Engineering tools for environmental bioprocess engineer

→Modeling & Models…

Some skills in setting up mathematical models for bioprocesses

Introduction to ASM:
Activated Sludge Model
WWTP modeling approach of International Water Association (IWA)

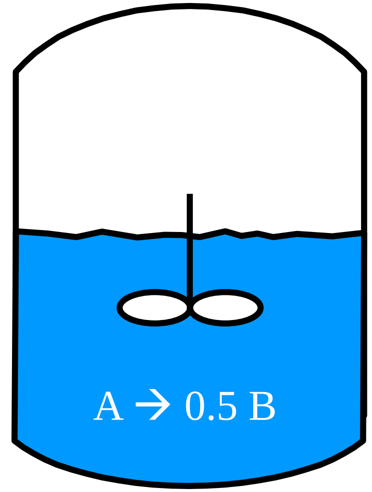
→For Simulation & Control

Some skills in control and simulation of biological processes

Introduction to Aquasim:
Computer program for the identification and simulation of aquatic systems

Models…? & Simulation

REACTION in a batch reactor of V=10 l :
Stoichiometry : A → 0.5 B
Process rate $r_A = k_A C_A$ with C_A [mg/l] ; C_{Ainit} = 1 [mg/l] ; k_A=1 [h^{-1}]



Stirred Batch Reactor

Plot the concentration of A and B as a function of time
→ Dynamic answer of the process !!!

??? HOW ???

$$\frac{d(C_A V)}{dt} = -r_A V \qquad (In = Out = 0)$$

$$\frac{d(C_B V)}{dt} = \frac{1}{2}(r_A V) \qquad as\ V = Cst$$

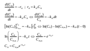
1 – Mass Balance for each compound

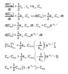
$$\frac{d(C_A)}{dt} = -r_A \ ; \ \frac{d(C_B)}{dt} = \frac{1}{2} r_A \ ; \ r_A = k_A . C_A$$

2 – Analytical Integration

$$C_A = C_{A,in} e^{-k_A . t}$$

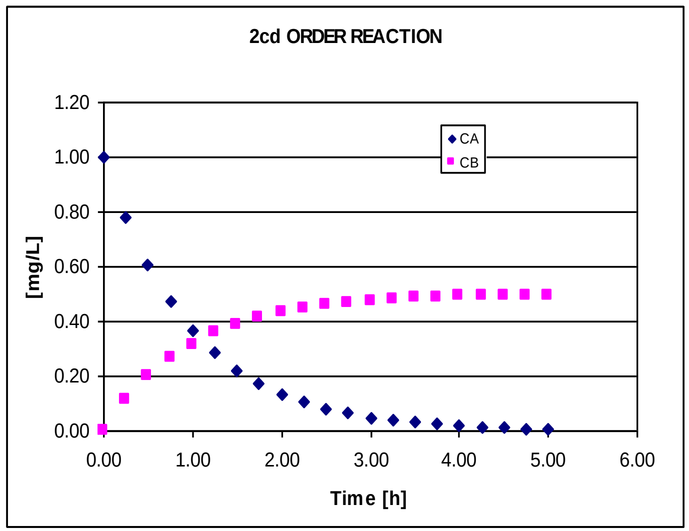
$$C_B = \frac{1}{2} C_{A,in} \left(1 - e^{-k_A . t}\right) + C_{B,0}$$





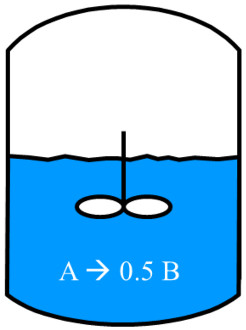
2 – Computation →

⇔ Simple !!!



kA	1	1/h
Cain	1	mg/L
Time	CA	CB
0.00	1.00	0.00
0.25	0.78	0.11
0.50	0.61	0.20
0.75	0.47	0.26
1.00	0.37	0.32
1.25	0.29	0.36
1.50	0.22	0.39
1.75	0.17	0.41
2.00	0.14	0.43
2.25	0.11	0.45
2.50	0.08	0.46
2.75	0.06	0.47
3.00	0.05	0.48
3.25	0.04	0.48
3.50	0.03	0.48
3.75	0.02	0.49
4.00	0.02	0.49
4.25	0.01	0.49
4.50	0.01	0.49
4.75	0.01	0.50
5.00	0.01	0.50

