Comparison with measured oxygen consumption



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XH	1592 mg/L
XS	25 mg/L
Total X	**1617 mg/L**
Measured:	**2090 mg/L**

Components of a WWTP model

Development of a biokinetic model for AS plants

Model B - Aerobic degradation of soluble and particulate organic C

Simulation results

- oxygen consumption well modelled
- sludge production underestimated (Experiment 2.1 g COD / L; Simulation 1.6)

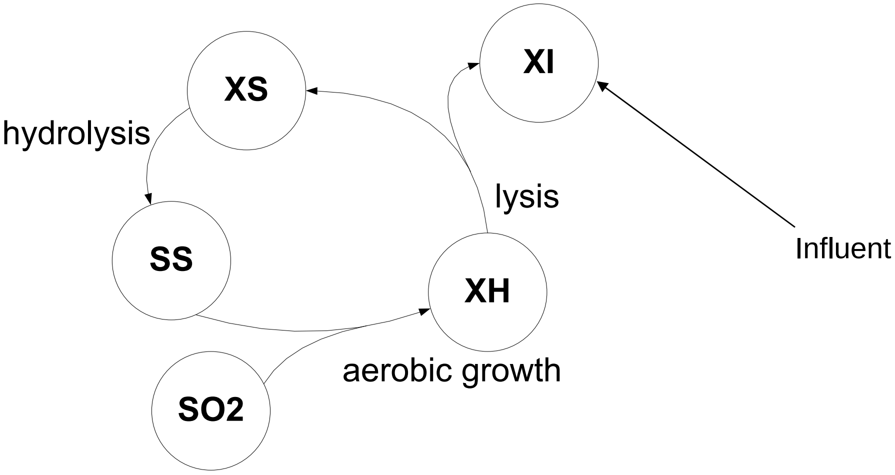
Extension

- inert particulate matter XI, that is not degradable and accumulates in the sludge

Components of a WWTP model

Development of a biokinetic model for AS plants

Model C - Non-degradable particulate matter



Components of a WWTP model

Development of a biokinetic model for AS plants

Model C - Non-degradable particulate matter

Components

1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. Heterotrophic biomass XH
5. Slowly biodegradable particulate organic matter XS
6. **Non-degradable particulate matter XI**

Processes

1. Aerobic growths of heterotrophic organisms
2. Lysis of heterotrophic organisms
3. (Aerobic) Hydrolysis (transformation of XS to SS)

Components of a WWTP model

Development of a biokinetic model for AS plants

Model C - Non-degradable particulate matter

Component	SO2	SI	SS	XH	XS	XI	Process rate r_i
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	+1			$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$
Lysis				-1	**$1-f_I$**	**f_I**	$b_H \cdot XH$
Hydrolysis			+1		-1		$k_H \cdot \frac{XS/XH}{K_X+XS/XH} \cdot \frac{SO2}{K_{Hyd,O2}+SO2} \cdot XH$

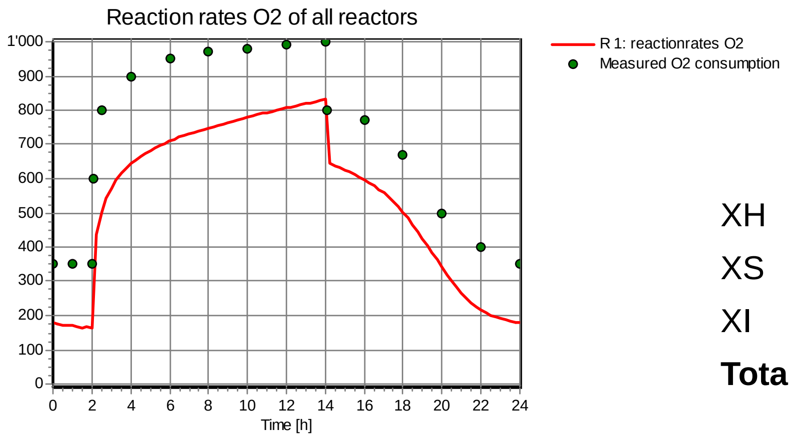
f_I = 0.08 g COD(XI)/g COD(BM) ... Inert matter generation during lysis

Influent: COD = 570 mg/L ➔ XI = 100 mg/L; XS = 330 mg/L; SS = 110 mg/L; SI = 30 mg/L

Components of a WWTP model

Development of a biokinetic model for AS plants

Model C - Comparison of simulated and measured oxygen consumption



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XH	1241 mg/L
XS	17 mg/L
XI	742 mg/L
Total X	**2000 mg/L**

Components of a WWTP model
Development of a biokinetic model for AS plants

Model C - Non-degradable particulate matter

Simulation results
- sludge concentration fits
- oxygen consumption too low

Extension
- consideration of oxygen consumption due to nitrification
- effluent of experimental plant: 20 mg$_{NO3-N}$/l (mean value) ➔ nitrification occurred although sludge age only 2.5 days

---

Components of a WWTP model
Development of a biokinetic model for AS plants

Model D - Nitrification

Components
1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. **Soluble Ammonia SNH4**
5. **Soluble Nitrate (and Nitrite) SNO3**
6. Heterotrophic biomass XH
7. Slowly biodegradable particulate organic matter XS
8. Non-degradable particulate matter XI
9. **Autotrophic biomass XA**

