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BIOMATH
Department of Applied Mathematics,
Biometrics and Process Control

Sewage Treatment:
Conversion Process Modelling

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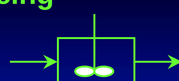
Overall modelling principle: Mass Balancing

Mass Balance for component:



$$\boxed{\frac{dM}{dt} = \frac{d(VC)}{dt} = \underbrace{Q_{in}C_{in} - Q_{out}C_{out}}_{\text{transport}} + \underbrace{rV}_{\text{conversion}}}$$

with
- M: Mass of compound in system (g)
- C: Concentration of compound (g/m^3)
- V: Volume of system (m^3)
- Q: flow rate (m^3/h)
- r: volumetric conversion rate ($g/m^3.h$)

Sewage treatment: a biological process

A culture of collaborating organisms do the job

Biological growth

- Growth = multiplication of organisms
- Requirements for growth:
  - nutrients (biomass = $C_5H_7O_2N$, + P, S, ...)
  - favourable environmental conditions (pH, temperature)
- Basic reaction :

C-source + NH_4 + PO_4 + H^+ ==> Biomass

+ electron acceptor (O_2, NO_3) + byproducts

+ electron donor (C-source) (H_2O, CO_2, N_2, NO_3)

Biological conversion

- Because biomass grows (or at least wants to), a number of compounds are converted, e.g.
  - Organic pollutants --> CO_2 + waste biomass
  - NH_4 --> NO_3
  - NO_3 --> N_2
  - PO_4 --> Poly-P stored in waste biomass
  - Organic pollutants --> biogas (CH_4 + CO_2)
- How much is converted ?
  - Rate of the conversion reaction ==> KINETICS
  - Ratio of conversions of the different compounds ==> STOICHIOMETRY

Reaction stoichiometry

Suppose the following reaction takes place:

$C_{18}H_{19}O_9N + O_2 + H^+ \rightarrow C_5H_7O_2N + CO_2 + H_2O$

for each “molecule” of pollutants degraded, a <u>proportional</u> amount of other components will be used (left of arrow) or produced (right of arrow)

We can therefore write:

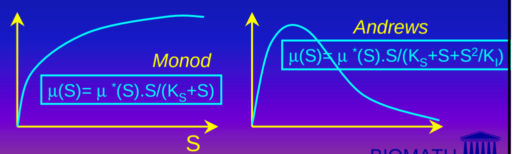
$a\ C_{18}H_{19}O_9N + b\ O_2 + c\ H^+ \rightarrow d\ C_5H_7O_2N + e\ CO_2 + f\ H_2O$

a,b,c,d,e,f are called <u>yield</u> or <u>stoichiometric</u> coefficients

note that one of the coefficients can be chosen = 1

Reaction kinetics

- A reaction will not occur (reaction rate = 0) when its <u>sources (substrates)</u> are absent
  - components on the left of the reaction arrow
- A reaction will have a maximum rate
  - when all sources are in excess
  - the rate may go down again when source increases further



Conversion rates

Take the conversion above

a $C_{18}H_{19}O_9N$ + b O_2 + c H^+ --> 1 $C_5H_7O_2N$ + d CO_2 + e H_2O

Suppose the reaction kinetics: $\rho(S)=\mu^*(S).X.S/(K_S+S)$

- Monod kinetics in the substrate concentration
- first order in the biomass concentration

The conversion of each component is then:

$C_{18}H_{19}O_9N$	: - a. $\rho(S)$	$C_5H_7O_2N$	: + 1. $\rho(S)$
O_2	: - b. $\rho(S)$	CO_2	: + d. $\rho(S)$
H^+	: - c. $\rho(S)$	H_2O	: + e. $\rho(S)$

Conversion rates (cont'd)

The conversion of each component is :

$C_{18}H_{19}O_9N$	: - a. $\rho(S)$	$C_5H_7O_2N$	: + 1. $\rho(S)$
O_2	: - b. $\rho(S)$	CO_2	: + d. $\rho(S)$
H^+	: - c. $\rho(S)$	H_2O	: + e. $\rho(S)$

<u>In general:</u>

Conversion rate of a component consists of 3 parts:

- sign (+/-) dependent on whether it is used or produced
- stoichiometric coefficient (ν) in the reaction
- rate (ρ) of the reaction

$$r(S) = \text{sign}(j)\ \nu_j.\rho$$

Conversion rates (cont'd)

- What if parallel reactions with same components ?

