Aalto University
School of Engineering

Modelling and Control of Water and wastewater treatment processes

WAT - E2130
Lecture 2 Modeling treatment processes and biological phenomena

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Lecture outline

MODELLING TREATMENT PROCESSES

Reactors and hydraulics

Reactions

Mass balances

EXERCISE BREAK

Using dynamic input in SUMO

Homework 1: 1&2

MODELING BIOLOGICAL PHENOMENA

Main biological processes

Process kinetics (Monod)

Principles of biological models

ACTIVATED SLUDGE MODELS

Gujer matrix

ASM model family

EXERCISE BREAK

Using dynamic input in SUMO

Homework 1: 3

Reactions and mass balances

Reaction rate

- Reaction: A + B ⟷ C + D
- Reaction rate in liquid phase =

$$r_{\text{reaction, A}} = k_r \, c_A^{\,n} \, c_B^{\,m}$$

- $r_{\text{reaction, A}}$ units are moles or mass of A / time * volume
- c_A = concentration of A (moles or mass / volume)
- c_B = concentration of B (moles or mass / volume)
- k_r = reaction rate constant (units depend on the form of the rate equation)
- n, m = order of the reaction, the general case
  - n^{th} order, m^{th} order, $n+m^{th}$ order
  - Most common orders of reaction 0, ½, 1, 2, 3
  - In water engineering the reaction order is usually already known (unless you are doing research)

Examples of reaction rates

$$2NO + O_2 \rightarrow 2NO_2$$

$$r_{reaction,NO} = k_r c_{NO}^2 c_{O_2}$$

- Oxidation of nitric oxide to nitrogen peroxide
- Elementary reaction: the order of the reaction matches the stoichiometry of the reaction

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

$$r_{reaction,CO} = k_r c_{CO} c_{H_2O}^{0.5} c_{O_2}^{0.25}$$

- In many cases the order of the reaction rate equation does not match the stoichiometry:
- Oxidation of carbon monoxide to carbon dioxide
- The reaction mechanisms is complex including water molecules, which are not shown in the total reaction equation

Determining reaction rate constants

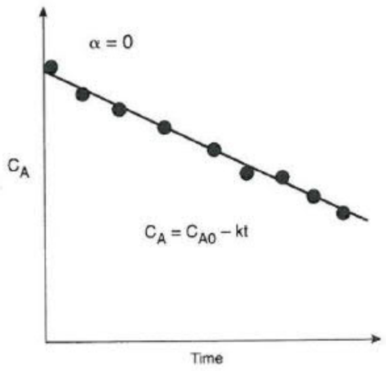


Figure 5-3 Zero-order reaction.

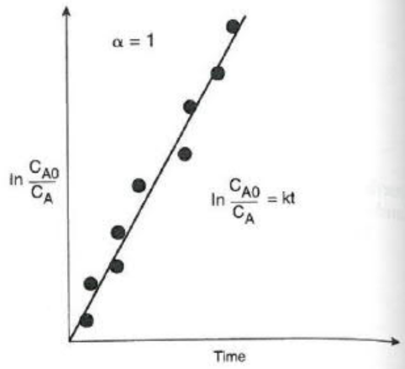


Figure 5-4 First-order reaction.

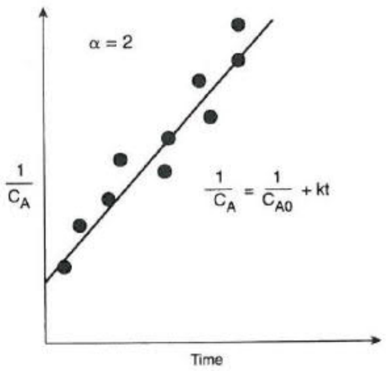


Figure 5-5 Second-order reaction.

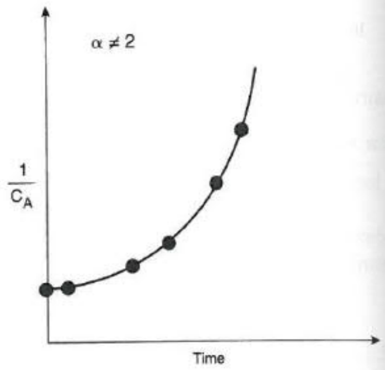


Figure 5-6 Plot of reciprocal concentration as a function of time.

- Experimental methods
  - The order of reaction cannot be deduced from the reaction equation
- Differential method
- Integralmethod:

  A-> reaction products

  - Zeroth order reaction

    $C_A = C_{A0} - kt$
  - First order reaction

    $\ln (C_{A0}/C_A) = kt$
  - Second order reaction

    $1/C_A - 1/C_{A0} = kt$

General mass balance

- Also called material balances
- ”A mass balance is a tool to keep track of how much substance is in a given region of space at a given time”
- Conservation of mass, or <u>rate</u> at which substance i enters, exit, reacts and accumulates

Rate of change of mass of *i* stored in the system	=	Rate at which *i* enters the system from outside	−	Rate at which *i* exits the system to the outside	+	Rate at which *i* is generated inside the reactor	−	Rate at which *i* is destroyed inside the reactor

- Rate: mass/time, volume/time, moles/time (… …)

Mass balance and system boundaries

Accumulation in system	=	Input to system	–	Output from system	+	Generation in system	–	Consumption in system

Even shorter:

ACC = IN – OUT + GEN – CON

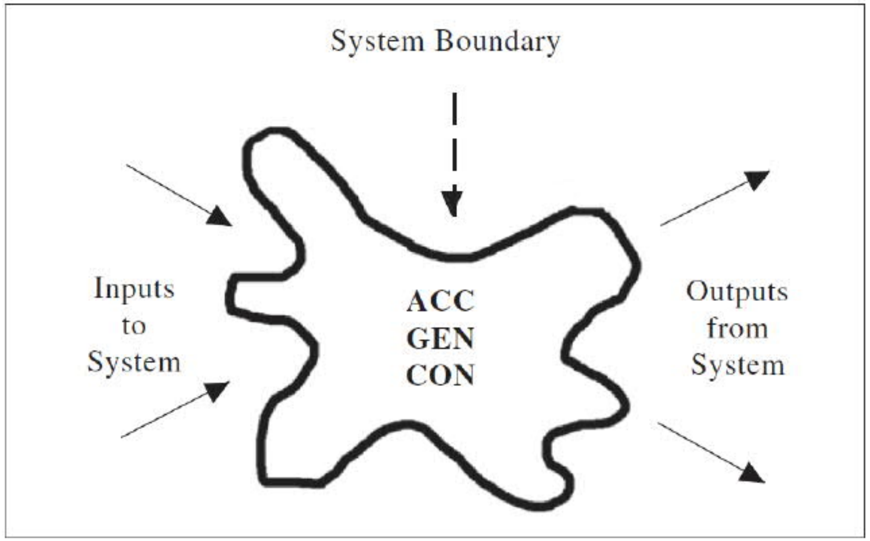
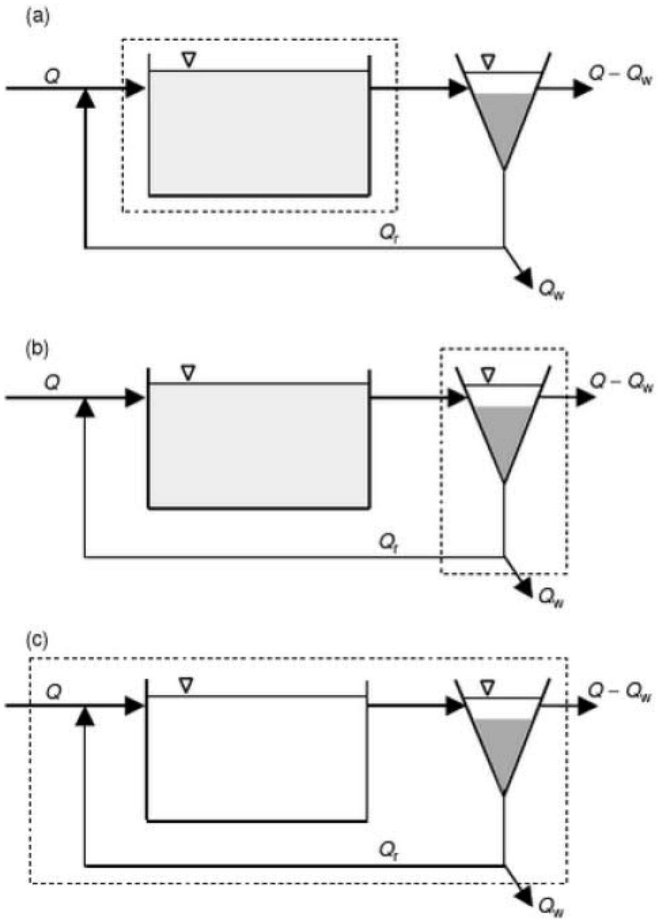


