Mathematical modelling of wastewater treatment technologies in industrial water circuits

P. Grau, I. Lizarralde and L. Sancho

ceit
ik4 research alliance

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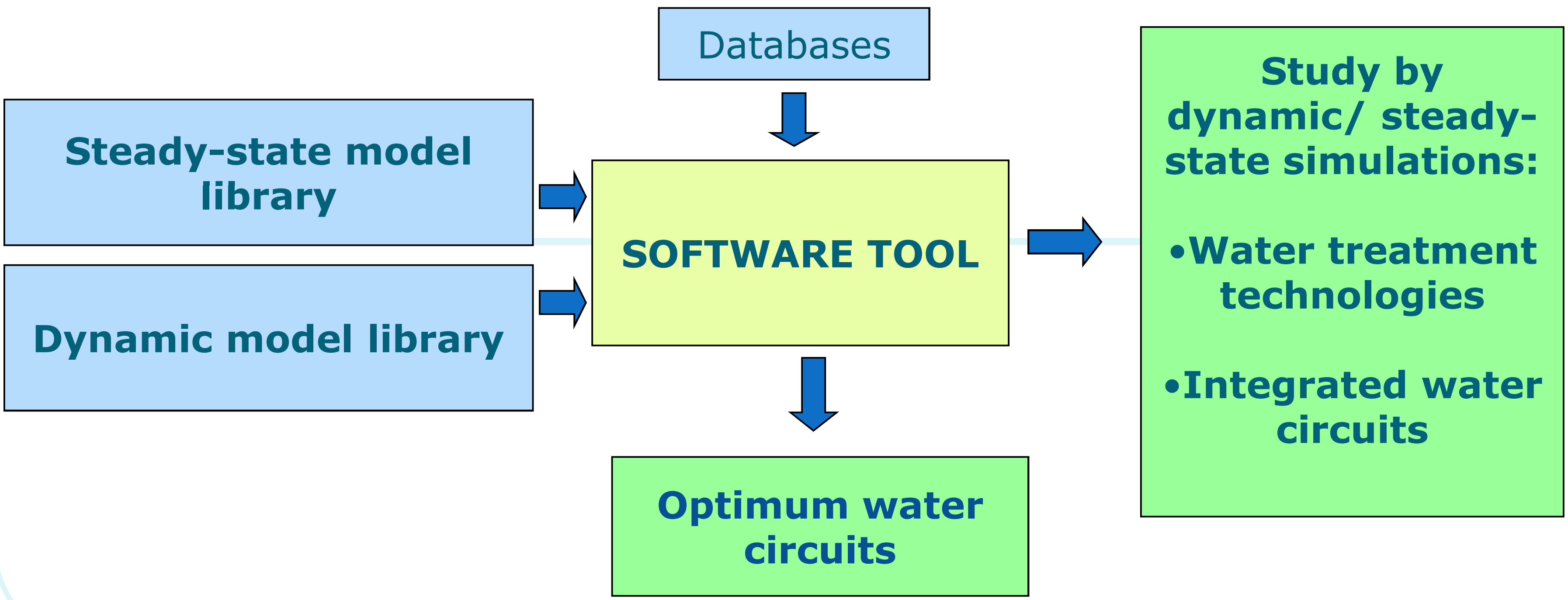
Introduction and Objectives

- Rising costs and scarcity of water encourages the study of new water treatment technologies and strategies for reusing water in water networks in mills
- The wide variety of technologies, the different water qualities at each point in the network and the multiple sources/sinks make difficult to find the optimum solution
- The use of mathematical models and simulation tools can be very helpful on this task
- Objective:
  - To develop a library of mathematical models able to reproduce the behaviour of some traditional and novel wastewater treatments

Part of the **WQMT**



Library of Unit-Process models

Biological Unit Processes
Activated Sludge unit
MBR
MBBR
Anaerobic unit (UASB)
Denutritor
Chemical Unit processes
AOPs
Disinfection (O_3, Cl_2, UV)
Coagulation-flocculation