Components of a WWTP model

Development of a biokinetic model for AS plants

Model D - Nitrification

Processes

1. Aerobic growths of heterotrophic organisms
2. Lysis of heterotrophic organisms
3. (Aerobic) Hydrolysis (transformation of XS to SS)
4. **Aerobic growth of autotrophic organisms (Nitrifiers)**
5. **Lysis of autotrophic organisms**

Components of a WWTP model

Development of a biokinetic model for AS plants

Model D – Nitrification: Stoichiometry

Process/Component	SO2	SI	SS	**SNH**	**SNO**	XH	XS	XI	**XA**
Heterotrophic growth	$1-\frac{1}{Y_H}$		$-\frac{1}{Y_H}$	$i_N \cdot \frac{1-Y_H}{Y_H}$		+1			
Heterotrophic lysis						-1	$1-f_I$	f_I	
Hydrolysis			+1				-1		
Autotrophic growth	$\frac{Y_A-4.57}{Y_A}$			$-i_N-\frac{1}{Y_A}$	$\frac{1}{Y_A}$				+1
Autotrophic lysis							$1-f_I$	f_I	-1

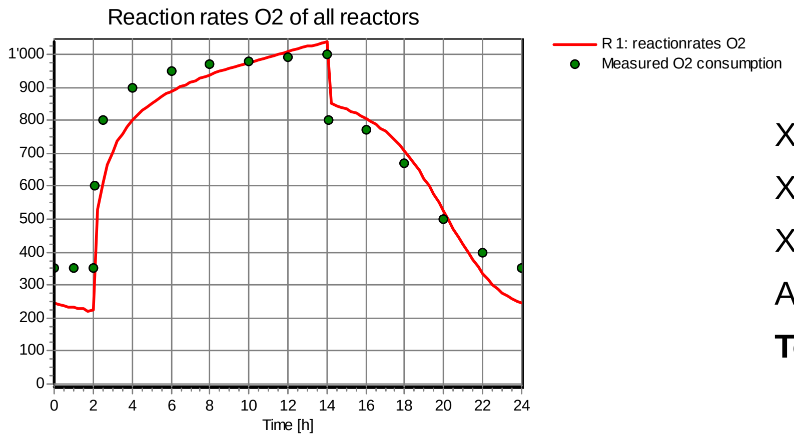
Components of a WWTP model
Development of a biokinetic model for AS plants

Model D – Nitrification: Kinetics

Process	Process rate
Heterotrophic growth	$\mu_H \cdot \frac{SO2}{K_{H,O2}+SO2} \cdot \frac{SS}{K_{H,SS}+SS} \cdot XH$
Heterotrophic lysis	$b_H \cdot XH$
Hydrolysis	$k_H \cdot \frac{XS/XH}{K_X+XS/XH} \cdot \frac{SO2}{K_{Hyd,O2}+SO2} \cdot XH$
Autotrophic growth (nitrification)	$\mu_A \cdot \frac{SO2}{K_{A,O2}+SO2} \cdot \frac{SNH}{K_{A,SNH}+SNH} \cdot XA$
Autotrophic lysis	$b_A \cdot XA$

Components of a WWTP model
Development of a biokinetic model for AS plants

Model D - Comparison of simulated and measured oxygen consumption



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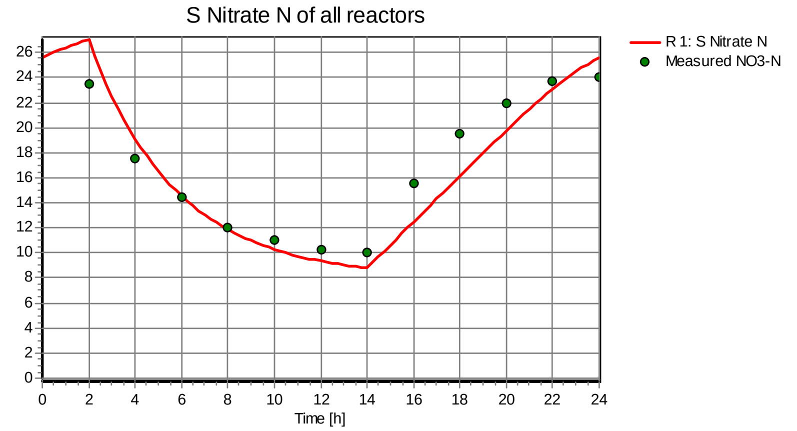
XH	1124 mg/L
XS	17 mg/L
XI	769 mg/L
AUT	721 mg/L
Total X	**1931 mg/L**

Components of a WWTP model
Development of a biokinetic model for AS plants

Model D - Comparison of simulated and measured effluent nitrate concentration



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Components of a WWTP model
Development of a biokinetic model for AS plants

Model E – Denitrification

Components

1. Soluble oxygen SO2
2. Soluble biodegradable organic matter SS
3. Soluble inert organic matter SI
4. Soluble Ammonia SNH4
5. Soluble Nitrate (and Nitrite) SNO3
6. Heterotrophic biomass XH
7. Slowly biodegradable particulate organic matter XS
8. Non-degradable particulate matter XI
9. Autotrophic biomass XA