Figure 1.01. Conceptual diagram of a system.

Control volumes

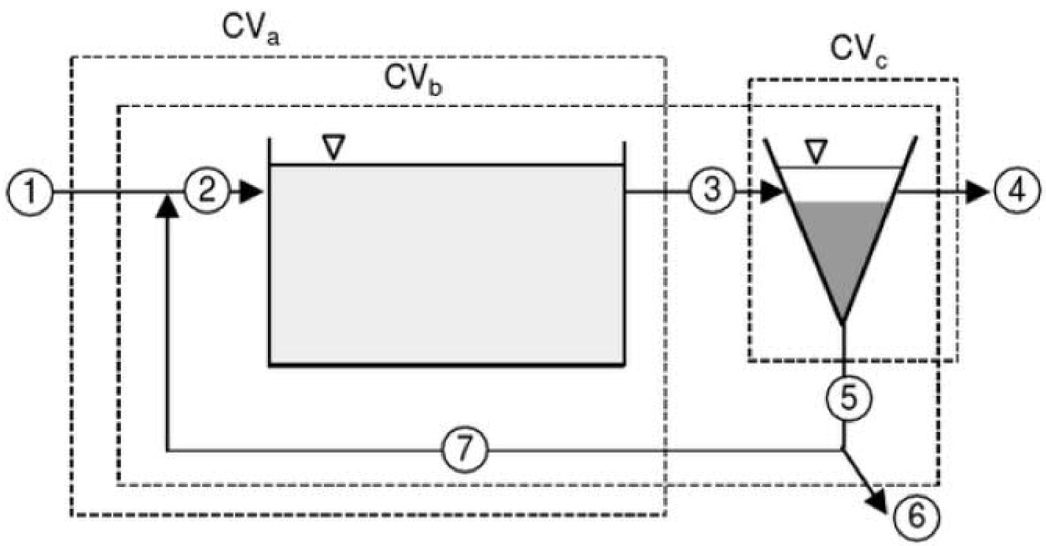


To choose the control volumes

- An open reactor and a settling basin
- With recycle of settled solids to the reactor influent
- Waste stream from the recycle stream
- Balance boundaries shown with broken line
- Q = Influent flow rate
- Q_r = Recycle stream flow rate
- Q_w = waste stream flow rate

In the picture the mass balances have been already utilized to calculate flow rates

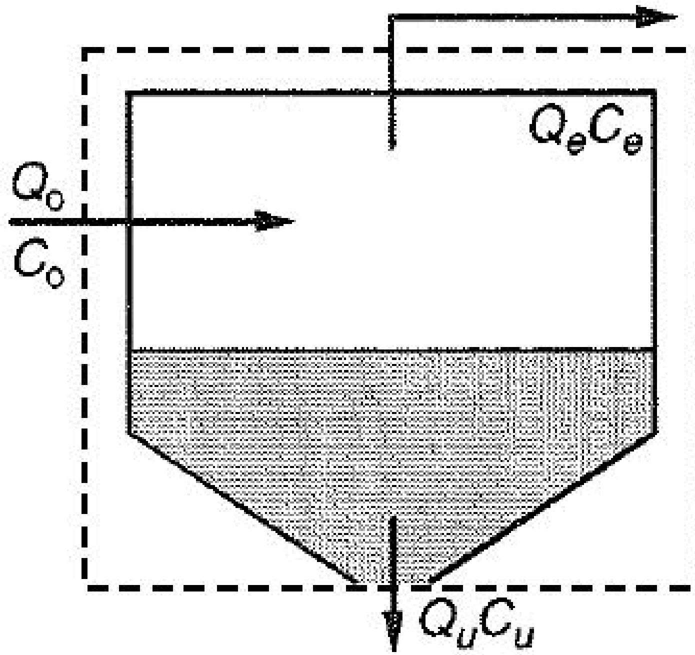
Marking the control volumes



Various control volumes for mass balances that are useful for solving the example problem.