Water – Solids separation Unit Processes
Settler
DAF
MF, UF
NF, RO
3FM
FACT
Evapoconcentrator
Electrodialysis

Mathematical structure of the models

- IWM: common method to construct mathematical models that guarantees mass and heat energy continuity
  - Definition of a Common Components List
    - Gathers all relevant components/measurements in internal processes in the mills and wastewater treatment technologies

- Definition of mass and heat balances for all components
- Definition of operational and capital costs functions

Modelling of Biological units

- Describe the COD removal:
  - Aerobic conditions:
    - ASU, MBR, MBBR
  - Anaerobic conditions:
    - UASB (COD and $SO_4^=$ removal)
- COD removal is described according to the endogenous respiration model (Lawrence and McCarty 1970)

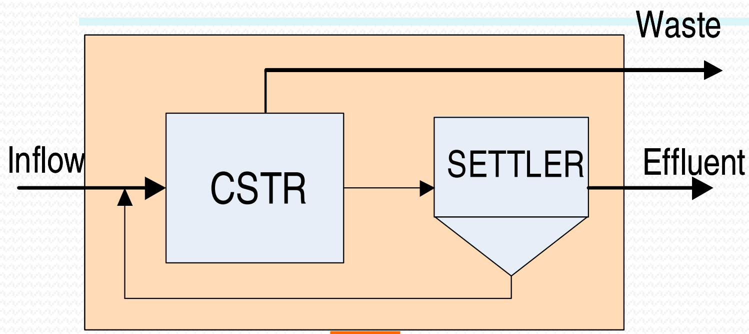
	S_S	X_{BH}	X_{end}	S_o
X_{BH} growth	-1	Y_H		$-(1-Y_H)$
X_{BH} decay		-1	f_{end}	$-(1-f_{end})$

$$\rho = \frac{\mu_H}{Y_H} \cdot \frac{S_S}{K_S + S_S} X_{BH}$$

$$\rho = b_H \cdot X_{BH}$$

- Steady-state equations are generated applying mass balances to the control volume of each biological technology

Biological models: **Activated Sludge Unit (ASU)**



$$TSS_{max} \approx 3500 \ \ mg/l$$

$$SRT \approx 8 \ d$$

Mass balance

Effluent Quality

$$BOD_{eff} = \frac{K_s\left[(1-f_{ns}) + SRT \cdot b_H\right]}{SRT(\mu_H - b_H) - (1-f_{ns})}$$

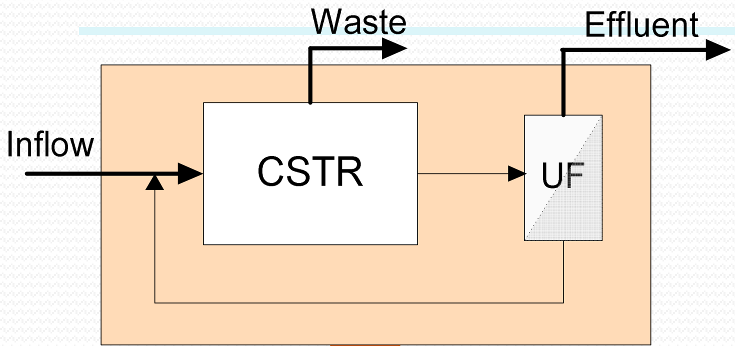
Variables related with costs

$$V_{ASU} = \frac{HRT_{min}}{Q_{inf}} \qquad Q_w = \frac{V_{ASU}}{SRT}$$

$$DO_{req} = \frac{V_{ASU}}{1000} \cdot \left[\frac{(1-Y_H) \cdot S_{COD}}{HRT} + (1-f_{end}) \cdot b_H \cdot X_{BH,LM}\right]$$

$$HRT_{min} = \frac{1}{TSS_{max}} \cdot \left[\frac{\left(\frac{SRT \cdot Y_H \cdot (BOD_0 - BOD_{ef})}{1 + b_H \cdot SRT} + f_{end} \cdot b_H \cdot SRT \cdot \frac{SRT \cdot Y_H \cdot (BOD_0 - BOD_{ef})}{1 + b_H \cdot SRT} + X_{I,0} \cdot SRT\right)}{f_{COD\_TSS}} + X_{II,0} \cdot SRT\right]$$

