Data assimilation for prediction of ammonium in wastewater treatment plant: from physical to data driven models

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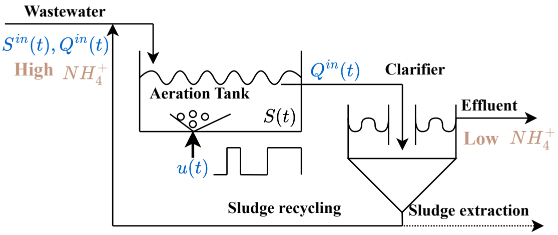
Outline

1. Wastewater Treatment Plants
2. Possible models for ammonium concentration
3. Model's calibration with data assimilation
4. Simulated Results
5. First real results

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



- Municipal plants.
- **Input** : NH_4^+ (ammonium) high.
  - $Q^{in}(t)$, inflow.
  - $S^{in}(t)$, inlet concentration.
- **Output** : NH_4^+ low.

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

How ? : By **controlling** the addition of oxygen in the aeration tank with $u(t)$.

Aeration control

The removal of nitrogen is carried out by alternating between :

- **Aeration phases** (energy-intensive) : oxygen is added using a compressor.
- **Non-aeration** phases : complete absence of oxygen.

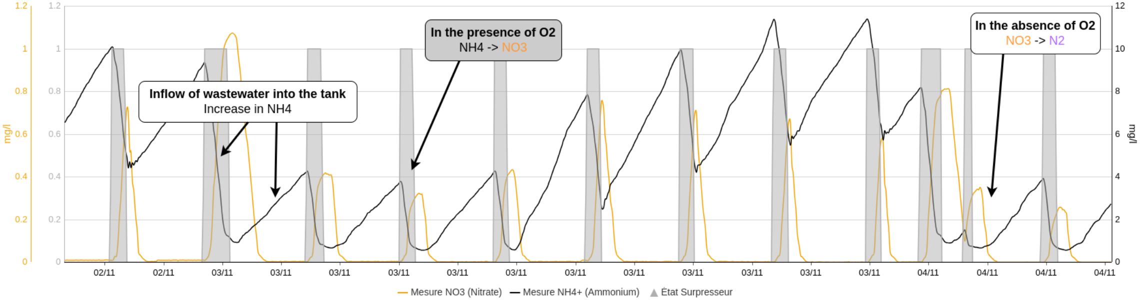


Figure – Nitrogen removal in the aeration tank.

Problems

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

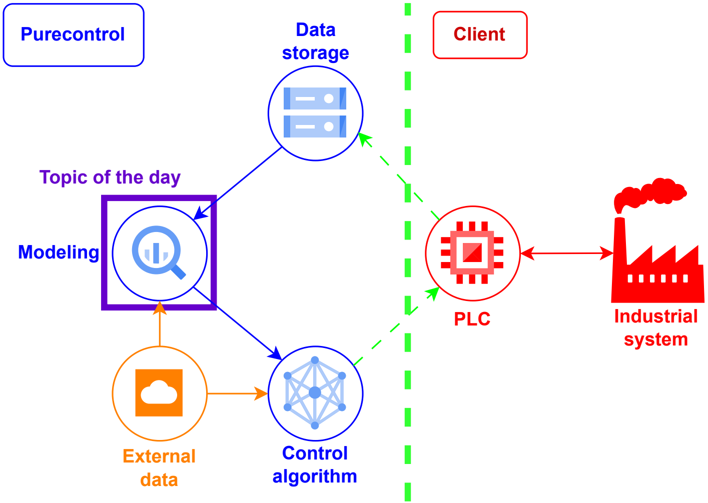
Feedforward/Scheduling Control.

→

Condition

Dynamic model (NH_4^+).