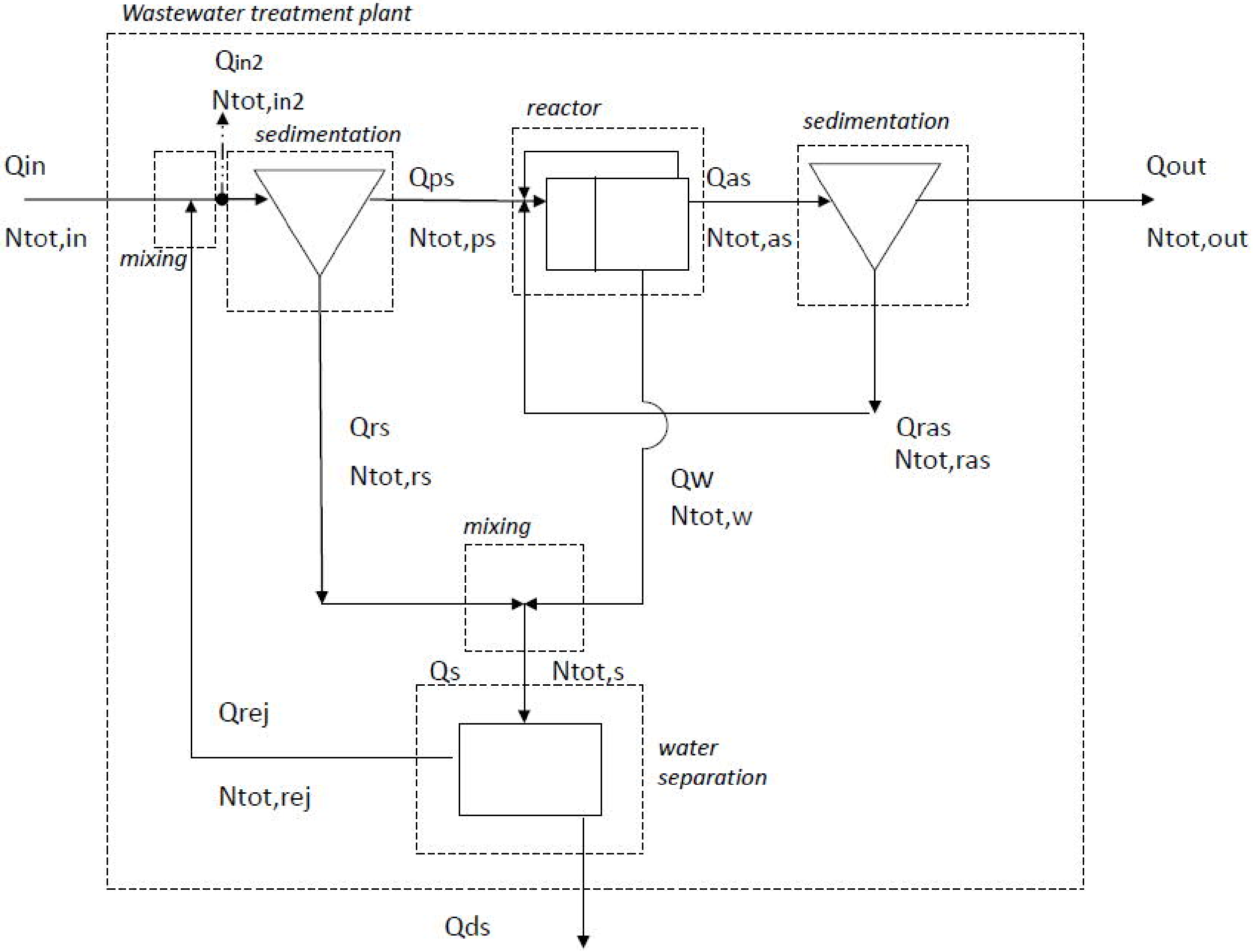
Mark down the flow rates and control volumes

Example: Thickener



- $Q_0 = Q_u + Q_e$
- $Q_0C_0 = Q_uC_u + Q_eC_e$

Wastewater treatment plant balance as a block diagram



- The diagram shows both flow and nitrogen

ps = primary sedimentation
as = activated sludge
ras = return activated sludge
w = waste sludge
rs = raw sludge from promary sedimentation
rej = reject water from sludge drying
s = sludge
ds = dried sludge

Systems and processes

Practical problems are classified according to the type of system and the nature of the process occurring in the system, as follows:

Closed system [Controlled mass]	Zero material* is transferred in or out of the system [during the time period of interest]. i.e. in the material balance equation: IN = OUT = 0 A process occurring in a closed system is called a BATCH process.
Open system [Controlled volume]	Material is transferred in and/or out of the system. i.e. in the material balance equation: IN $\neq$ 0 and/or OUT $\neq$ 0 A process occurring in an open system is called a CONTINUOUS process.
Steady-state process	A process in which all conditions are invariant with time. i.e. at steady-state: Rate ACC = 0 for all quantities.
Unsteady-state process	A process in which one or more conditions vary with time [these are *transient* conditions], i.e. at unsteady-state: Rate ACC $\neq$ 0 for one or more quantities.

* *Energy can be transferred in and/or out of both closed and open systems.*

Steps of calculating the mass balances

1. Draw a diagram and balance boundary/ies
2. Write down all known quantities
3. Identify and assign symbols to all unknown quantities
4. Determine the appropiate set of equations to solve the unknowns
5. Solve the unknowns

Reactors and hydraulics in models

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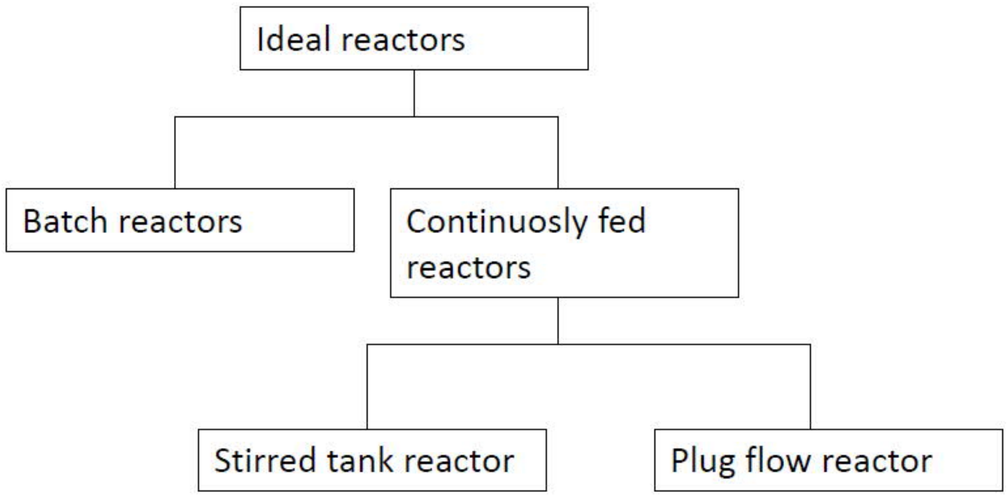
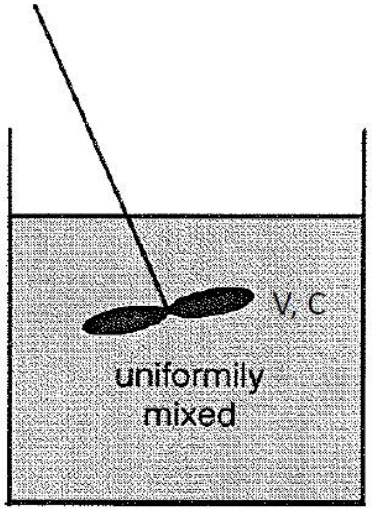
Reactor types

Designing reactors



Batch reactor



- The reaction is let run until the desired yield is reached
- No flow in or out
- => The end products are available only after the reaction time is finished
- For a constant volume V:

$$V\frac{dC}{dt} = Vr_c$$

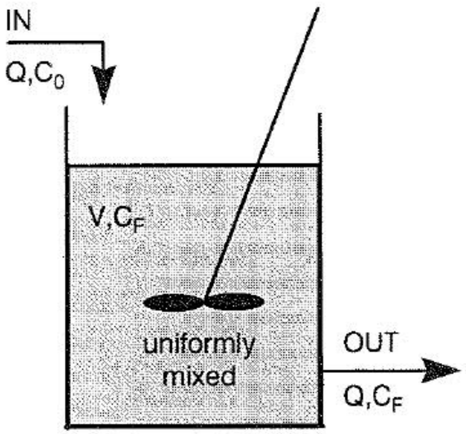
$$\frac{dC}{dt} = r_c$$

for a first-order reaction where C is consumed from an initial concentration of C_O:

$$r_C = -kC$$

Integrated form with solved concentration by time: $C = C_O \exp(-kt)$

Continuous flow stirred tank reactor, CFSTR or CSTR



- Flow in and out = Q
- Tank volume = V
- Influent concentration = C_0
- Effluent concentration = C_F
- Completely mixed
- The concentration of the end products in the reactor = concentration in the outflow
  - The yield is limited because the influent is mixed to the whole tank volume

