A stochastic expectation maximization algorithm for the estimation of wastewater treatment plant ammonium concentration

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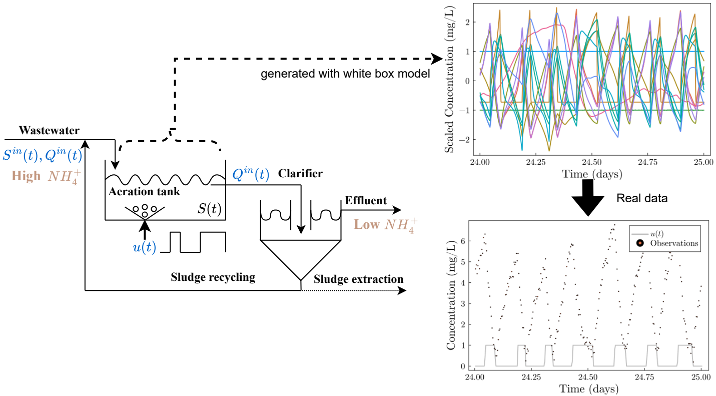
28 June 2024

Zoom on the secondary treatment of **Alternated Activated Sludge Plants** (AAS) :



- Municipal plants.
- **Input** : High NH_4^+.
- **Output** : Low NH_4^+.
- Control oxygen.
- **Interaction** of species.
- Few noised sensors.

Objective : Reduce concentration of NH_4^+ coming from inlet water (nitrogen removal).

Socio-economic Context

- **Increase** in environmental standards.
- Increase in **price** of energy.
- Increase in **variability** of energy.

Consequence : Minimize electric consumption.

Wastewater Treatment Plants

- **Complex** and **stochastic** system.
- **Expensive** and **unreliable** sensors.
- Controlled by **rudimentary** controllers.

Consequence : Finding new control algorithms.

Possible solution

Feedforward/Scheduling Control.

→

Condition

Dynamic model (NH_4^+).

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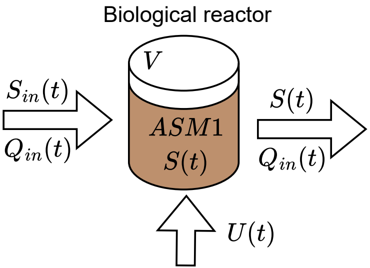
Outline

Development of family of **ASM's physic based** model

$$\frac{\partial S(t)}{\partial t} = \frac{Q^{in}(t)}{V}(S^{in}(t) - S(t)) + r(t, S(t), u(t))$$

- $S(t)$, **unknown** concentration of species.
- V, **unknown** volume of the reactor.
- $(Q^{in}(t), S^{in}(t))$, **known** inflow and inlet concentration.
- $u(t)$, **known** control applied to the system.



Possible models

Main objective : precise NH_4^+ predictions over 24h horizon.

- **Problem** : complex physic model.
- **Criteria** :
  - Easy control integration.
  - Observable.
  - Good generalization.

Solution : Grey box model

Reduced physic based model.

Table 2 Process kinetics and stoichiometry for carbon oxidation, nitrification, and dentrification

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

Simplified physic-based model :

$$\frac{\partial S_{NH}(t)}{\partial t} = \frac{Q^{in}(t)}{V}\left[S_{NH}^{in}(t) - S_{NH}(t)\right] - \beta u(t)\frac{S_{NH}(t)}{S_{NH}(t) + K}$$

with V, β and K **unknown** parameters.

Discretization :

$$S_{NH}[t+h] = S_{NH}[t] + h\left[\frac{Q^{in}[t]}{V}\left[S_{NH}^{in}[t] - S_{NH}[t]\right] - \beta u[t]\frac{S_{NH}[t]}{S_{NH}[t] + K}\right]$$

Main question : How can I find the parameters of the model ?
(non linear + simplified model + noised observations)

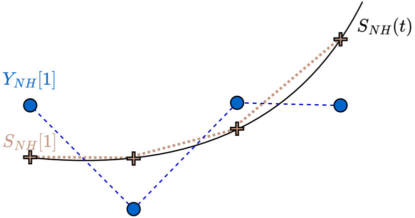
Outline

1. Proposed model
2. Proposed training procedure
3. Results

Training Dataset : $(Y_{NH}[i], \dots, Y_{NH}[N])$

Prediction Error Minimization : replace $S_{NH}[i]$ by observations $Y_{NH}[i]$

$$min_{V,\beta,K} \sum_{t=1}^{N-1} \left[Y_{NH}[t+1] - \left(Y_{NH}[t] + h \left[\frac{Q^{in}[t]}{V} \left[S^{in}_{NH}[t] - Y_{NH}[t] \right] - \beta u[t] \frac{Y_{NH}[t]}{Y_{NH}[t] + K} \right] \right) \right]^2$$



New question : How can I deal with noises ?