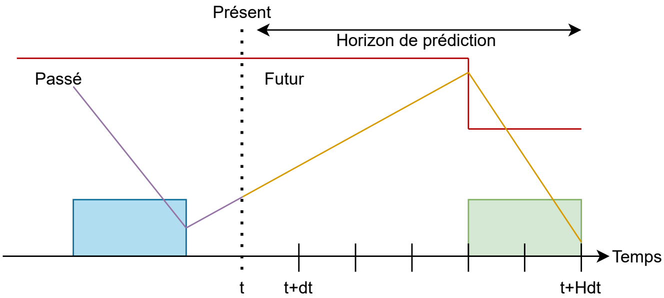
Purecontrol Solution for Energy Optimization



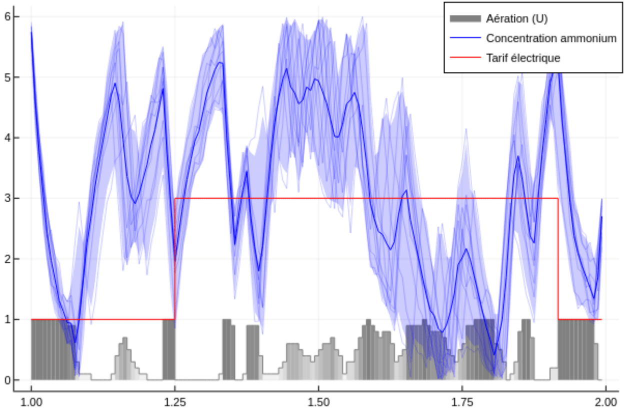
Model Predictive Control (MPC)

What is MPC ?

Model Predictive Control (MPC) predicts the system's future behavior using a dynamic model, allowing the generation of optimal control actions.



Recalculated at each time step *dt* $\Longrightarrow$ **dynamic adaptation** to system variations.



Prediction Objective

24-hour stochastic prediction of ammonium (NH_4^+).

Modeling Requirements

Calibration of parameters and uncertainties.

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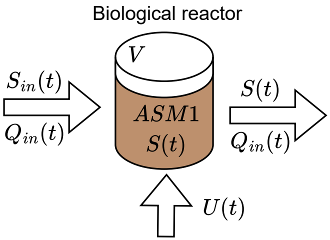
Well-known physic model

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.

Our Case Study

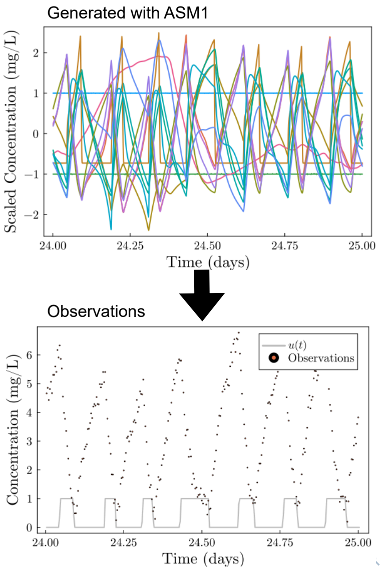
Main objective : High-precision NH_4^+ predictions over a 24-hour horizon.

Problem decomposition :

$$P(S(t), S_{in}(t)) = \overbrace{P(S(t)|S_{in}(t))}^{\text{NH}_4\text{ Dynamics}} \times \overbrace{P(S_{in}(t))}^{\text{Inlet Estimation}}$$

System characteristics :

- Medium Dimensionality
- Strong Interactions & High Uncertainty
- Partial Observability



White-box model : Reduced ASM1 model

$$\frac{\partial S(t)}{\partial t} = \overbrace{\frac{Q^{in}(t)}{V}(S^{in}(t) - S(t))}^{\text{Not modified}} + \overbrace{r(t, S(t), u(t))}^{\text{Modified part}}$$

- **Problem** :
  - Complex physic model.
  - 13 species.
  - Many parameters.
- **Solution** : Reduced ASM1 Model
  - 5 species
  - Still 21 parameters.

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

Figure – Matrix representation of the ASM1 model.

Simplified Physics-Based Model :

$$\frac{\partial S_{NH}(t)}{\partial t} = \underbrace{\frac{Q^{in}(t)}{V}\left[S_{NH}^{in}(t) - S_{NH}(t)\right]}_{\text{Not modified}} - \underbrace{\beta u(t)\frac{S_{NH}(t)}{S_{NH}(t)+K}}_{\text{Modified part}}$$

where V, β, and K are **unknown** parameters.

Key Remarks :

- **Simple** yet effective model.
- Few parameters, lacking direct **physical interpretation**.
- Based on multiple **assumptions** whose validity is **uncertain**.