Steady-flow of water conditions: $Q_{in} = Q_{out} = Q$ and $\frac{dV}{dt} = 0$

Mass Inflow + Mass generated = Mass outflow + Mass accumulated

$$QC_O + Vr_C = QC + V\frac{dC}{dt}$$

$$C_O - C + \frac{V}{Q}r_C = \frac{V}{Q}\frac{dC}{dt}$$

Continues on next page

CSTR (continues)

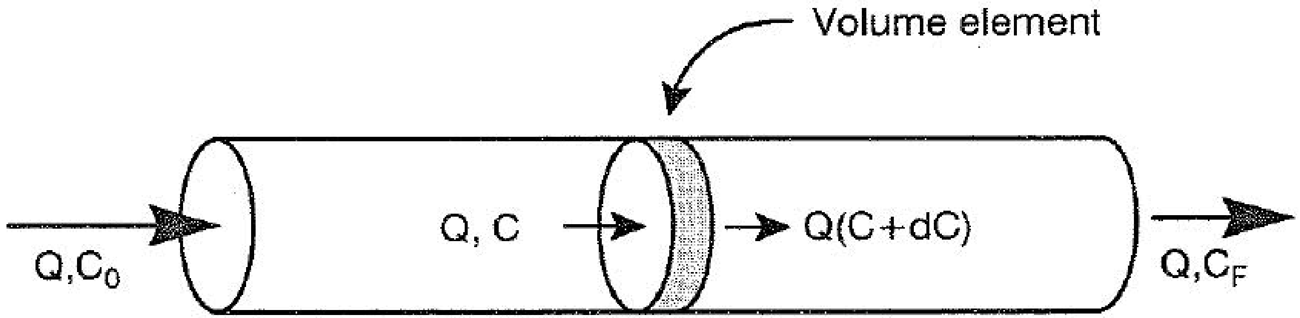
From previous page

$$C_O - C + \frac{V}{Q} r_C = \frac{V}{Q} \frac{dC}{dt}$$

Definition: Retention time = hydraulic residence time = the time required for a reaction

$$\theta = \frac{V}{Q}$$

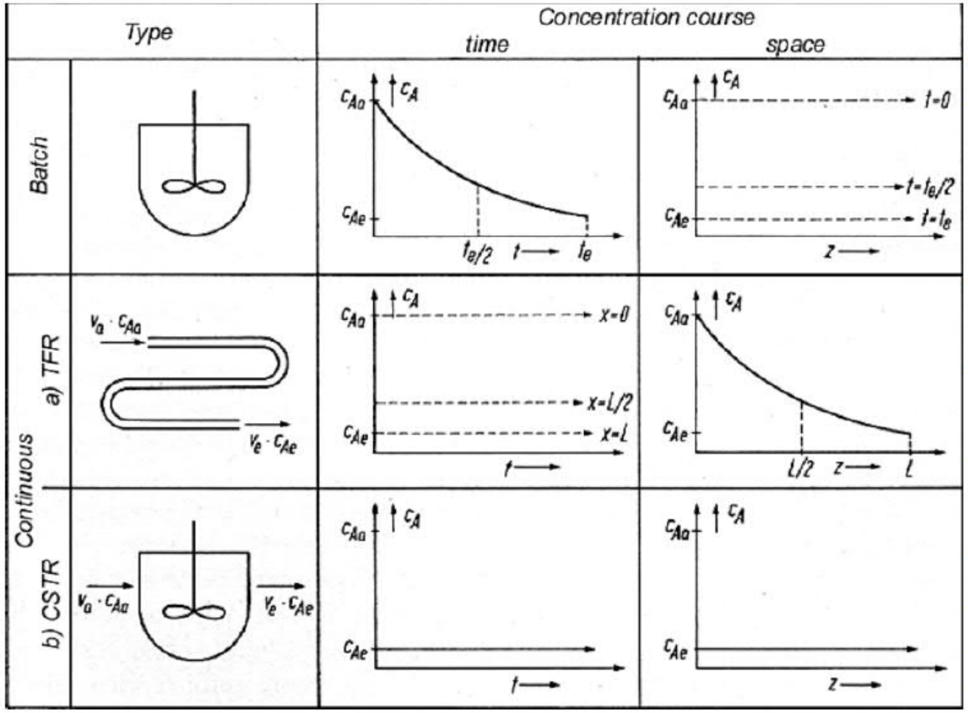
Plug flow reactor PFR



- Continuous flow reactor
- Influent fed to one end of the reactor
- Effluent drawn from the other end
- No mixing
- Reaction advances along the length of the reactor
- Concentrations different in the influent and effluent
- Hydraulic retention time is the same as for CFSTR

$$\theta = \frac{V}{Q}$$

Ideal reactors

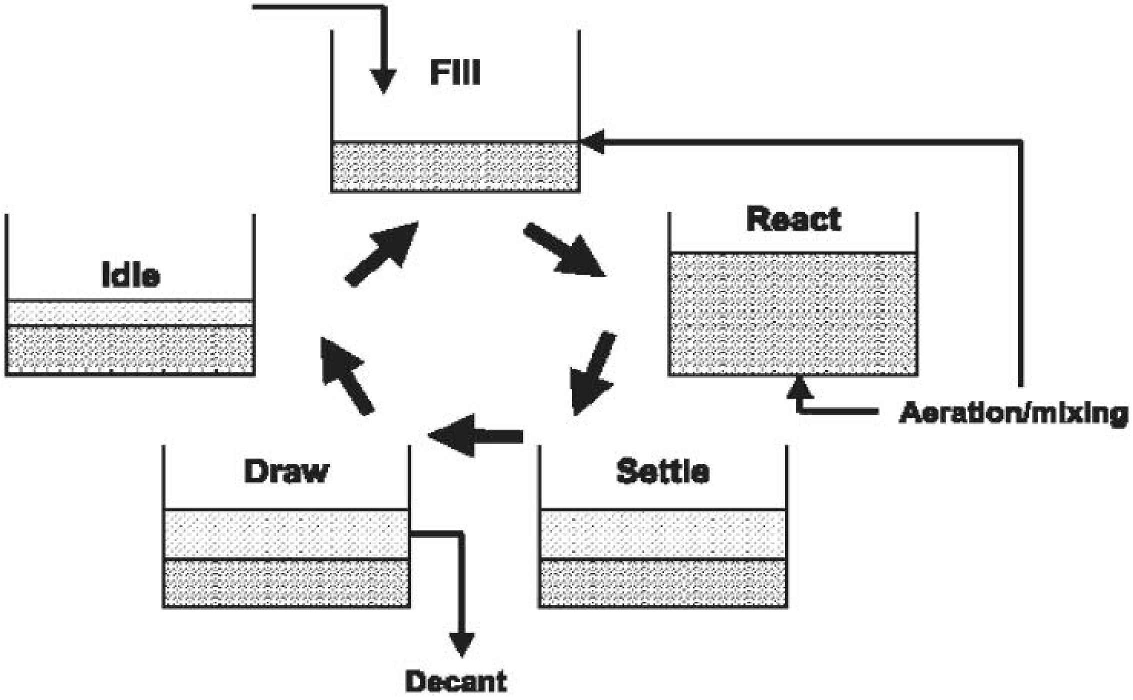


<u>the batch stirred tank reactor:</u> concentration is constant in the whole tank, but it is dropping down with the time. The reactor is **<u>not</u> stationary in (both) space <u>and</u> time.**