  a $C_{18}H_{19}O_9N$ + b O_2 + c H^+ --> 1 $C_5H_7O_2N$ + d CO_2 + e H_2O

  f CO_2 + g O_2 + h NH_4^+ --> 1 $C_5H_7O_2N$ + i NO_3 + j H_2O + j H^+

- ==> $C_5H_7O_2N$, O_2, CO_2, H^+, H_2O occur more than once

$C_5H_7O_2N$	: + 1. ρ_1 + 1. ρ_2
O_2	: - b. ρ_1 - g. ρ_2
CO_2	: + d. ρ_1 - f. ρ_2
H^+	: - c. ρ_1 + j. ρ_2

General conversion model

- For the i-th component, S_i:

$$r(S_i) = \Sigma_j \text{ sign}(ji)\ v_{ji}.\rho_j$$

where

ρ_j = the rate of the j-th reaction in which S_i participates

v_{ji} = the stoichiometric coefficient for S_i in the j-th reaction

sign(ji) = sign (+/-) indicating whether S_i is substrate or product in the j-th reaction

Temperature effect on conversion rate

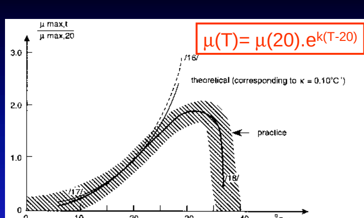


Fig 3.7 *Nitrification as a function of temperature. As opposed to the other biological processes in wastewater treatment, thermophilic nitrifying bacteria are unknown.*

Rule of thumb: Doubling of reaction rate for temperature increase with 10ºC

Yearly temperature evolution

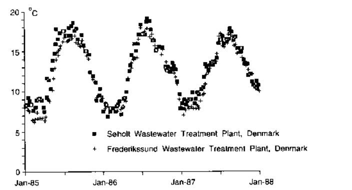
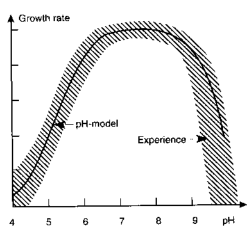


Fig 1.12 *Temperature variation in activated sludge tanks, Søholt and Frederikssund wastewater treatment plants (Denmark) /23/.*

Winter period is critical for process performance, especially for nitrification, since this is the slowest

pH effect on conversion rates

$\mu(pH) = \mu(pH_{opt}).K_{pH}/(K_{pH} - 1 + 10^{|pH-pHopt|})$



Process is changing the system pH by production of H^+ (e.g. nitrification, digestion) or OH^- (denitrification)

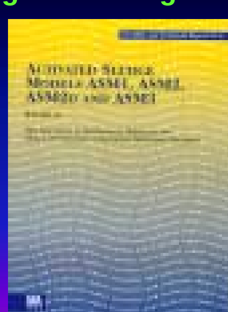
"The" starting point for Activated Sludge Modelling

Henze, M., Gujer, W., Takashi, M. and van Loosdrecht, M. (2000)

Activated Sludge Models ASM1, ASM2, ASM2D and ASM3.

Scientific and Technical Report No. 9

IWA Publishing, London.



Activated Sludge Model No 1

- Henze et al. (1987)
- Innovations:
  - Nomenclature: Solubles: symbol S
    Particulates: symbol X
  - Focus on:
    - Sludge production
    - Oxygen consumption
    - Nitrogen removal
  - COD based modelling ==> Mass balancing
  - Peterson matrix
- Now: basis for sewer / river water quality models

Peterson (1965) matrix notation

Components, Processes, Stoichiometry & Kinetics:

Continuity

Mass Balance

Component → i / j Process ↓	1 X_B	2 S_S	3 S_O	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1 Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\hat{\mu} S_S}{K_S + S_S} X_B$
2 Decay	−1		−1	bX_B
Observed Conversion Rates $ML^{-3}T^{-1}$	$r_i = \sum_j r_{ij} = \sum_j \nu_{ij}\rho_j$			Kinetic Parameters: Maximum specific growth rate: $\hat{\mu}$ Half-velocity constant: K_S Specific decay rate: b
Stoichiometric Parameters: True growth yield: Y	Biomass $[M(COD)\ L^{-3}]$	Substrate $[M(COD)\ L^{-3}]$	Oxygen (negative COD) $[M(-COD)\ L^{-3}]$	