Black-box Model : Linear State Space Model vs. Local Linear Regression

Linear State Space Model

$$S(t+1) = AS(t) + Bu(t) + CE(t) + \eta_t$$

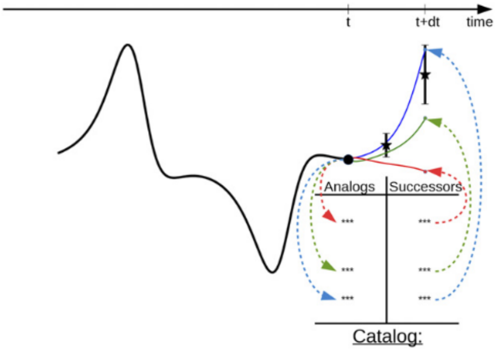
$$y(t) = HS(t) + \epsilon_t$$

Key Properties :

- **No physical meaning.**
- Assumes **global linearity**.
- Only based on **data-driven** methods.

Local Linear Regression

- Linear Regression on the k nearest neighbors.



Model Comparison

White-box

- **Based on physical laws.**
- **Requires many parameters** (often hard to estimate).
- Large number of species.
- High interpretability but may be too rigid.

Grey-box

- Uses simplified **mechanistic models** with data-driven corrections.
- **Reduces the number of parameters** compared to White-box.
- Trade-off between interpretability and flexibility.

Black-box

- **Fully data-driven.**
- Uses statistical or machine learning models.
- **No physical meaning**, purely empirical.
- Flexible but requires a lot of data and may lack generalization.

How to reconstruct the hidden concentrations and quantify the uncertainty ?

State Space Model structure

Separation of the model into two parts

- **Transition equation :**

$$S[t+h] = \text{ChoosenModel}(S[t], U[t], E[t]) + \eta_t, \quad \eta_t \sim \mathcal{N}(0, \Sigma_\eta)$$

- **Observation equation :**

$$Y_{NH}[t] = H(S[t]) + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \Sigma_\epsilon)$$

How can I find **jointly** the **hidden** variables, the **parameters** of the model and the **uncertainties** ?

Methods for Uncertainty Quantification and Latent Space Reconstruction

White-box

- **Main interest :** Latent states reconstruction using observers (Gernaey et al., 2004).
- **Parameter Estimation :** Often neglected due to model complexity (Chachuat, 2001).
- **Uncertainty Handling :** Rarely integrated directly ; relies on a posteriori sensitivity analysis (Boulkroune, 2008).

Grey-box

- **Hybrid Calibration :** Combines mechanistic models with data-driven parameter tuning (Stare et al., 2006).
- **Uncertainty Handling :** Few models explicitly calibrate both parameters and uncertainty (Stentoft et al., 2018).
- **Key Challenge :** Ensuring consistency between physics-based and ML components.

Black-box

- **Fully Data-driven :** Requires large datasets ; lacks physical interpretability.
- **Uncertainty Estimation :** Difficult to quantify and integrate into assimilation frameworks (Alvi et al., 2023).
- **Recent Advances :** Local linear regression improves performance while reducing complexity (Chau et al., 2021).

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Grey-box calibration example

- **Transition equation :**

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

- **Observation equation :**

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

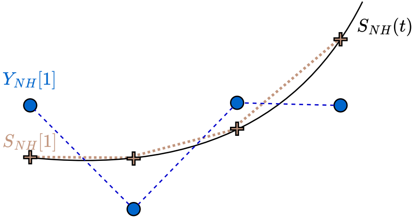
Majority of studies assume no observation noise during training.

Standard training : Prediction Error Minimization (PEM)

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

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

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



How to **adapt** to **hidden** variables and **observation** noise ?

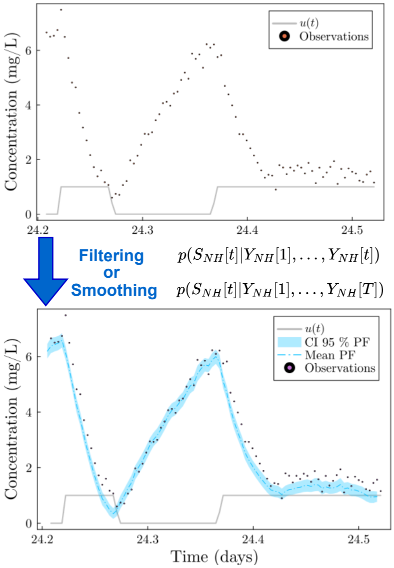
Data Assimilation

Data assimilation integrates real-world observations into models.