<u>the continuous plug (tubular) flow reactor:</u> concentration is constant over the time at different length positions along the tube. The concentration drops down along the reactor length. The reactor is **<u>not</u> stationary in (both) space <u>and</u> time.**

<u>the continuous stirred tank reactor:</u> concentration is stationary in space and time. The reactor is **stationary in space <u>and</u> time**. (not in the start-up- , shutdown- or disturbed operation phase)

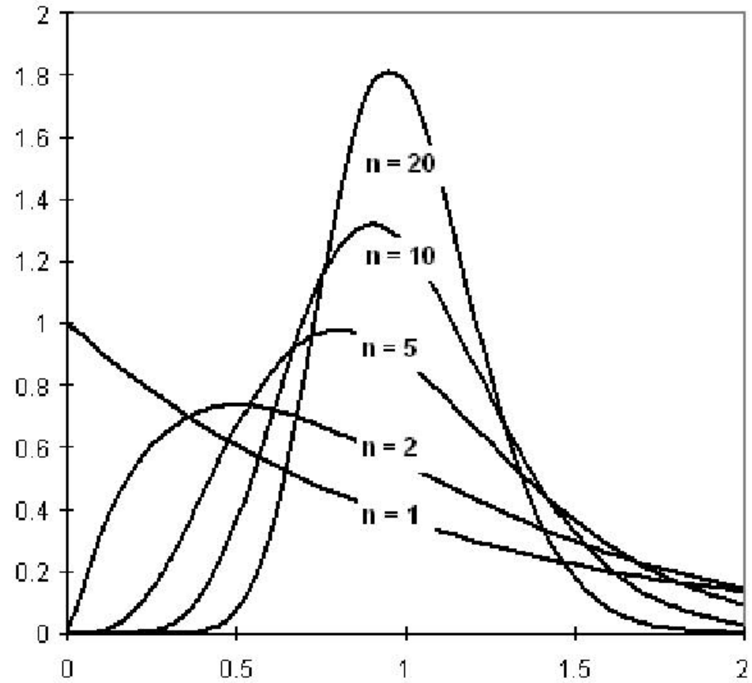
Sequencing batch reactor SBR



All phases happen in the same tank sequentially

Reactor hydraulics

- Usually real reactors have a character between a completely mixed and a plug-flow reactor (≠ ideal reactors)
- Split in “N zones”
- Based on dimensions, flow, turbulence
- Empirical (i.e. flow varies)
- N can be measured (dye test)



Modeling biological phenomena

Model Processes in full plant models

- Biological processes
  - Biological growth processes
  - Decay processes
  - Hydrolysis reactions
  - Fermentation
  - Ammonification
  - Phosphorus release / uptake
- Physico-chemical processes
  - Precipitation
  - Gas-liquid transfer
  - Settling
  - Mixing

Classification of bacteria

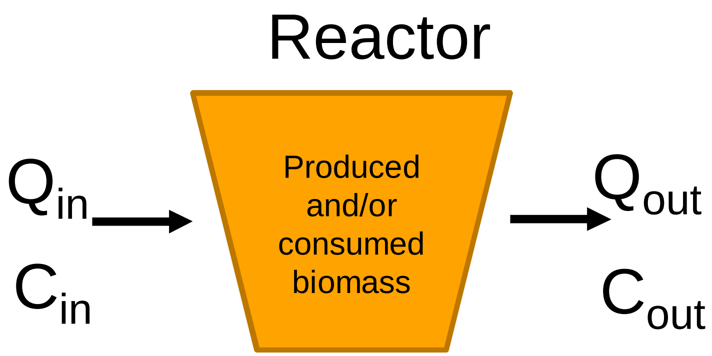
Carbon source	Energy source	Relationship to oxygen	Temperature
- Autotrophs - Heterotrophs	- Light - Chemical compounds	- Aerobic - Anaerobic - Facultative	- Psychrophilic - Mesophilic - Thermophilic

Biological processes in water and wastewater treatment

Type of bacteria	Common reaction name	Carbon source	Electron donor (substrate oxidized)	Electron acceptor	Products
Aerobic heterotrophic	Aerobic oxidation	Organic compounds	Organic compounds	O_2	CO_2, H_2O
Aerobic autotrophic	Nitrification	CO_2	NH_4^+, NO_2^-	O_2	NO_2^-, NO_3^-
	Iron oxidation	CO_2	Fe(II)	O_2	Ferric Iron Fe(III)
	Sulfur oxidation	CO_2	H_2S, S^0, $S_2O_3^{2-}$	O_2	SO_4^{2-}
Facultative heterotrophic	Denitrification anoxic reaction	Organic compounds	Organic compounds	NO_2^-, NO_3^-	N_2, CO_2, H_2O
Anaerobic heterotrophic	Acid fermentation	Organic compounds	Organic compounds	Organic compounds	Volatile fatty acids (VFAs) (acetate, propionate, butyrate)
	Iron reduction	Organic compounds	Organic compounds	Fe(III)	Fe(II), CO_2, H_2O
	Sulfate reduction	Organic compounds	Organic compounds	SO_4	H_2S, CO_2, H_2O
	Methanogenesis	Organic compounds	Volatile fatty acids (VFAs)	CO_2	Methane

Tchopanoglous

Basics of mass balance and biological reactions



Bacterial reactions in modelling the wastewater treatment processes are based on bioaccumulation and bacterial metabolism