Mass balancing

- Vertical summation of

  Stoichiometry term * Kinetics

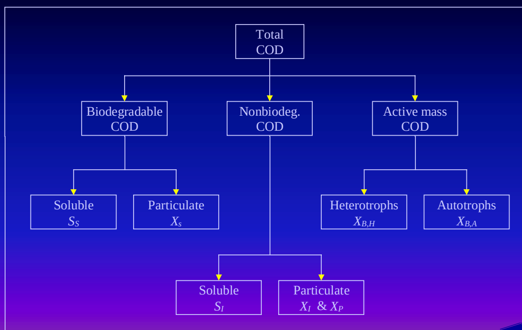
  terms gives total conversion

$$r(S_i) = \Sigma_j \text{ sign}(ji)\ v_{ji}.\rho_j$$

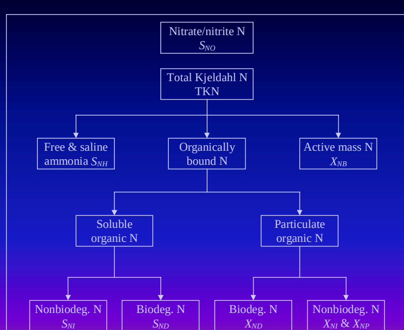
Add the transport terms ==> the mass balance !

$$\boxed{\frac{dM}{dt} = \frac{d(V \cdot S)}{dt} = Q_{in} \cdot S_{in} - Q_{out} \cdot S_{out} + V \cdot r(S)}$$

ASM1: COD-components



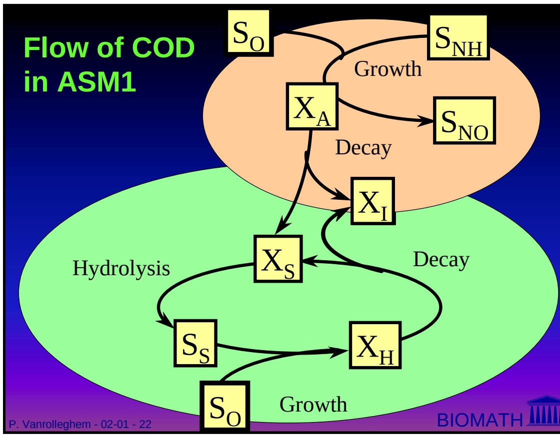
ASM1: N-components



ASM1: Processes

1) Growth of biomass
   - heterotrophs
     - aerobic
     - anoxic
   - autotrophs (nitrification)
2) Decay of biomass
   - heterotrophs
   - autotrophs
3) Ammonification of organic nitrogen (KjN --> NH_4)
4) Hydrolysis of particulate organic matter

Flow of COD in ASM1



ASM1: Peterson matrix

Component (i) → ↓ Process (j)	1 S_I	2 S_S	3 X_I	4 X_S	5 X_{BH}	6 X_{BA}	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)
1 Aerobic growth of heterotrophic biomass		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\mu_{\max H}\frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}X_{BH}$
2 Anoxic growth of heterotrophic biomass		$-\frac{1}{Y_H}$			1					$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}$ $-\frac{i_{XB}}{14}$	$\eta_g\mu_{\max H}\frac{S_S}{K_S+S_S}\frac{K_{OH}}{K_{OH}+S_O}$ $\frac{S_{NO}}{K_{NO}+S_{NO}}X_{BH}$
3 Aerobic growth of autotrophic biomass						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\mu_{\max A}\frac{S_{NH}}{K_{NH}+S_{NH}}\frac{S_O}{K_{OA}+S_O}X_{BA}$
4 Decay of heterotrophic biomass				$1-f_P$	-1		f_P					$i_{XB}-f_P i_{X}$		$b_H X_{BH}$
5 Decay of autotrophic biomass				$1-f_P$		-1	f_P					$i_{XB}-f_P i_{X}$		$b_A X_{BA}$
6 Ammonification of soluble organic nitrogen										1	-1		$1/14$	$k_a S_{ND} X_{BH}$
7 Hydrolysis of slowly biodegradable substrate		1		-1										$k_h\frac{X_S/X_{BH}}{K_X+X_S/X_{BH}}\frac{S_O}{K_{OH}+S_O}$ $+\eta_h\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}X_{BH}$
8 Hydrolysis of organic nitrogen											1	-1		$\rho_7(X_{ND}/X_S)$

Continuity calculations

- Horizontal summation of stoichiometric/composition coefficients should equal 0 !

$$\Sigma_i\, v_{ji}.i_{ki} = 0$$

if and only if: - consistent units have been used
- all substrates/products are included

This can be done for COD, N, P, Charge, Mass

Sets of equations allow to find v_{ij} !