Components of a WWTP model

Development of a biokinetic model for AS plants

Model E – Denitrification

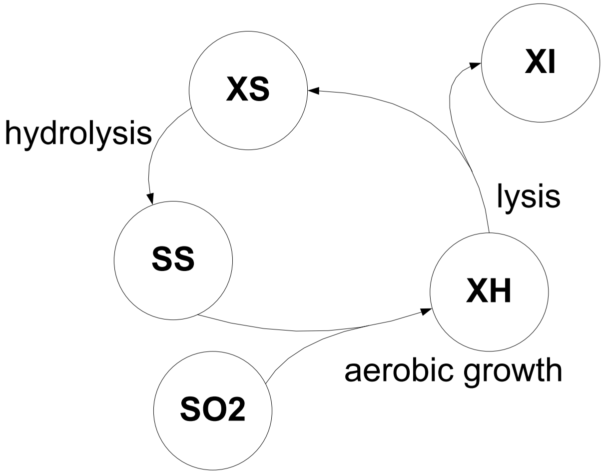
Processes

1. Aerobic growths of heterotrophic organisms
2. Lysis of heterotrophic organisms
3. (Aerobic) Hydrolysis (transformation of XS to SS)
4. Aerobic growth of autotrophic organisms (Nitrifiers)
5. Lysis of autotrophic organisms
6. **Anoxic growths of heterotrophic organisms (denitrification)**
7. **(Anoxic) Hydrolysis**

Components of a WWTP model

Development of a biokinetic model for AS plants

Model C - Aerobic growth

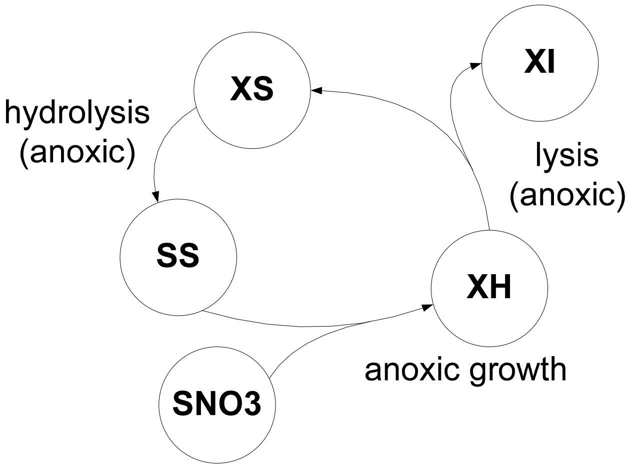


Components of a WWTP model

Development of a biokinetic model for AS plants

University of Natural Resources and Life Sciences, Vienna
Department of
Water, Atmosphere, and Environment

Model E – Denitrification

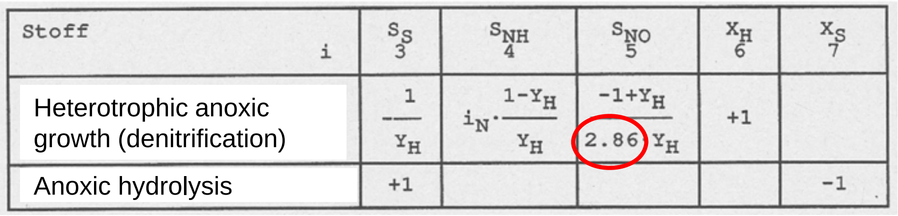


Components of a WWTP model

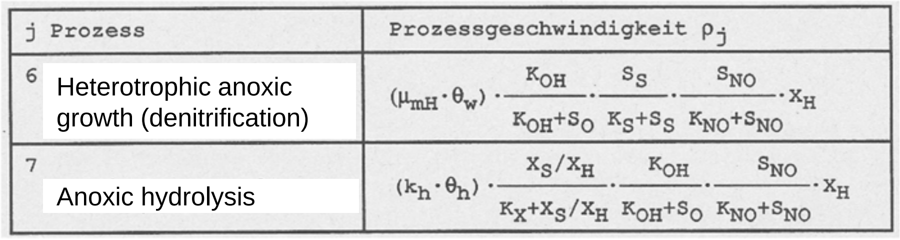
Development of a biokinetic model for AS plants

University of Natural Resources and Life Sciences, Vienna
Department of
Water, Atmosphere, and Environment

Model E – Denitrification



Stoff i	S_S 3	S_{NH} 4	S_{NO} 5	X_H 6	X_S 7
Heterotrophic anoxic growth (denitrification)	$\frac{1}{Y_H}$	$i_N \cdot \frac{1-Y_H}{Y_H}$	$\frac{-1+Y_H}{2.86 \cdot Y_H}$	+1	
Anoxic hydrolysis	+1				-1



j Prozess	Prozessgeschwindigkeit ρ_j
6 Heterotrophic anoxic growth (denitrification)	$(\mu_{mH} \cdot \theta_w) \cdot \frac{K_{OH}}{K_{OH}+S_O} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_{NO}}{K_{NO}+S_{NO}} \cdot X_H$
7 Anoxic hydrolysis	$(k_h \cdot \theta_h) \cdot \frac{X_S/X_H}{K_X+X_S/X_H} \cdot \frac{K_{OH}}{K_{OH}+S_O} \cdot \frac{S_{NO}}{K_{NO}+S_{NO}} \cdot X_H$