Separation of the model into two parts

- **Transition equation :**

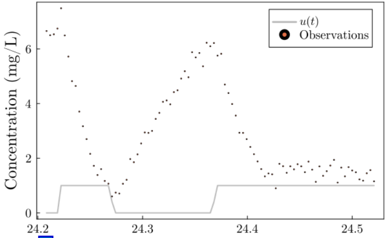
$$S_{NH}[t+h] = S_{NH}[t] + h\left[\frac{Q^{in}[t]}{V}\left[S_{NH}^{in}[t] - S_{NH}[t]\right] - \beta u[t]\frac{S_{NH}[t]}{S_{NH}[t]+K}\right] + w_t, \quad w_t \sim \mathcal{N}(0, \sigma_\epsilon^2)$$

- **Observation equation :**

$$Y_{NH}[t] = S_{NH}[t] + v_t, \quad v_t \sim \mathcal{N}(0, \sigma_m^2)$$

New question : How can I find jointly the hidden variable $S_{NH}[t]$ and the parameters of the model ?

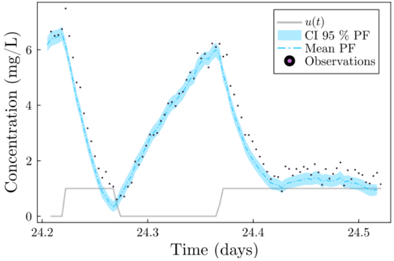
Filtering and Smoothing : Estimation of the latent variables



Filtering $p(S_{NH}[t]|Y_{NH}[1], \ldots, Y_{NH}[t])$

or

Smoothing $p(S_{NH}[t]|Y_{NH}[1], \ldots, Y_{NH}[T])$



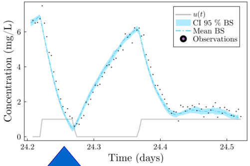
Condition : Known parameters.

- **Linear model**
  - Kalman Filter and Smoother
- **Nonlinear model**
  - ◇ Linearization
    - Extended Kalman Filter and Smoother
  - ◇ Sequential Monte Carlo
    - Ensemble Kalman Smoother and Filter
    - Particle Filter and Backward Smoother

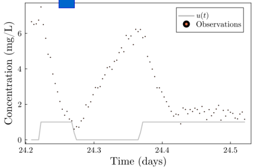
Monte-Carlo Expectation Maximization (MCEM)

$\hat{S}_{NH}[1], \ldots, \hat{S}_{NH}[T]$

E-Step



Filtering => Smoothing



M-Step

$$\hat{w}[t] = \left[\hat{S}_{NH}[i+1] - \left(\hat{S}_{NH}[i] + h\left[\frac{Q^{in}[t]}{V}[S^{in}_{NH}[t] - \hat{S}_{NH}[i]] - \beta u[t]\frac{\hat{S}_{NH}[i]}{\hat{S}_{NH}[i]+K}\right]\right)\right]$$

$$\hat{v}[t] = Y_{NH}[t] - \hat{S}_{NH}[t]$$

Residual's computation using smoothed values

$$min_{V,\beta,K,\sigma_m,\sigma_\epsilon} \sum_{i=1}^{N-1} \left[\log(\sigma_m^2) + \frac{\hat{w}[i]^2}{\sigma_m^2}\right] + \left[\log(\sigma_\epsilon^2) + \frac{\hat{v}[i]^2}{\sigma_\epsilon^2}\right]$$

Maximization of likelihood

$V, \beta, K, \sigma_\epsilon, \sigma_m$

Main objective : precise NH_4^+ predictions over 24h horizon.

WTTPs dynamics

- complex
- disturbances
- noises
- partially observed
- non-linearities
- ...

