Mathematical Modelling of Wastewater Treatment Plants

Part II: The Modelling Process

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Outline

- Types of models
- Modeling strategy
- System identification (parameter identification)
- Example of a simple two-sate variable dynamic system

References:
Olsson, G. and Newell, B. (1999). Wastewater Treatment Systems. IWA Publishing, 742 p.
Jeppsson, U. (1996). Modelling Aspects of Wastewater Treatment Processes. Ph.D. Thesis, Lund University, 428 p.

Types of models

- Lab/bench scale models
- Physical models
- Mathematical models
- Qualitative models
- Linguistic models
- Visual models

Mathematical models

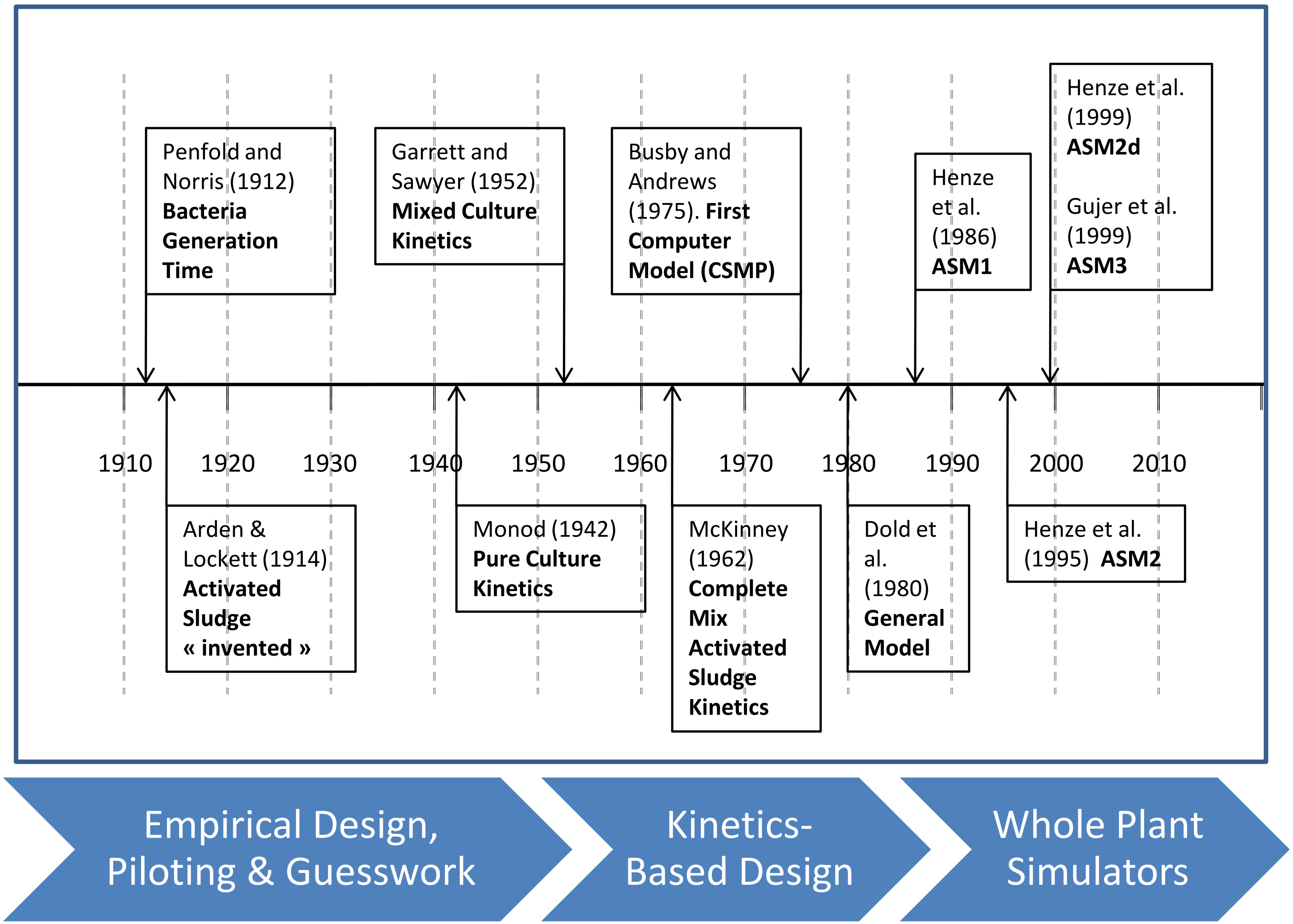
- A mathematical model is a representation (simplification) of reality, designed to help us understand the processes that are taking place in the plant
- To represent the same process, models can be very simple or they can be extremely complex
- From an engineering perspective, models should be “as simple as possible, but no simpler”
- Need to be concerned with model « identifiability »