Components of a WWTP model

Development of a biokinetic model for AS plants

Model E – Denitrification – Stoichiometry

Denitrification (C-source = CH_2O = formaldehyde):

$5\ CH_2O + 4\ NO_3^- + 4\ H^+ \rightarrow 5\ CO_2 + 2\ N_2(aq) + 7\ H_2O$
(4 x 14) = 56g NO_3-N for (5 x 30) = 150g $CH_2O \rightarrow 2.679\ g_{CH2O} / g_{NO3N}$

Oxidation:

$CH_2O + O_2(aq) \rightarrow CO_2 + H_2O$
32g O_2 for 30g $CH_2O \rightarrow 1.067 g_{O2} / g_{CH2O}$

2.679 x 1.067 = **$2.86\ g_{O2} / g_{NO3N}$**

Components of a WWTP model

Development of a biokinetic model for AS plants

Models for phosphorus removal

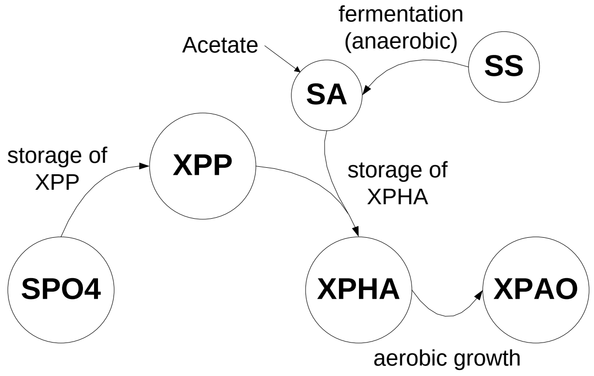
1) Biological P-Removal (Bio-P)
- „Luxury Uptake“ (e.g. Acinetobacter)
- XPAO = P-accumulating organisms

2) Chemical P-Precipitation
- $Me(PO_4)_x(OH)_{3-3x}$ ... Me … metal
- 1/x = b ... Stoichiometric ratio for dosing of Me

Components of a WWTP model

Development of a biokinetic model for AS plants

Model for Bio-P (EBPR – Enhanced Biological Phosphorus Removal) e.g. ASM2



XPHA ... cell-internal organic storage product of XPAO (Poly-hydroxy-alkanoates)

XPP ... cell-internal inorganic storage product of XPAO (Poly-Phosphat)

Components of a WWTP model

Development of a biokinetic model for AS plants

Model for chemical P precipitation (chemical equilibrium)

Components

- Soluble phosphorus (orthophosphate) SPO4
- Soluble Iron SFe
- Iron-hydroxide XFeOH
- Iron-phosphate XFeP

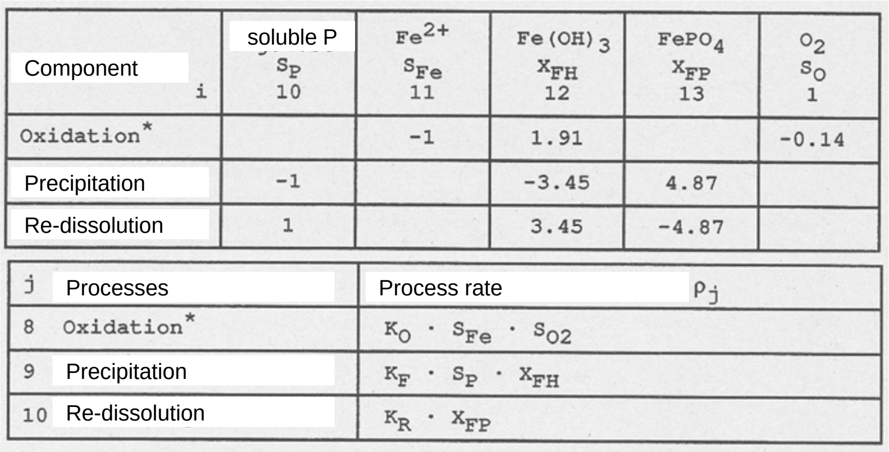
Processes

- Oxidation $Fe^{2+} \rightarrow Fe^{3+}$
- Precipitation SPO4 ➔ XFeP
- Re-dissolution XFeP ➔ SPO4

Components of a WWTP model

Development of a biokinetic model for AS plants

Model F - Model for chemical P precipitation



Component i	soluble P S_P 10	Fe^{2+} S_{Fe} 11	$Fe(OH)_3$ X_{FH} 12	$FePO_4$ X_{FP} 13	O_2 S_O 1
Oxidation*		-1	1.91		-0.14
Precipitation	-1		-3.45	4.87	
Re-dissolution	1		3.45	-4.87	

j	Processes	Process rate ρ_j
8	Oxidation*	$K_O \cdot S_{Fe} \cdot S_{O2}$
9	Precipitation	$K_F \cdot S_P \cdot X_{FH}$
10	Re-dissolution	$K_R \cdot X_{FP}$

Components of a WWTP model

IWA Activated Sludge Models

IWA – International Water Association (since 2000)
IAWQ – International Association on Water Quality (1990-2000)
IAWPRC – International Association on Water Pollution Research and Control (<1990)

Components of a WWTP model

IWA Activated Sludge Models

IWA Activated Sludge Model No.1 (ASM1, 1987)