Biological models: **Membrane Bioreactor (MBR)**



$$TSS_{max} \approx 10000\ mg/l$$

$$SRT \approx 35\ d$$

Mass balance

Effluent Quality

$$BOD_{eff} = \frac{K_s\left[(1-f_{ns}) + SRT \cdot b_H\right]}{SRT(\mu_H - b_H) - (1-f_{ns})}$$

Variables related with costs

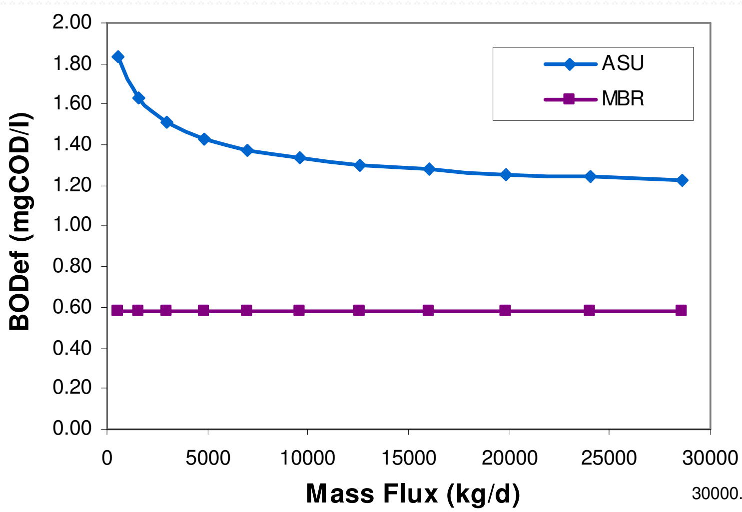
$$V_{MBR} = \frac{HRT_{min}}{Q_{inf}} \qquad Q_w = \frac{V_{MBR}}{SRT}$$

$$DO_{req} = \frac{V_{MBR}}{1000} \cdot \left[\frac{(1-Y_H) \cdot S_{COD}}{HRT} + (1-f_{end}) \cdot b_H \cdot X_{BH,LM}\right]$$

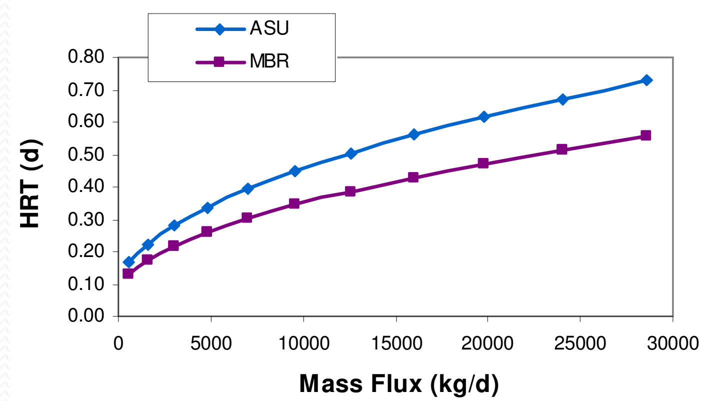
$$HRT_{min} = \frac{1}{TSS_{max}} \cdot \left[\frac{\left(\frac{SRT \cdot Y_H \cdot (BOD_0 - BOD_{ef})}{1 + b_H \cdot SRT} + f_{end} \cdot b_H \cdot SRT \cdot \frac{SRT \cdot Y_H \cdot (BOD_0 - BOD_{ef})}{1 + b_H \cdot SRT} + X_{I,0} \cdot SRT\right)}{f_{COD\_TSS}} + X_{II,0} \cdot SRT\right]$$