Mathematical models

- The objective is to conceptualize our knowledge of a process or a physical system in a mathematical description of the process
- Once we have a working model we can use it for:
  - Design
  - Operation
  - Research
  - Performance assessment / plant audit
  - Training of operators
  - Forecast and planning purposes
- Modelling of the activated sludge process is not new …

Activated Sludge Modeling Timeline

(adapted from Bruce Johnson, CH2M Hill, 2009)



Modelling Strategy

1. Functional process specification
2. Define your modelling objectives
    a. Purpose
    b. Accuracy
    c. Boundary conditions
    d. Time-scale
    e. Etc.
3. Model type (L vs NL, D vs Continuous, etc.)
4. Model development
5. Model verification
6. Model calibration / validation
7. Use the model for its intended purpose

Modelling Objectives

1. Define the purpose of the model (what will it be used for?)
    - Design
    - Research
    - Process control and operation
    - Forecasting
    - Performance analysis / audit
    - Education / learning / training
    - Etc.
  – A design-based model will be very different than a model developed for research purposes (e.g., CAPDETWorks vs GPS-X)
  – Hierarchical modeling (a hierarchy of models)
2. Define System Boundaries
    - A component of a reactor
    - The reactor itself
    - Liquid line
    - Entire plant (liquid and sludge line processes)

Modelling Objectives

3. Define time scale of interest
    - Dynamics of processes will vary from

      seconds & minutes (e.g., dissolved oxygen dynamics)

      to

      days and/or weeks (biomass growth)

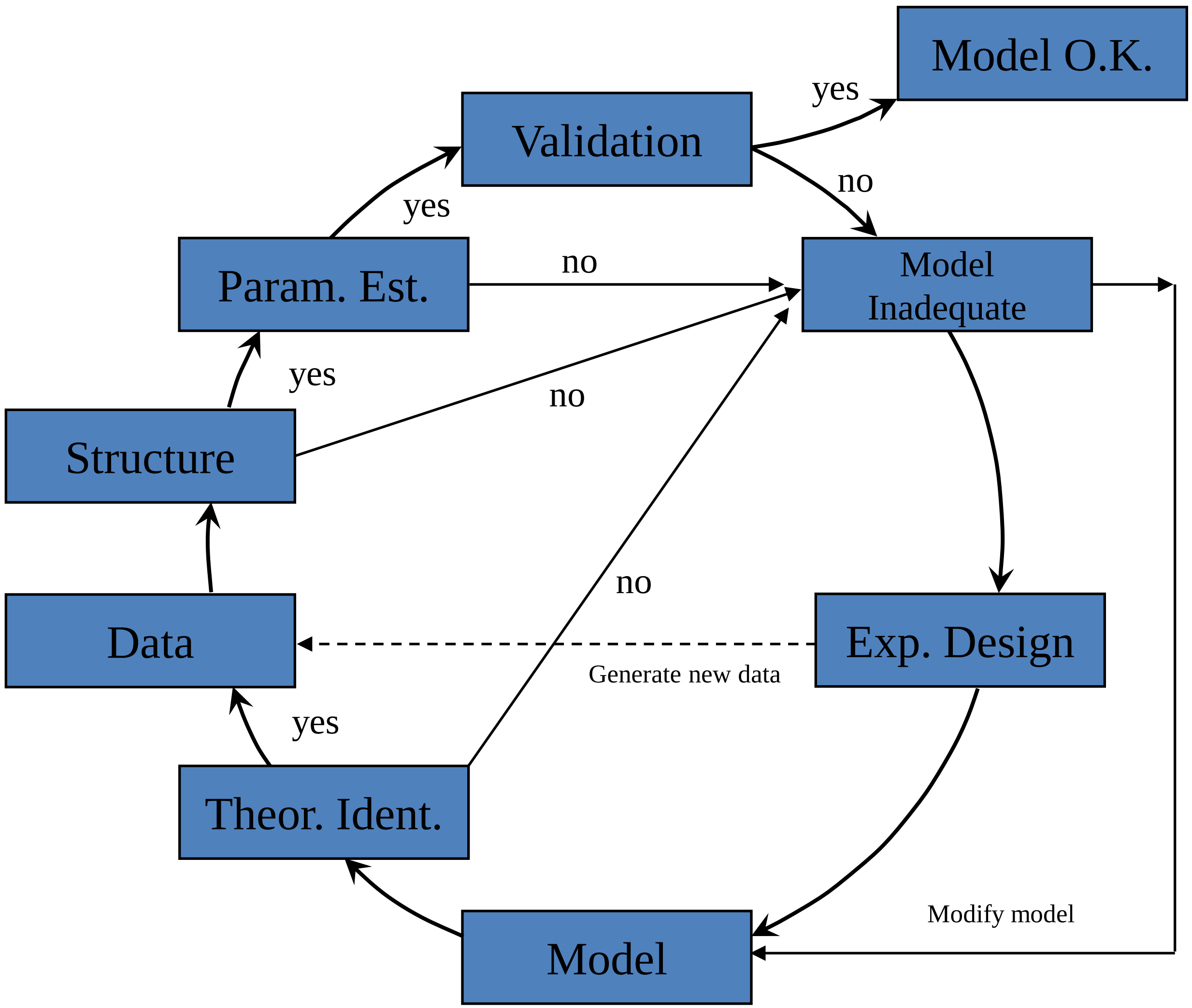
      Depending on your modeling objectives, model formulation and solution will be dependent on the time scale of interest