Fundamentals

- 13 components and 8 processes
- Describes oxygen consumption, sludge production and nitrogen elimination
- Mass balances for C and N
- Standard model for numerical simulation of activated sludge plants

References

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Components of a WWTP model

IWA Activated Sludge Models

ASM1 – components

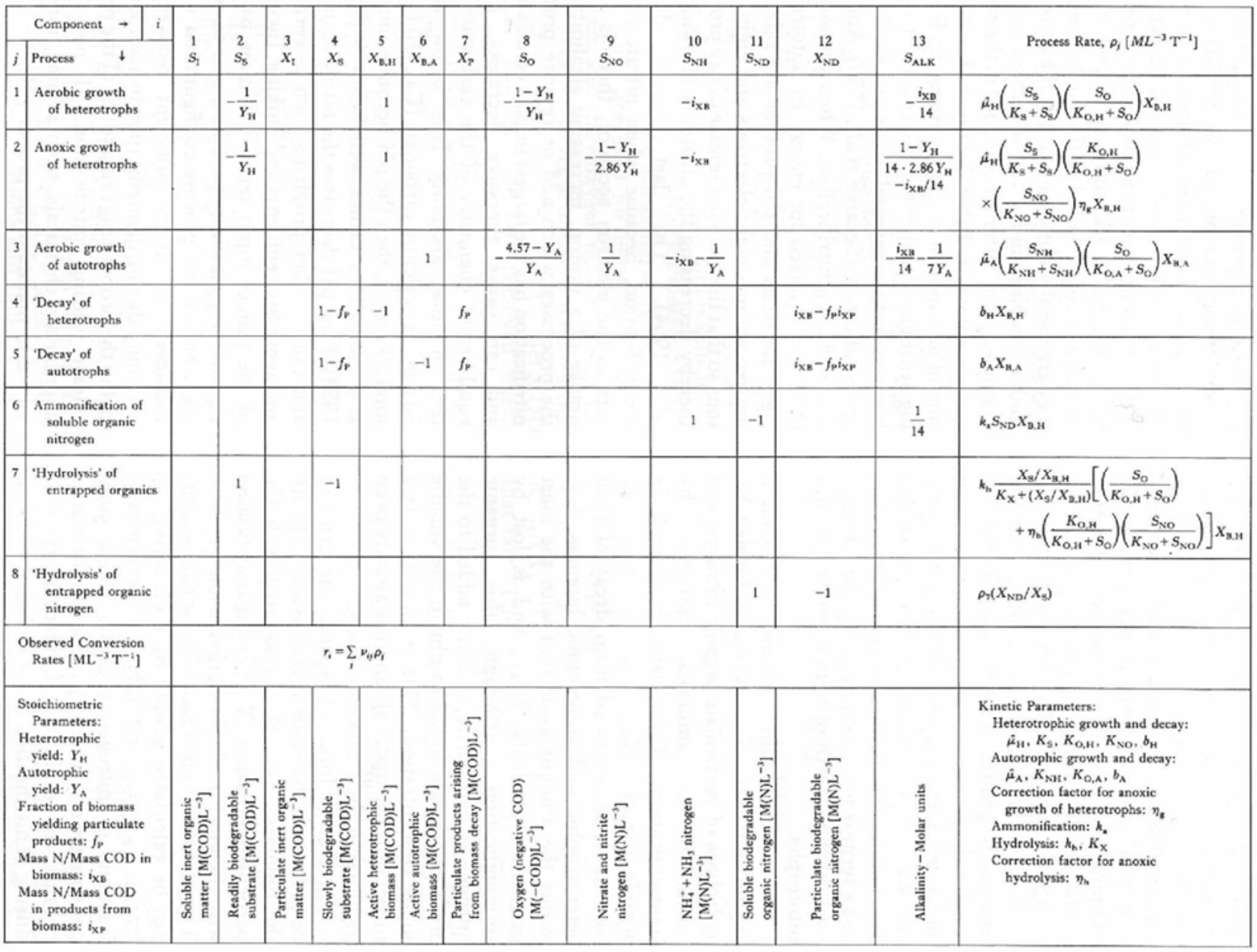
1. SI: Soluble inert organic matter
2. SS: Soluble biodegradable organic matter
3. XS: Slowly biodegradable particulate organic matter
4. XI: Non-degradable particulate matter
5. XBH: Heterotrophic biomass
6. XBA: Autotrophic biomass
7. **XP: Particulate products of decay processes**
8. SO: Soluble oxygen
9. SNO: Soluble nitrate and nitrite nitrogen
10. SNH: Soluble ammonia nitrogen
11. **SND: Soluble organic nitrogen**
12. **XND: Particulate organic nitrogen**
13. **SALK: Alkalinity**

Components of a WWTP model

IWA Activated Sludge Models

ASM1 – processes

1. Aerobic growths of heterotrophic organisms
2. Anoxic growths of heterotrophic organisms (denitrification)
3. Aerobic growth of autotrophic organisms (nitrification)
4. Lysis of heterotrophic organisms
5. Lysis of autotrophic Organisms
6. **Ammonification**
7. Aerobic Hydrolysis
8. Anoxic Hydrolysis