Models…? & Simulation



Stirred Batch Reactor

Simple process : - 1 compound
- with 1 kinetic process (linear)
- in 1 reactor in batch mode V=cst,

→ (Very) SIMPLE …

In Wastewater Treatment Plants

→ Complexity ↑

1. Complexity increases due to # compounds :
   - More than13 (ASM Activated Sludge)
   - Up to 25 (ADM Anaerobic Digestion)

Compounds	
Dissolved compounds	
S_{O_2}	Dissolved oxygen
S_I	Soluble inert organics
S_S	Readily biodegradable substrates
S_{NH_4}	Ammonium
S_{N_2}	Dinitrogen, released by denitrification
S_{NOX}	Nitrite plus nitrate
S_{ALK}	Alkalinity, bicarbonate
Particulate compounds	
X_I	Inert particulate organics
X_S	Slowly biodegradable substrates
X_H	Heterotrophic biomass
X_{STO}	Organics stored by heterotrophs
X_A	Autotrophic, nitrifying biomass
X_{SS}	Total suspended solids

Models…? & Simulation

In Wastewater Treatment Plants → Complexity ↑

2. Complexity increase with more than 12 complex multi-parameter multivariate kinetic processes : $r_A = k_A . C_A$ → $r_S = q_S^{max} (C_S / C_S + k_S) . C_X$

3. Complexity due to:
- multiple reactors
- multiple steps and treatment lines
- multiple operating mode batch, continuous and sequencing

Dynamic answer of such complex model
CANNOT be solved analytically !!!

This can be achieved with the followings tools:

- Modeling approach/tool which can cope with model complexity: **Matrix formulation** in ASM created by IWA task group
- Computing environment with **numeric integration**, identification and **simulation** such AQUASIM

1 Hydrolysis

Heterotrophic organisms,

2 Aerobic storage of S_S

3 Anoxic storage of S_S

4 Aerobic growth

5 Anoxic growth (denitrification)

6 Aerobic endogenous respiration

7 Anoxic endogenous respiration

8 Aerobic respiration of X_{STO}

9 Anoxic respiration of X_{STO}

Autotrophic organisms, ni

10 Aerobic growth of X_A, nitrification

11 Aerobic endogenous respiration

12 Anoxic endogenous respiration

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→Modeling & Models…

ASM - Activated Sludge Model
This modeling formulation has been popularized in the 80' by specialists and professionals (IWA – Modeling task groups International Water Association)

- This modeling was first used for Activated Sludge Model (ASM1→ASM3)
- And then used for Anaerobic Digestion Model (ADM1)

→For Simulation & Control

AQUASIM a software tool designed for the simulation and identification of aquatic systems in the laboratory, in technical plants and in natural environment.

1. Simulation
2. Parameter sensitivity
3. Parameter Identification

In GBE course → Assignment #1 = Self training to ASM + Aquasim
- Introduction to ASM modelling
- Tutorial + Use of Aquasim (Dynamic Simulation)

Modeling → For Simulation and Control

More about WWTP Modeling, Design and Control → Simulation Benchmark

It's the result of 2 COST (European Union) programs

1. COST682 « Integrated Wastewater Management » 1992-1998 Focusing on optimization of design and control of dynamic biological wastewater processes
2. COST624 "Efficiency and optimization of biological wastewater treatments" 1998-2002 to increase knowledge about microbial biosystems and integrated wastewater treatments for sustainable development

→ COST « Simulation Benchmark » Manual

It consists of a complete protocol for evaluation of efficiency and control strategy of Activated Sludge wastewater treatments

→ Full description of the WWTP modeling system with

1. Description of implementation on multiple simulation environments dedicated to WWTP (with specificities, adaptations, tunings and bias)
2. Check of steady state and dynamic answers
3. Comparison of performance and quality of control strategy

See Official COST Report

The COST Simulation Benchmark Description and Simulator Manual.pdf

(in Readings folder)