4. Define the desired accuracy

Model Type

- Mechanistic vs Black-Box (I/O or ARMAX)
- Deterministic vs stochastic
- Continuous vs discrete
- Distributed vs lumped
- Time domain vs frequency domain

Mechanistic, deterministic, time-domain, continuous distributed models



Adapted from
Jeppsson (1996)

System Identification

- Are the model parameters identifiable?
  - Are they uniquely identifiable ? i.e., is there a unique solution?
  - Are they locally identifiable ? i.e., finite number of solutions, i.e., parameter values
  - Are they unidentifiable ? i.e.,

A Simple Example – Two-State Variable System

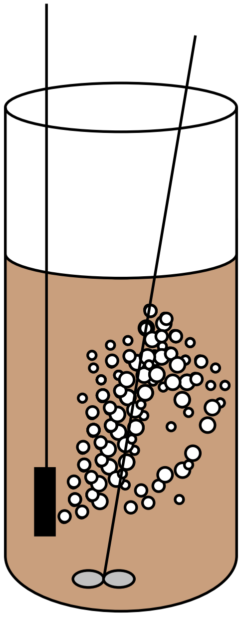
Substrate S; Biomass X

Consider:

$$\frac{dX}{dt} = \mu(S)X - bX \qquad (1)$$

$$\frac{dS}{dt} = -\frac{1}{Y}\mu(S)X \qquad (2)$$

$$\mu(S) = \frac{\hat{\mu}S}{K_S + S} \qquad (3)$$



Assume X and S are measureable.

Can all 4 parameters K_S , $\hat{\mu}$, Y , b be uniquely determined from perfect data? In other words, is the system globally identifiable?

Let $X_0 = X(0)$; $S_0=S(0)$

$$X'(0) = \frac{\hat{\mu} S_0}{K_S + S_0} X_0 - bX_0 = X_1 \qquad (4)$$

$$S'(0) = -\frac{1}{Y}\frac{\hat{\mu} S_0}{K_S + S_0} X_0 = S_1 \qquad (5)$$

$$\mu = \frac{\hat{\mu} S_0}{K_S + S_0}$$

$$X_1 = (\mu - b) X_0$$

$$S_1 = -\frac{\mu}{Y} X_0$$

Take the first-order Taylor series expansion of Eq. (1) and (2) at time t=0

$$X''(0) = (\mu - b)X_1 + \frac{\mu K_S X_0 S_1}{(K_S + S_0)S_0} = X_2 \qquad (6)$$

$$S''(0) = -\frac{\mu}{Y}\left(X_1 + \frac{\mu K_S X_0 S_1}{(K_S + S_0)S_0}\right) = S_2 \qquad (7)$$