Key Challenges :

- **Reconstructing Hidden States :**
  - **Sequential Methods :** More time-consuming but provide stronger theoretical guarantees.
  - Variational Methods : Minimization of a cost function.
- **Calibrating Model Parameters and Uncertainties :**
  - Direct Likelihood Maximization : Involves challenging steps such as differentiating over sequential methods (which can be unstable).
  - Maximizing the complete likelihood with the **Expectation-Maximization** algorithm.

Filtering and Smoothing : Estimation of the latent variables

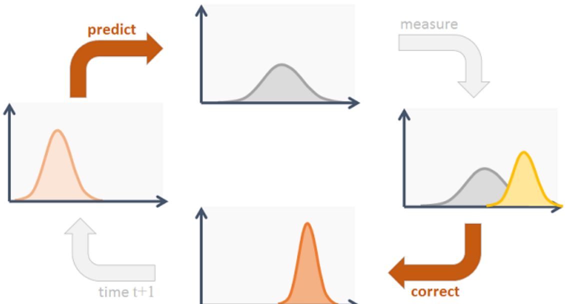


Condition : Known parameters.

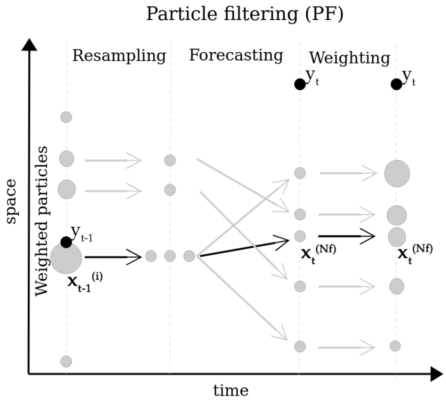
- **Linear model**
  - Kalman Filter and Smoother
- **Nonlinear model**
  - ◇ Linearization
    - Extended Kalman Filter and Smoother
  - ◇ Sequential Monte Carlo
    - Ensemble Kalman Smoother and Filter
    - Particle Filter and Backward Smoother

Kalman Filter and Particle Filter

Kalman Filter



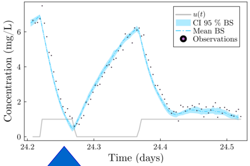
Particle Filter



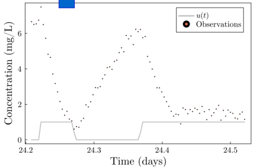
Monte-Carlo Expectation Maximization (MCEM)

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

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

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

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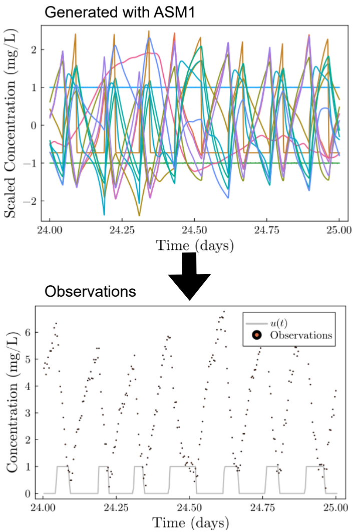
Experimental Setup

Objective :

- **Evaluate** model performance.
- Assess the **quality** of **uncertainty calibration**.

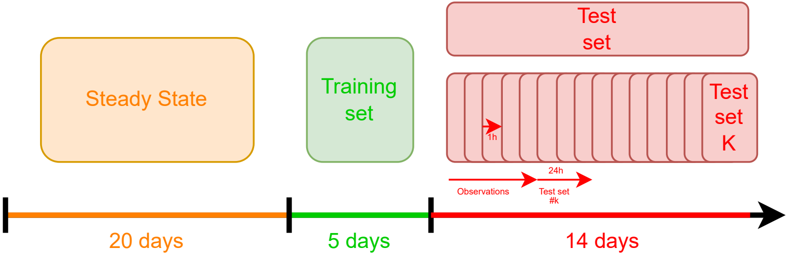
Experimental Design :

- Data generated from a simulator based on **ASM1**.
- ORP-based aeration control.
- **Diverse** external conditions.
- **Training :** 5 days | **Testing :** next 14 days.
- **Repeated** 10 times for each condition.