Sequential Monte-Carlo (SMC)
+
Expectation Maximization (EM)

VS

Standard Prediction Error Minimization (PEM)

$\Rightarrow NH_4^+$ model

Outline

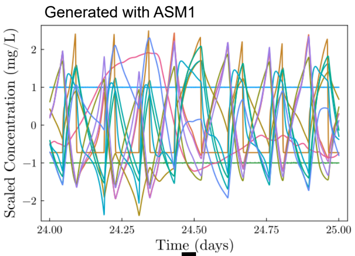
Experimental Setup

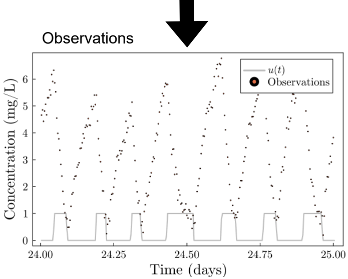
Objective :

- **Good** performance of **grey box** model.
- Comparison between **SSM** approaches and **PEM**.

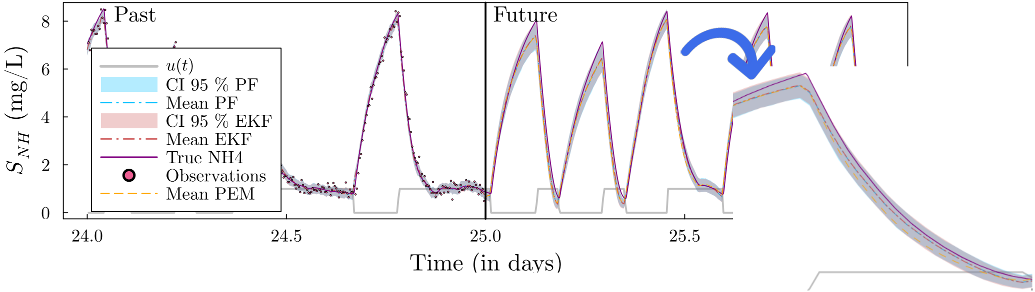
Experimental Setup :

- Data generated from a simulator using **ASM1**.
- ORP control.
- **Various** external conditions.
- 5 day for training and next day for testing.
- **Repeat** experience 10 times for each condition.



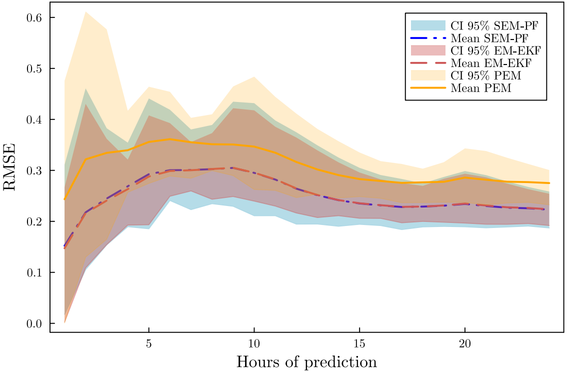


Filtering concentration



- **Reduced model** performs well.
- Model trained with **PEM** : no **Confidence Interval** and **bias** during aeration.

RMSE according to horizon



- **State Space Model** representation outperforms classical PEM criterion.
- RMSE **stabilizes** with extension of prediction horizon.
- **Decrease** of performance around 5 hours.
- **Probability coverage** : 86 %.

- No **differences** between EKF and PF.

- **Accurate** estimation of **observation** noise.
- Parameters in **physical** ranges.
- Difference between **SSM** approaches and **PEM**.

Parameters	Proposed (SEM-PF)	EM-EKS	PEM criterion
V	1122 ± 43	1122 ± 44	1131 ± 39
β	231 ± 7	231 ± 7	258 ± 9
K	0.42 ± 0.07	0.42 ± 0.07	0.700 ± 0.060
σ_m	0.08 ± 0.003	0.08 ± 0.004	-
σ_ϵ	0.19 ± 0.004	0.19 ± 0.004	-

Table – Parameter Estimation over different intervals and inlet concentrations (Mean ± Standard deviation).

Conclusion :

- **Precise** NH_4^+ predictions over 24h horizon.
  - Low RMSE.
  - **Well-calibrated** confidence interval.
- **State Space Model** representation outperforms classical **PEM** criterion.

Perspectives :

- Estimation of **inlet** concentration.
- **Integration** of other sensors (like oxygen or ORP).
- **Comparison** of different types of model : white, grey and black box models.

Thank you for your attention
Questions ?