Growth and decay

$$\frac{dX}{dt} = \mu X - bX$$

Substrate consumption

$$\frac{dS}{dt} = -\frac{1}{Y}\mu X$$

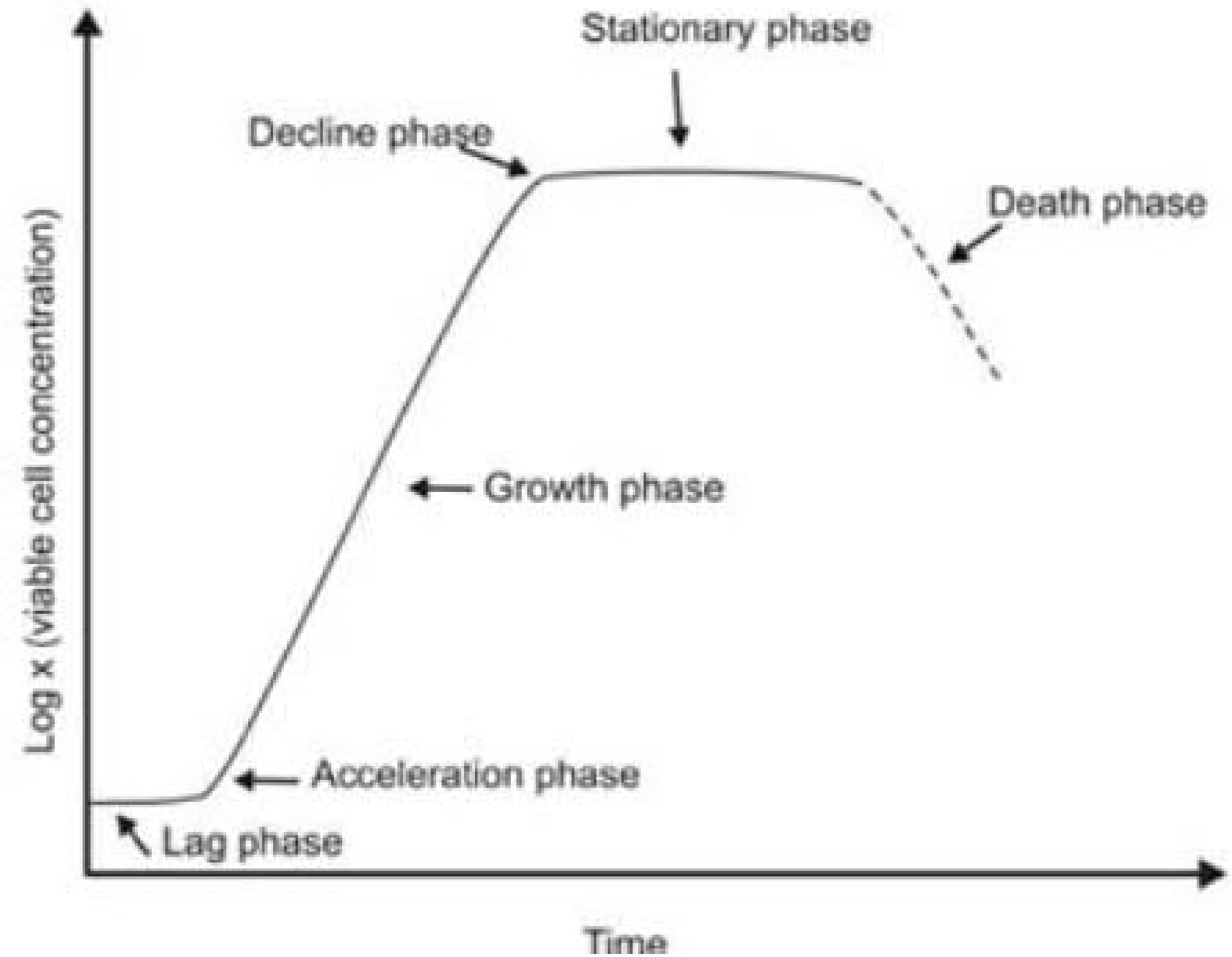
Monod Kinetics

$$\mu = \hat{\mu}\frac{S}{K_S + S}$$

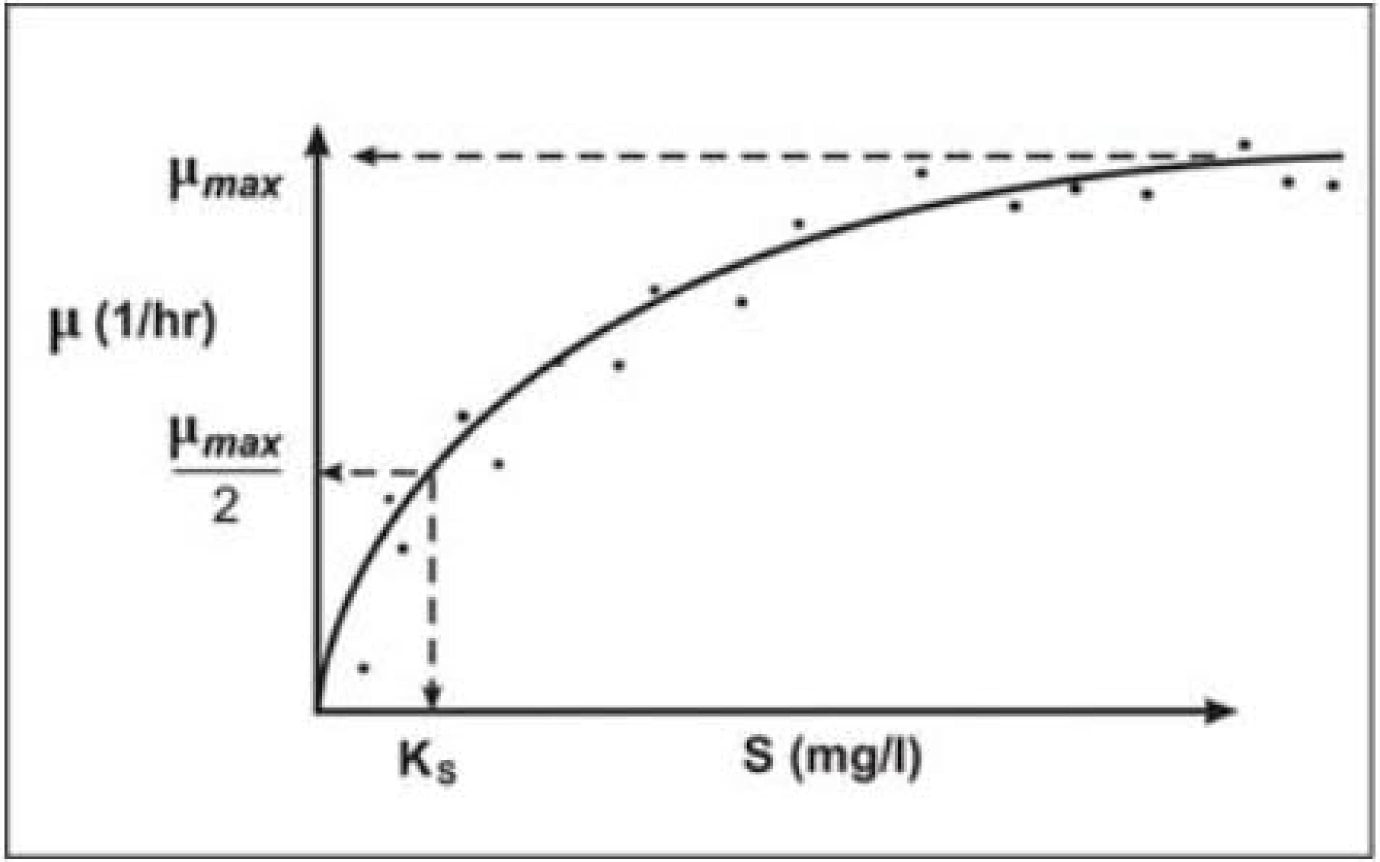
Substrate + Nutrients + (Oxygen) → Biomass + Energy

Applied from M. Mulas

Typical growth curve for microbial population in batch reactor



Monod's kinetics



$$\mu = \mu_{max}\left(\frac{S}{S+K_S}\right)$$

State and Composition Variables

- State variables are fundamental variables in the modelled biological reactios and they are calculated in each juction point in the model

- For state variables S refers to soluble and X to particulate material or substrate
  - Ss = soluble substrate
  - Snh = soluble free and ionized ammonia
  - Xs = particulate substrate etc.