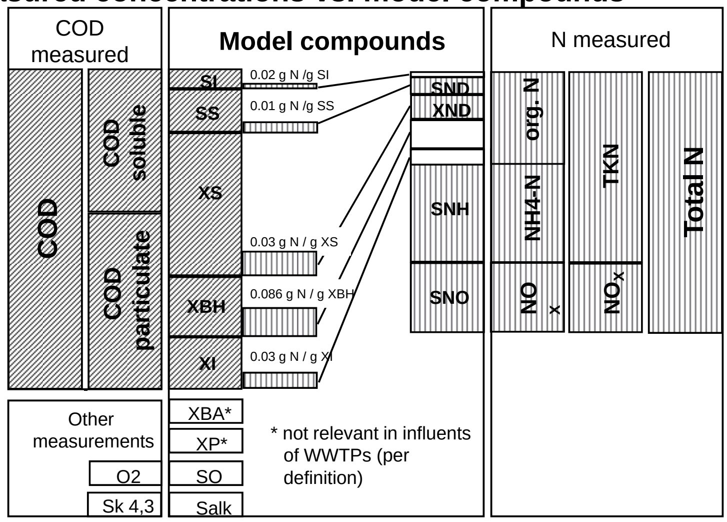


j	Component → i Process ↓	1 S_I	2 S_S	3 X_I	4 X_S	5 $X_{B,H}$	6 $X_{B,A}$	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	11 S_{ND}	12 X_{ND}	13 S_{ALK}	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)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

Components of a WWTP model

IWA Activated Sludge Models

ASM1 – measured concentrations vs. model compounds



Components of a WWTP model

IWA Activated Sludge Models

ASM1 – limitations

1. a constant value of pH,
2. constant coefficients in the rate equations,
3. constant stoichiometric factors, and
4. a limited temperature range from 10°C to 25°C.

Components of a WWTP model

IWA Activated Sludge Models

IWA Activated Sludge Model No.2 (ASM2, 1995)

- ASM1 (C+N) + Bio-P + chemical P-precipitation
- org. N + org. P modelled as part of COD
- 19 components und 19 processes

IWA Activated Sludge Model No.2d (ASM2d, 1999)

- ASM2 + more accurate Bio-P Model
- 19 components und 21 processes

Components of a WWTP model

IWA Activated Sludge Models

IWA Activated Sludge Model No.3 (ASM3, 1999)

Fundamentals

- new C-degradation in relation to ASM1 (cell-internal storage products)
- without P (extensions for P are existing)
- 13 components and 12 processes

References

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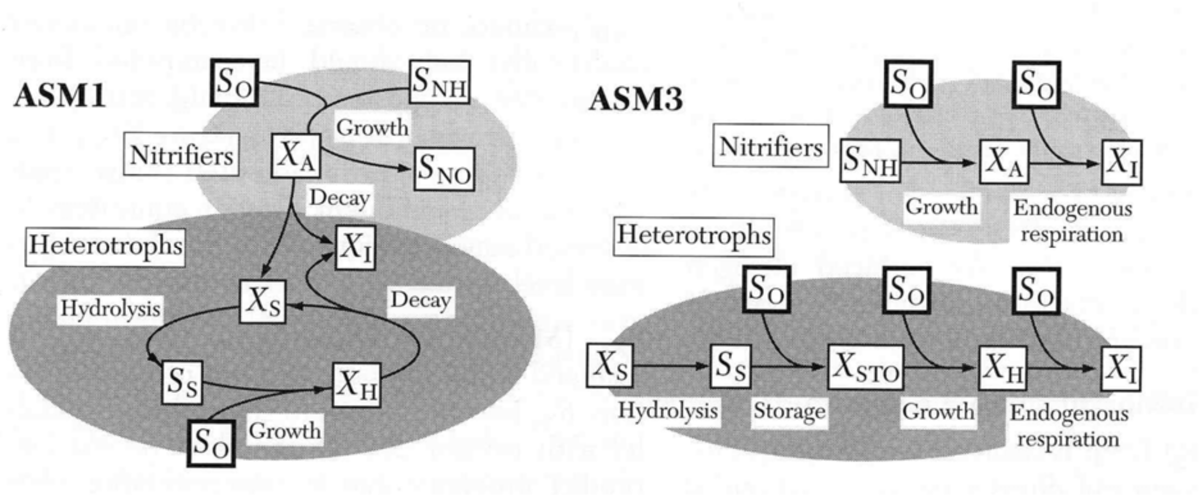
Components of a WWTP model