Solve (4), (5), (6) and (7) for K_S , $\hat{\mu}$, Y , b

Solve for parameters

$$K_S = \frac{S_2 S_0^2 X_0 - S_1 S_0^2 X_1}{S_1^2 X_0 - S_2 S_0 X_0 + S_1 S_0 X_1}$$

$$\mu = \frac{X_2 X_0 S_1 - X_1^2 S_1}{S_2 X_0^2 - S_1 X_1 X_0}$$

$$\hat{\mu} = \frac{\left(X_2 X_0 S_1 - X_1^2 S_1\right)\left(K_S + S_0\right)}{S_2 S_0 X_0^2 - S_1 S_0 X_1 X_0}$$

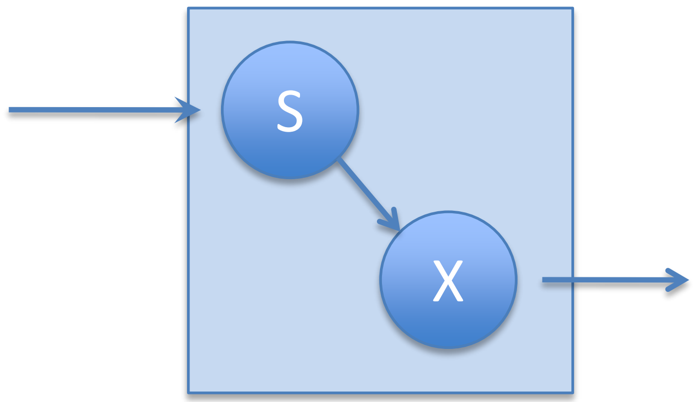
$$b = \frac{S_1 X_2 - S_2 X_1}{S_2 X_0 - S_1 X_1}$$

$$Y = \frac{X_1^2 - X_1 X_0}{S_2 X_0 - S_1 X_1}$$

Accordingly, the process parameters are identifiable.

If measurements are noise-corrupted
Then parameters are not uniquely
Identifiable!

Modelling of a Single Substrate System



$Q_{in} = Q_{out} = Q$ → Constant Volume Reactor

Input – Output = Accumulation - Reaction

- Biomass (X_H):

$$QX_{H,in} - QX_{H,out} = \frac{d(VX_H)}{dt} - r_H V$$

$$r_{X_H} = \hat{\mu}\left(\frac{S_S}{K_S + S_S}\right) X_H$$

$$X_{H,in} = 0$$

$$\text{CSTR} \rightarrow X_{H,out} = X_H$$

$$\frac{dX_H}{dt} = \left(\hat{\mu}\left(\frac{S_S}{K_S + S_S}\right) X_H - \frac{X_H}{\theta}\right)$$

- Substrate (S_S):

$$QS_{S,in} - QS_{S,out} = \frac{d(VS_S)}{dt} - r_S V$$

$$r_{S_S} = -\frac{1}{Y_H}\hat{\mu}\left(\frac{S_S}{K_S + S_S}\right) X_H$$

$$\text{CSTR} \rightarrow S_{S,out} = S_S$$

$$\frac{dS_S}{dt} = \frac{1}{\theta}\left((S_{S,in} - S_S) - \frac{1}{Y_H}\hat{\mu}\left(\frac{S_S}{K_S + S_S}\right) X_H\right)$$

Solve these two NODE using numerical methods techniques.
Matlab, Simulink, ACSL, etc.

Two-State / One Process Model in Petersen Matrix Format

Processes ↓	Components (state-variables)		Process rate Kinetics
	Substrate, S_S	Biomass, X_H	
Aerobic heterotrophic growth	$-\frac{1}{Y_H}$	1	$\hat{\mu}\left(\frac{S_S}{K_S + S_S}\right)X_H$

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				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\cdot\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57}{Y_A}+1$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
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 [$ML^{-3}T^{-1}$]	$r_i=\sum_j \nu_{ij}\rho_j$									$r_i=\sum_j \nu_{ij}\rho_j$				
	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

Part III

Dynamic Modelling of the Activated Sludge Process (ASM1)