- Composition variables are formed as follows:
  - COD = Ss + Xs + Si + Xi + Xii

- Depending on the model, there might be from 19 to 65 state variables!
  - The more state variables, the more laborous calibration…

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Activated sludge – a typical plant model

Michela Mulas

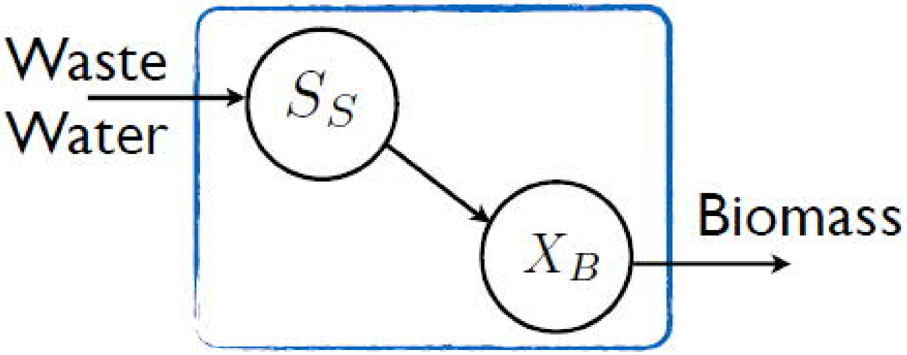
Modelling activated sludge process

A simple bioreactor model

The basic principles in biological wastewater treatment are based on the physical-biological phenomena, **biofloculation**, and a purely biological phenomenon, the **bacterial metabolism**

Growth	**Biomass** X_B	$\mu X_B - b X_B$
Decay	**Substrate** S_s	$-\frac{1}{Y}\mu X_B$
Monod kinetics	$\mu = \hat{\mu}\frac{S_S}{K_S + S_S}$	

Modelling activated sludge process
Single nutrient



The microorganisms absorb the nutrient for the wastewater using it to grow and to produce more biomass

Biomass

$$\frac{d}{dt}(VX_B) = Q_{in}X_{B,in} - Q_{out}X_{B,out} + Vr_B$$

Substrate

$$\frac{d}{dt}(VS_s) = Q_{in}S_{s,in} - Q_{out}S_{s,out} + Vr_S$$

Modelling activated sludge process

Single nutrient

Component → ↓ Process	1 Substrate S_S	2 Biomass X_B	Reaction
Biomass Growth	$-\frac{1}{Y}$	1	$\hat{\mu}\frac{S_S}{K_N+S_S}X_B$

Biomass

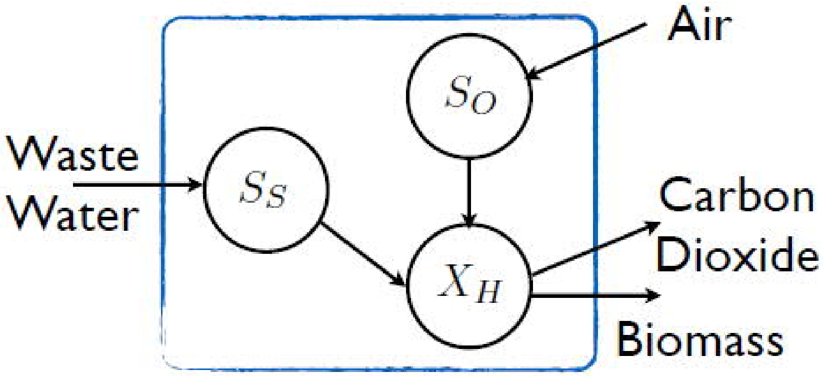
$$\frac{d}{dt}(VX_B) = Q_{in}X_{B,in} - Q_{out}X_{B,out} + Vr_B$$

Substrate

$$\frac{d}{dt}(VS_s) = Q_{in}S_{s,in} - Q_{out}S_{s,out} + Vr_S$$

Modelling activated sludge process

Carbon removal



The carbonaceous nutrient and dissolved oxygen are assorbed by the microorganisms which grow to produce more biomass

Biomass

$$\frac{d}{dt}(VX_H) = Q_{in}X_{H,in} - Q_{out}X_{H,out} + Vr_H$$

Substrate

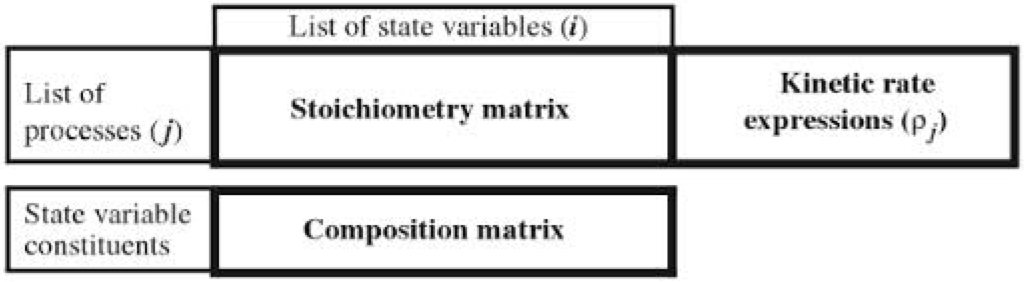
$$\frac{d}{dt}(VS_s) = Q_{in}S_{s,in} - Q_{out}S_{s,out} + Vr_S$$

Oxygen

$$\frac{d}{dt}(VS_o) = Q_{in}S_{o,in} - Q_{out}S_{o,out} + Vr_o + K_La\left(S_{o,sat} - S_o\right)V$$

Gujer Matrix

- Commonly applied matrix to present biological reactions
- Employed in the Activated Sludege Models (ASM1, ASM2 and ASM3)



The Gujer matrix (Guidelines for using Activated Sludge Models, 2013)

- Consists of three parts:
  - Stoichiometric matrix
    - Includes the stoichiometry of each reaction, usually expressed in the same unit
  - Compositions matrix
    - Includes the balance of the variables composition
  - Kinetic rates
    - Kinetic rates for each reaction in the matrix

Understanding the Gujer matrix

Three components

Two fundamental processes

Continuity

Mass Balance

Component →	i	1 X_B	2 S_S	3 S_O	Process Rate, ρ_j $[ML^{-3} T^{-1}]$
j Process ↓					
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:
Stoichiometric Parameters: True growth yield: Y		Biomass [M(COD) L^{-3}]	Substrate [M(COD) L^{-3}]	Oxygen (negative COD) [M(−COD) L^{-3}]	Maximum specific growth rate: $\hat{\mu}$; Half-velocity constant: K_S; Specific decay rate: b