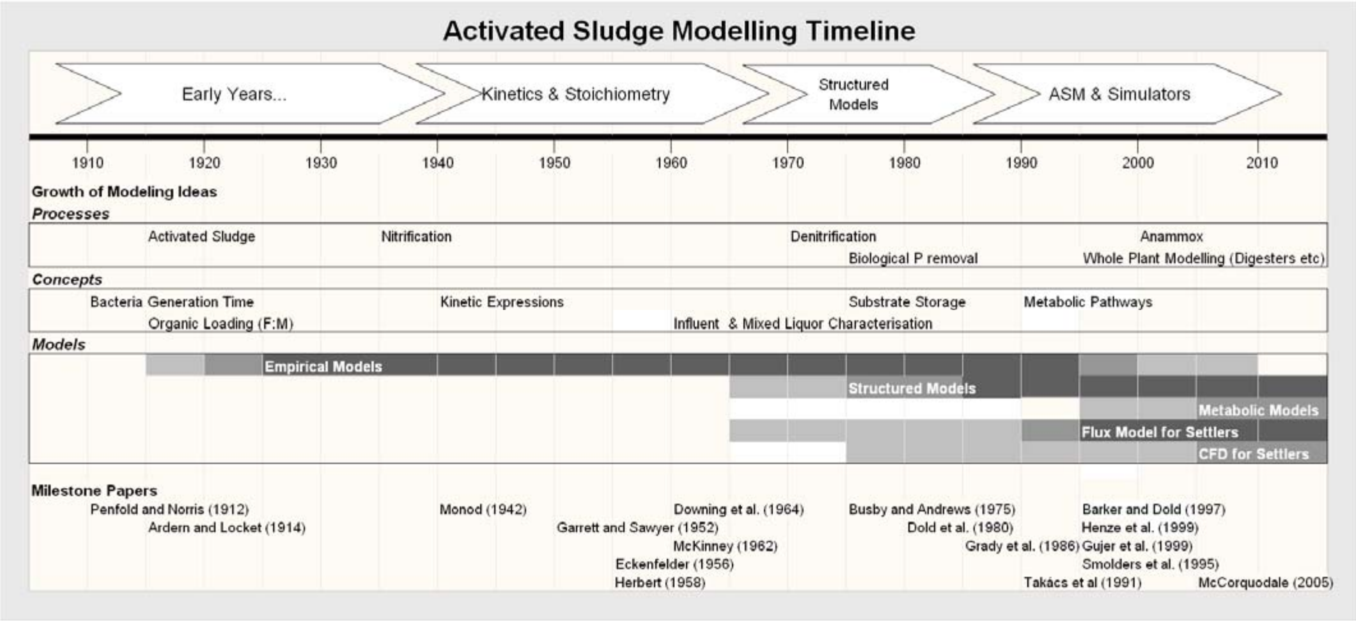
IWA Activated Sludge Models

Differences ASM1 - ASM3



Components of a WWTP model

Development of a biokinetic model for AS plants



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Components of a WWTP model

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Components of a WWTP model

Development of a biokinetic model for AS plants

Brief history of AS modelling

Before 1983: different approaches: C and N removal

- Empirical design
- Early models based on BOD, MLSS
- Experiments at University of Capetown (UCT) from 60s

1983 : IWA TG "Mathematical modelling for design and operation of biological wastewater treatment"

- ASM1 Henze *et al*., 1986 (Activated sludge Model n°1)

1995/1999: Bio-P removal included in IWA model series ASM2/2d

1997 : C/N/P model (Barker and Dold,1997)

Since then:

- New concepts C and N removal (ASM3), ASM3+Bio-P (EAWAG), metabolic model (Delft Univ.), UCTPHO+, elemental balances (Takács *et al*., 2006), …

Components of a WWTP model

Development of a biokinetic model for AS plants

Available biokinetic models

C and N removal

- ASM1
- ASM3, ASM3C

C/N and P removal

- ASM2, ASM2d, ASM3+Bio-P
- Barker & Dold
- UCTPHO+
- ASDM
- TUDelft

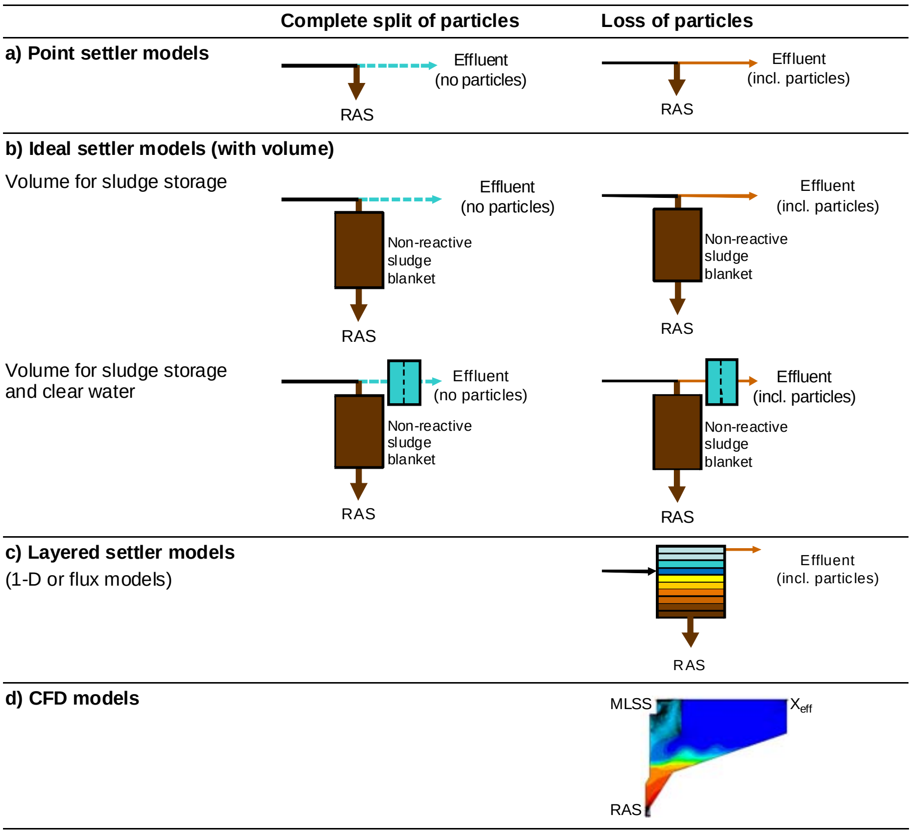
many others, modified models…

Components of a WWTP model

Models for secondary clarifiers

Secondary clarifiers

- Separation activated sludge / effluent
- Settling and thickening of AS
- Sludge storage in the case of rainfall events in mixed systems