--> Example: ASM3

j	Process Component i >	1	2	3	4	5	6	7	8	9	10	11	12	13
		S_O	S_I	S_S	S_{NH}	S_{N2}	S_{NO}	S_{HCO}	X_I	X_S	X_H	X_{STO}	X_A	X_{TS}
v	expressed as >	O_2	COD	COD	N	N	N	Mole	COD	COD	COD	COD	COD	TSS
1	Hydrolysis		f_{SI}	$1-f_{SI}$	y_1			z_1		-1				$-i_{XS}$
Heterotrophic organisms, denitrification														
2	Aerobic storage of COD	x_2		-1	y_2			z_2				Y_{STO}		t_2
3	Anoxic storage of COD			-1	y_3	$-x_3$	x_3	z_3				Y_{STO}		t_3
4	Aerobic growth	x_4			y_4			z_4			1	$-1/Y_H$		t_4
5	Anoxic growth (denitrification)				$-i_{NBM}$	$-x_5$	x_5	z_5			1	$-1/Y_H$		t_5
6	Aerobic endog. respiration	$-(1-f_I)$			y_6			z_6	f_I		-1			t_6
7	Anoxic endog. respiration				y_6	$-x_7$	x_7	z_7	f_I		-1			t_7
8	Aerobic respiration of PHA	-1										-1		-0.60
9	Anoxic respiration of PHA					$-x_9$	x_9	z_9				-1		-0.60
Autotrophic organisms, nitrification														
10	Nitrification	x_8			y_{10}		$1/Y_A$	z_{10}					1	i_{TSBM}
11	Aerobic endog. respiration	$-(1-f_I)$			y_{11}			z_{11}	f_I				-1	t_{11}
12	Anoxic endog. respiration				y_{12}	$-y_{12}$	y_{12}	z_{12}	f_I				-1	t_{12}
Composition matrix $\iota_{k,I}$														
k	Conservatives													
1	COD g COD	-1	1	1		-1.71	-4.57		1	1	1	1	1	
2	Nitrogen g N		i_{NSI}	i_{NSS}	1	1	1		i_{NXI}	i_{NXS}	i_{NBM}		i_{NBM}	
3	Ionic charge Mole +				1/14		-1/14	-1						
	Observables													
4	TSS g TSS								i_{TSXI}	i_{TSXS}	i_{TSBM}	0.60	i_{TSBM}	

ASM3 Composition matrix Solubles

Component expressed as >		S_O O_2	S_I COD	S_S COD	S_{NH} N	S_{N2} N	S_{NO} N	S_{HCO} Mole
Composition matrix $\iota_{k,i}$								
k	Conservatives							
1	COD g COD	-1	1	1		-1.71	-4.57	
2	Nitrogen g N		i_{NSI}	i_{NSS}	1	1	1	
3	Ionic charge Mole +				1/14		-1/14	-1
	Observables							
4	TSS g TSS							

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ASM3 Composition matrix Particulates

Component expressed as		X_I COD	X_S COD	X_H COD	X_{STO} COD	X_A COD	X_{TS} TSS
Composition matrix $\iota_{k,i}$							
k	Conservatives: Conservation equation						
1	COD g COD	1	1	1	1	1	
2	Nitrogen g N	i_{NXI}	i_{NXS}	i_{NBM}		i_{NBM}	
3	Ionic charge Mole +						
	Observables: Composition equation						
4	TSS g TSS	i_{TSXI}	i_{TSXS}	i_{TSBM}	0.60	i_{TSBM}	

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Consistency Check ASM3

Conservation eq.: $\sum_i \nu_{j,i} \cdot \iota_{k,i} = 0 \quad \text{for} \quad i = 1 \text{ to } 12$

for k = COD, N and ionic charge
yields j × k = 12 × 3 = 36 equations
which allow to predict all $\mathbf{x_j}$, $\mathbf{y_j}$, $\mathbf{z_j}$

TSS Composition equation

$$t_j = \nu_{j,TSS} = \sum_i \nu_{j,i} \cdot \iota_{TSS,i} \quad \text{for } i = 8 \text{ to } 12$$

yields j = 12 equations which
allow easily to predict all $\mathbf{t_j}$

Message !

- Mass balancing: $\boxed{\frac{dM}{dt} = \frac{d(VC)}{dt} = Q_{in}C_{in} - Q_{out}C_{out} + rV}$
- Peterson matrix: $\boxed{r(S_i) = \Sigma_j \text{ sign(ji) } \nu_{ji}.\rho_j}$
- Continuity calculations: $\boxed{\Sigma_i \nu_{ji}.i_{ki} = 0}$

allow to build models efficiently, check them
and communicate about them clearly