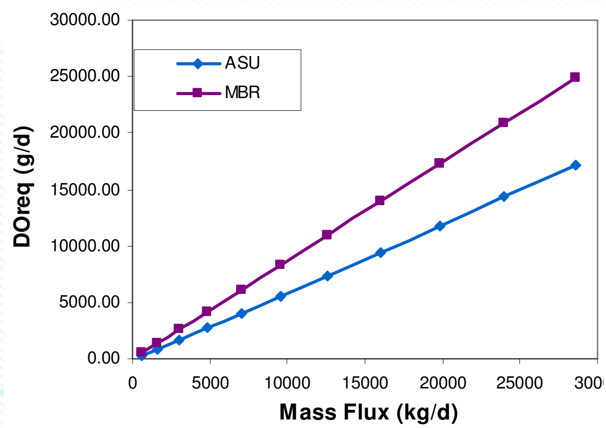
Comparison between ASU and MBR

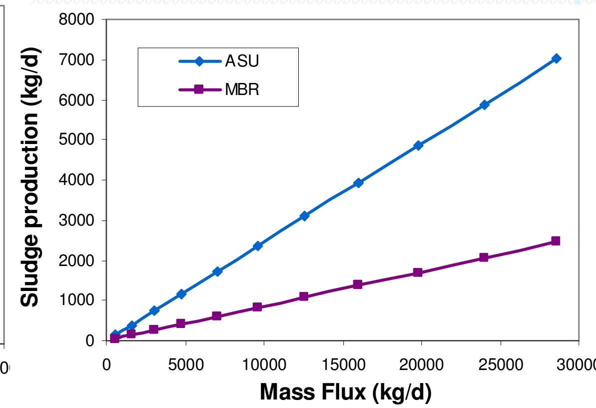
Effluent Quality



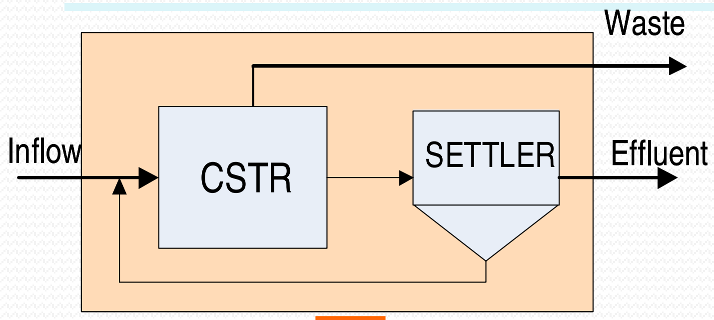
Variables related with costs







Biological models: **(UASB)**



$$TSS_{max} > 10000 \ mg/l$$

$$SRT > 30 \ d$$

$$V_{MBR} = \frac{HRT_{min}}{Q_{inf}}$$

Mass balance

Effluent Quality

$$COD_{SRB} = f_{COD\_SO4} \cdot SO_4{}^{=}{}_{inf}$$

$$S_{SO4=,eff} = \frac{K_s\left[(1-f_{ns}) + SRT\left(b_H + \frac{f_{ns}}{HRT}\right)\right]}{SRT\left(\mu_H - b_H - \frac{f_{ns}}{HRT}\right) - (1-f_{ns})}$$

$$S_{COD,eff} = \frac{K_s\left[(1-f_{ns}) + SRT\left(b_H + \frac{f_{ns}}{HRT}\right)\right]}{SRT\left(\mu_H - b_H - \frac{f_{ns}}{HRT}\right) - (1-f_{ns})}$$