Complete split of particles | **Loss of particles**

a) Point settler models

b) Ideal settler models (with volume)

Volume for sludge storage

Volume for sludge storage
and clear water

c) Layered settler models
(1-D or flux models)

d) CFD models

e) Reactive models

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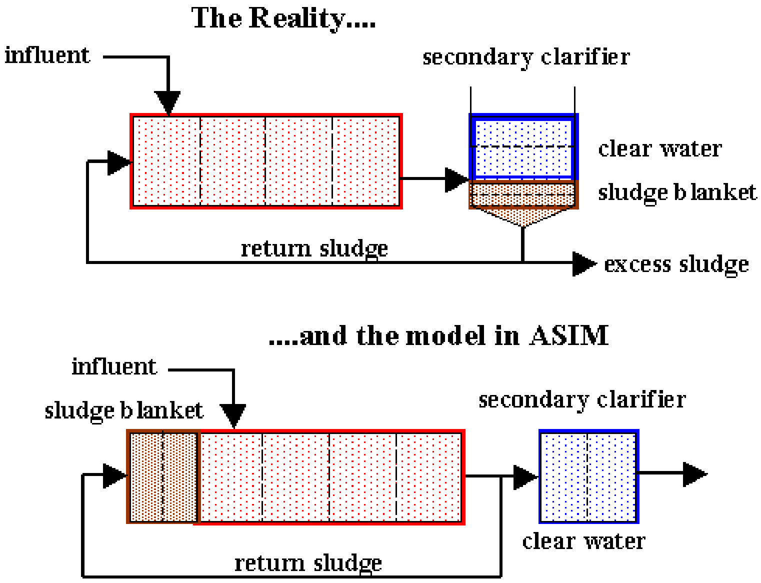
Components of a WWTP model

Models for secondary clarifiers



The Reality....

....and the model in ASIM

Secondary clarifier
model in ASIM

Components of a WWTP model

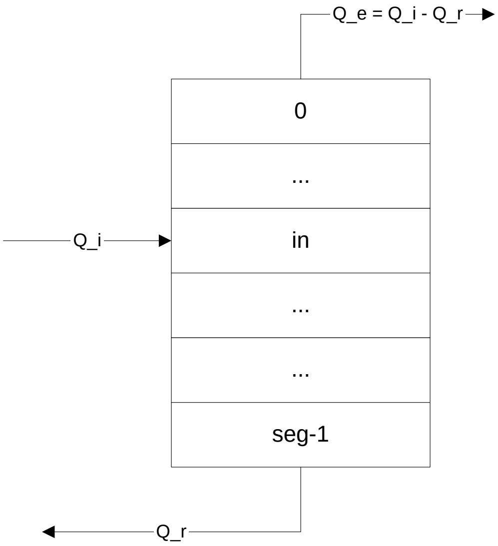
Models for secondary clarifiers

1D layered settler models

vertical transport due to

1. convection (with flowing water) and
2. sedimentation (relative to flowing water)

Q_i = influent
Q_r = recirculation
Q_e = effluent = Q_i – Q_r



Components of a WWTP model

Models for secondary clarifiers

1D layered settler models

Settling velocity

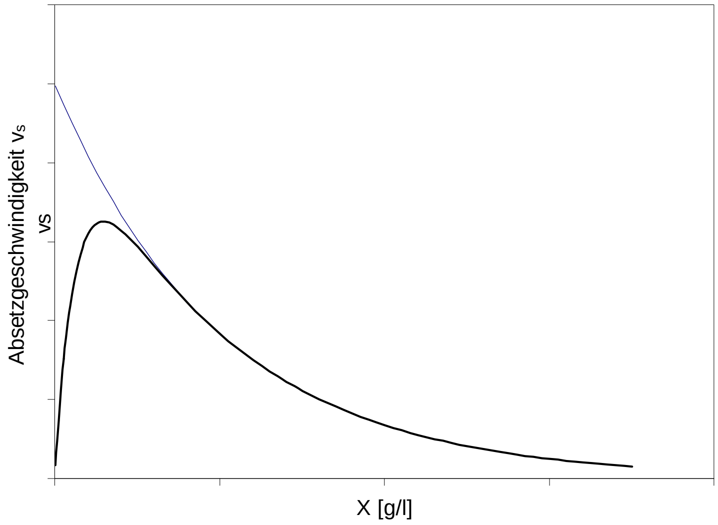
Most simple:

$$v_s = v_{s0} \cdot e^{-nX}$$

X < ➔ v_s too high

Double exponential form

$$v_s = v_{s0} \cdot e^{-nX} - v_{s0} \cdot e^{-mX}$$



Modelling exercise 1

Dynamic simulation of a AS plant

Introduction to ASIM

Objectives

1. Implementation of a AS plant into the ASIM simulation software
2. Optimisation on nitrogen elimination

Contact

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