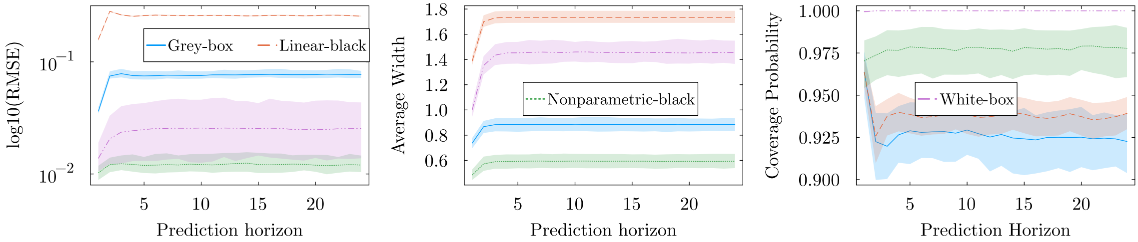
Metrics

New **observations** are assimilated **every hour**, and **24-hour predictions** are made.



- **Root Mean Squared Error (RMSE)** : Quantifies the average magnitude of errors between predicted and actual values.
- **Average Width (AW)** : Represents the mean width of prediction intervals.
- **Coverage Probability (CP)** : Measures the proportion of times the true value lies within the predicted interval.

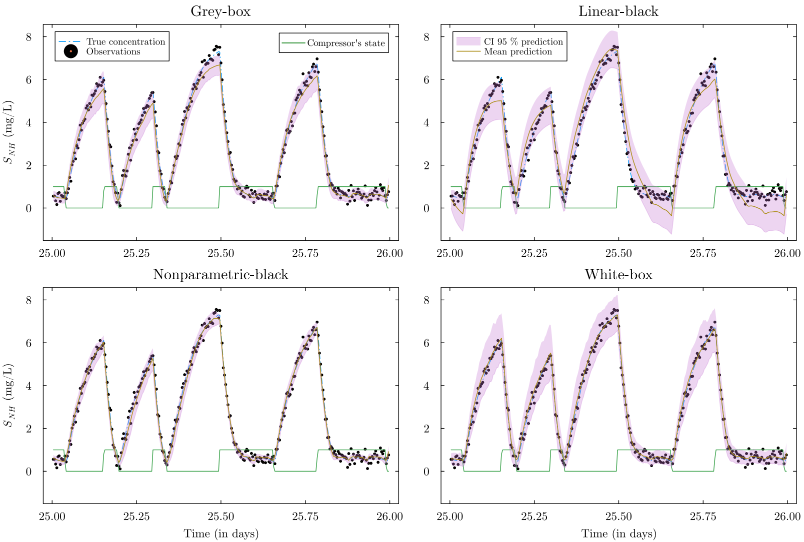
RMSE, AW, and CP Over Time Horizon



Key Observations :

- The **linear model** has the highest RMSE, while **LLR** achieves the best RMSE and AW.
- **White-box model** shows low RMSE but wide CI, indicating training instability.
- Most models are well-calibrated, except for the **white-box model**.

24h Model Predictions



Key Observations :

- **Linear model** fails to capture saturation at 0.
- **Grey-box model** shows bias at high concentrations.
- **White-box model** is well-calibrated but has wide confidence intervals.
- **LLR** achieves the best overall performance.

Estimated Parameters

Simulated observation standard deviation : 0.2 mg/L.

Model	Training Time (seconds)	Estimated Observation Standard Deviation	Estimated s_{NH} Standard Deviation
Grey-box	813	0.184	0.103
Linear Black-box	**162**	0.162	0.180
Nonparametric Black-box	3990	**0.197**	**0.062**
White-box	294000	0.189	0.109

Key Observations :

- All models provide accurate estimates of the observation standard deviation.
- **Linear model** is the fastest, while the **white-box** is extremely computationally expensive.
- **Nonparametric Black-box** achieves the lowest standard deviation for s_{NH}.