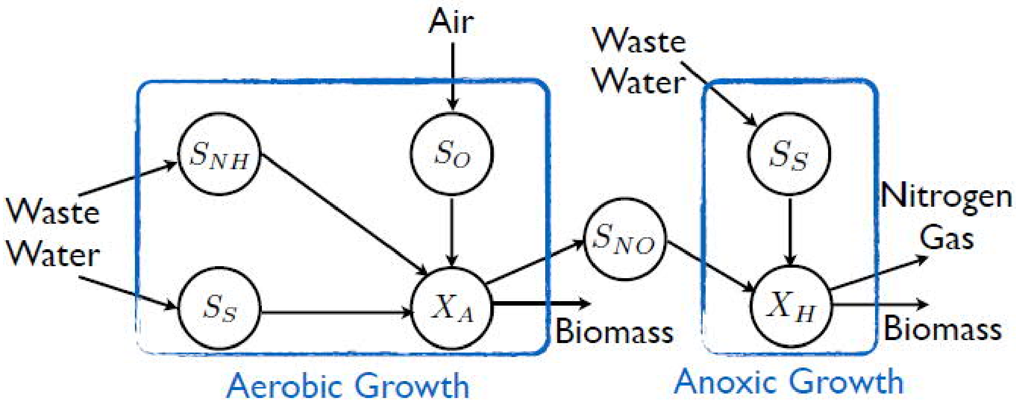
X – Particulate
C – Colloidal
S – Soluble

Modelling activated sludge process
Carbon removal

Component → ↓ Process	1 Nutrient	2 Biomass	3 Oxygen	Reaction
Aerobic growth of Heterotrophs	$-\frac{1}{Y_H}$	1	$\frac{Y_H-1}{Y_H}$	$\hat{\mu}\frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}X_H$
Decay of Heterotrophs	$1-f_P$	-1		$b_H X_H$

Modelling activated sludge process

Nitrogen removal



The simplest example of carbon and nitrogen removal involves:

- Heterotrophic biomass
- Autotrophic biomass
- Ammonia
- Oxygen
- Nitrate

The **aerobic growth of autotrophs** consumes soluble carbon, ammonia and dissolved oxygen to produce extra biomass and nitrate in solution. This steps can be further divided into two steps: producing nitrites and oxidizing the nitrites to nitrates

The **anoxic growth of heterotrophs** uses as source of oxygen and produce extra biomass and nitrogen gas

Gujer Matrix

- Reactions taking place in the activated sludge processes
  - Aerobic growth
  - Anoxic growth
  - Nitrification
  - Denitrification, etc.

Saturation function

Inhibition function

Electron equivalence

Component → ↓ Process	1 S_S	2 S_O	3 S_{NH}	4 S_{NO}	5 X_H	6 X_A	Kinetics
Aerobic growth of Heterotrophs	$-\frac{1}{Y_B}$	$\frac{Y_H-1}{Y_H}$	$-i_{XB}$		1		$\hat{\mu}_H \frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}X_H$
Anoxic growth of Heterotrophs	$-\frac{1}{Y_B}$		$-i_{XB}$	$\frac{Y_H-1}{2.86Y_H}$	1		$\hat{\mu}_H \frac{S_S}{K_S+S_S}\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\eta_g X_H$
Aerobic growth of Autotrophs		$\frac{Y_A-4.57}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$	$\frac{1}{Y_A}$		1	$\hat{\mu}_A \frac{S_{NH}}{K_{NH}+S_{NH}}\frac{S_O}{K_{OA}+S_O}X_H$
Decay of Heterotrophs	$1-f_P$		$i_{XB}-f_P i_{XP}$		−1		$b_H X_H$
Decay of Autotrophs	$1-f_P$		$i_{XB}-f_P i_{XP}$			−1	$b_A X_A$

Maximum rate

Decay factor

Matrix: M. Mulas

About the Kinetics

- Saturation function is used to increase the kinetic rate in certain environmental conditions
- Inhibition function is used to decrease the kinetic rate in certain environmental conditions

- Electron equivalence is calculated based on the stoichiometry of each reaction
  - Eg. It requires 4.57 g O_2 to convert 1 g of NH_4 to NO_3

- Different growth factors and maximum growth factors
  - Each reaction has their own factors
  - Usually they can be obtained empirically
  - *Important: Normally when modelling there is no need to calibrate the kinetic rates!*

Modelling activated sludge process

ASM's family

In 1987, the **International Association on Water Quality** formed a task group to promote the development and facilitate the application of practical model for design and operation of biological wastewater systems

ASM1

Organic and Nitrogen removal
- 13 State Variables
- 8 Reaction Rates
- 19 Parameters

ASM3

ASM2

Organic, Nitrogen and Phosphorus removal
- 19 State Variables
- 19 Reaction Rates
- 64 Parameters

ASM2d

Commonly Applied Activated Sludge Models

- ASM1
  - Activated Sludge Model NO 1
  - The first activated sludge model, published in the 80's
  - Employs 8 reactions and 13 state variables
    - In Gujer matrix this converts to 8 rows and 13 columns (+ title row and rate column)
- ASM3
  - Activated Sludge Model NO 3
  - The latest activated sludge model, published in 2001
  - Employs 12 reactions and 13 state variables
    - In Gujer matrix this converts to 12 rows and 13 columns (+ title row and rate column)
  - In addition to the reactions in ASM1, the storage reactions are considered

Model Processes in full plant models

- Biological growth processes
- Decay processes
- Hydrolysis reactions
- Fermentation
- Ammonification
- Phosphorus release / uptake
- Precipitation
- Gas-liquid transfer
- Settling
- Mixing

Modelling practices

International Water Association

IWA is a **global reference point** for water professionals, spanning the continuum between research and practice and covering all facets of the water cycle.

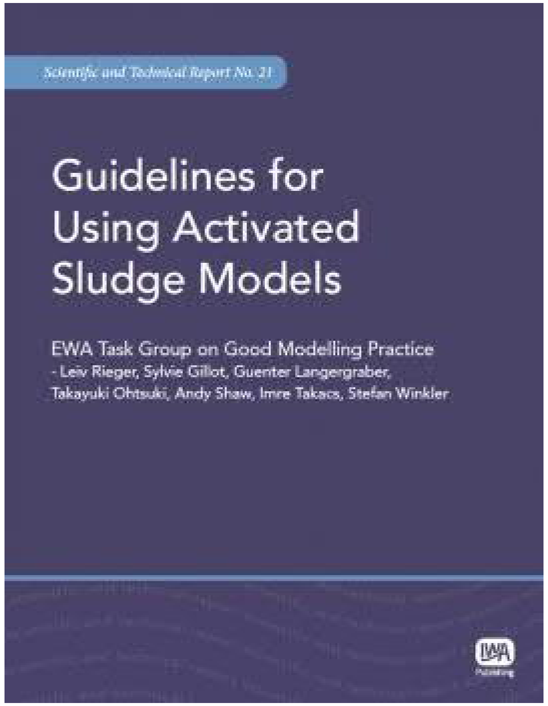
http://www.iwa-network.org/

The IWA network **facilitates multi-level cooperation** among its diverse membership groups, and sharing of the very best of knowledge on water science, research and management worldwide.

Modelling practices

Good modeling practice

GMP is a small team of modelers with wide international experience. Their goal is to **collect the experience and knowledge on activated sludge modeling** with the clear aim to provide guidance to practitioners. https://iwa-gmp-tg.irstea.fr/



Mathematical modeling has become a widely accepted tool for plant design and operation, training of process engineers and operators and a research tool.