Variables related with costs

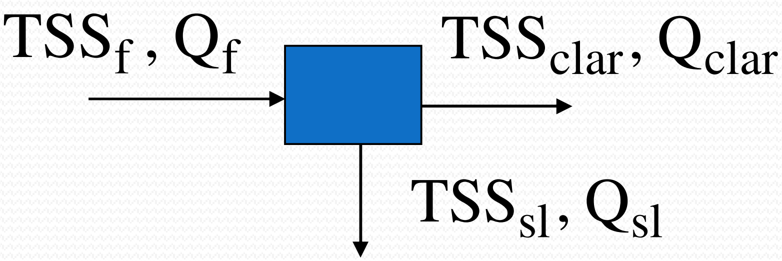
$$V_{UASB} = \frac{HRT_{min}}{Q_{inf}} \qquad Q_w = \frac{V_{UASB}}{SRT}$$

Water-Solids separation Units

- Units for separation of suspended solids and colloids (TSS and TCS)
  - Settler
  - Dissolved Air Flotation (DAF)
  - 3FM
  - MF-UF (% of dissolved particles TDS)
- Units for separation of TDS (organic and ions)
  - NF-RO
  - Evapoconcentrator
  - Electrodyalisis

Units for separation of TSS and TCS: **Settlers** and **DAFs**

- Water-Solid separation is based on efficiency rates for TSS and TCS



- **Settler (>1500 mg/l)**

$$TSS_{clar} = f_{X\_nss} \cdot TSS_f \cdot \frac{Q_f}{Q_{clar}}$$

$$TSS_{sl} = \left(1 - f_{X\_nss}\right) \cdot TSS_f \cdot \frac{Q_f}{Q_{sl}}$$

f_{X_nss} depends on the TSS setteability

- **DAF (≈ 1000 mg/l)**

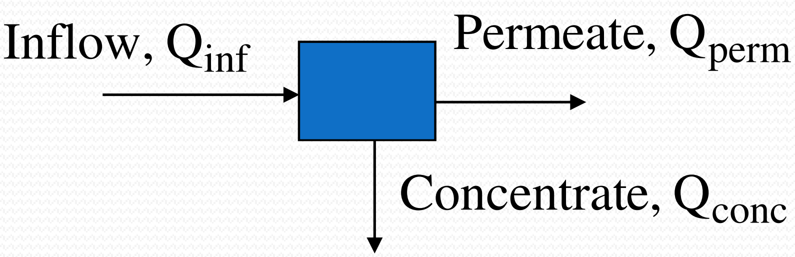
$$TSS_{clar} = f_{X\_nss} \cdot TSS_f \cdot \frac{Q_f}{Q_{clar}}$$

$$TSS_{sl} = \left(1 - f_{X\_float}\right) \cdot TSS_f \cdot \frac{Q_f}{Q_{sl}}$$

f_{X_float} depends on the air/solids ratio (a_S):
$f_{float} = 0.66a_S + 0.79$

Units for separation of TSS and TCS: **3FM** and **MF-UF**

- Water-Solid separation is driven by a pressure drop across the membrane



$$\begin{cases} Q_p = \dfrac{L_p \cdot \Delta P}{(1+FF)} \cdot A \qquad C_p = C_f \cdot \left(1 - \dfrac{R_C}{100}\right) \\ FF = \alpha_X \cdot TSS + \alpha_C \cdot TCS + \alpha_S \cdot TDS \end{cases}$$

- **3FM (2-5 μm)**
  - **TSS and TCS removal**
  - **Op. Costs:**

$$OP_{PE} = K_E \cdot P_E \cdot Q_{perm}$$

$$OP_{air} = K_E \cdot P_{air} \cdot Q_{air}$$

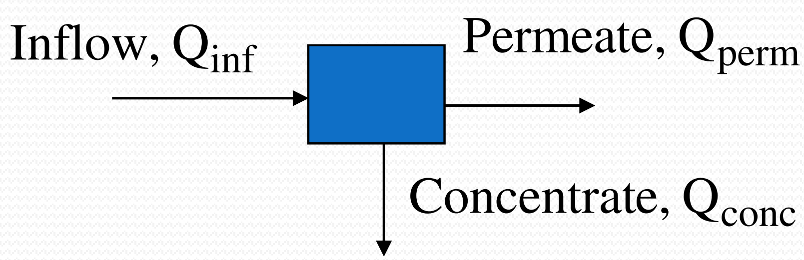
- **MF-UF (0.02-0.4 μm)**
  - **TSS, TCS and % TDS removal**
  - **Op. Costs:**