General Observations

Grey-box Model

- **Balanced** performance according to simplifications.
- Slight bias in high ammonium concentrations.
- Low computational cost.

Black-box Model

- **Best RMSE and AW** and well-calibrated confidence intervals for LLR.
- Linear version lacks expressivity (fails to model saturation).

White-box Model

- **Low RMSE** but large uncertainty intervals.
- Computationally expensive (long training time).
- **Unstable** training.

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First Real-World Experiment

Experimental Setup :

- **Period :** April 12 – May 8, 2023.
- **Location :** Acigné, France.
- **Facility :** Wastewater treatment plant (14,000 PE).
- **Sampling Frequency :** Every minute.

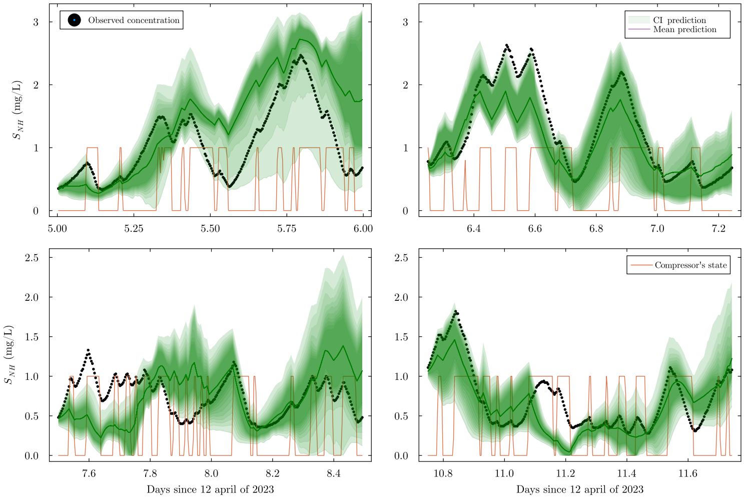
Available Data :

- **Inflow rate.**
- **Ammonium sensor measurements** (NH_4^+).
- No direct inlet concentration data.

Objective

Evaluate the performance of the non-parametric black-box model on real-world data.

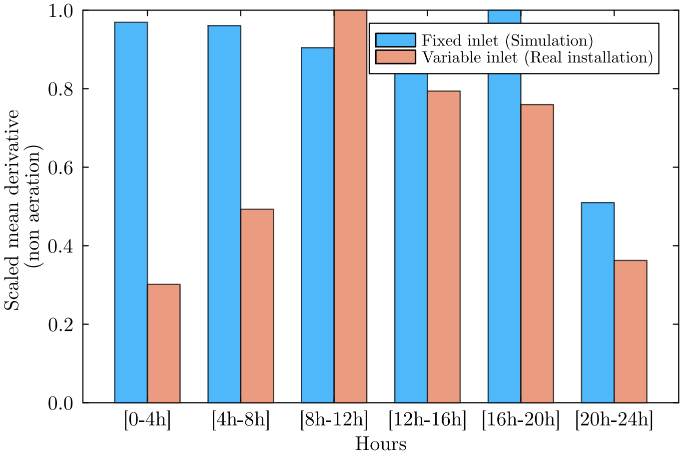
24h Model Predictions on Real Data



Key Observations :

- **Trend vs Amplitude :** Model struggles more with amplitude than trend.
- **Uncertainty Calibration :** Increased uncertainty, indicating good calibration.
- **Limitations :** Assumption of constant inlet concentrations is **violated** in real data.

Inlet Diurnal Variation in Catalog



Keys observations :

- **High Variability :** Significant fluctuations in the derivative within LLR catalogs.
- **Model Adjustment :** Need to incorporate **additional covariates** to improve performance.

Conclusion

- **Research Contributions** :
  - **Comparison** of various model types for ammonium prediction within a **data assimilation** framework.
  - The **non-parametric** black-box model outperformed all other models in terms of predictive **accuracy** and **uncertainty estimation**.
  - General trends were captured in **real data**, but performance still **needs improvement**.
- **Research Perspectives** :
  - Integration of heteroscedastic noise.
  - Enhancement of LLR on real data using covariates (e.g., rain, time of day, etc.).
  - Inlet concentration estimation.

Thank you for your attention

Questions ?

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