$$OP_{PE} = K_E \cdot P_E \cdot Q_{perm}$$

$$OP_{bwash} = K_E \cdot P_E \cdot (TSS + TCS + TDS) Q_{conc}$$

Units for separation of TDS:
RO, Evapoconcentrator and Electrodialysis

- All of them considered as instantaneous separation units:



Calculation of Q_{perm} and TDS_{perm} depend on the technology used

- Reverse Osmosis

$$Q_p = \frac{L_p \cdot (\Delta P - \Delta \Pi)}{(1 + FF)} \cdot A$$

$$\Delta \Pi = 1.19(T + 273) \cdot \left(\sum_{conc} m_i - \sum_{feed} m_i \right) \cdot \frac{0.76}{11}$$

$$C_p = C_f \left(\frac{B}{B + Q_p / A} \right)$$

- Electrodyalisis

$$C_p = C_f - \frac{\xi \cdot N \cdot I}{z \cdot F \cdot Q_p}$$

- Evapoconcentrator

$$C_p = C_f \text{ for volatile compounds}$$

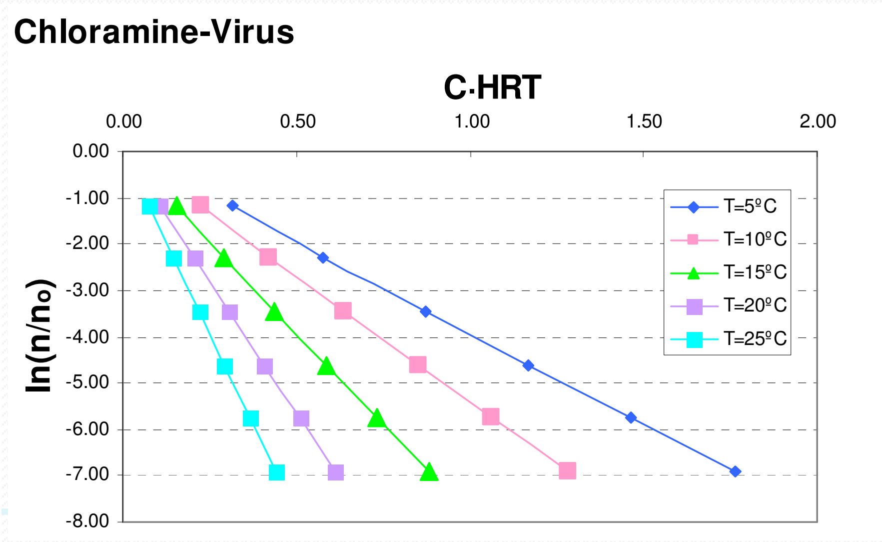
$$C_p = 0 \text{ for non volatile compounds}$$

Chemical Unit processes: **Disinfection**

- Inactivation related to contact time given by Chick's law:

$$\ln \frac{N_t}{N_o} = -k \cdot C^n \cdot HRT^m$$

- k values depend on:
  - Disinfectant: Ozone, chloramine, chlorine, UV radiation
  - Pathogens: bacteria (e-coli, legionella), virus, cyst, crystosporidium, egg-nematode
  - Temperature
  - pH



Conclusions

- A library of mathematical models able to describe a set of traditional and novel wastewater treatment technologies has been developed
  - Describe the fate of the most relevant and critical components in water networks
  - Models are compatible and directly connectable among them
  - Consider all relevant variables to calculate investment and operational costs associated to each treatment
- Current and future tasks
  - Implementation and verification of the models in the software tool
  - Calibration of the models with experimental data