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Sources and propagation of uncertainty in N2O model predictions

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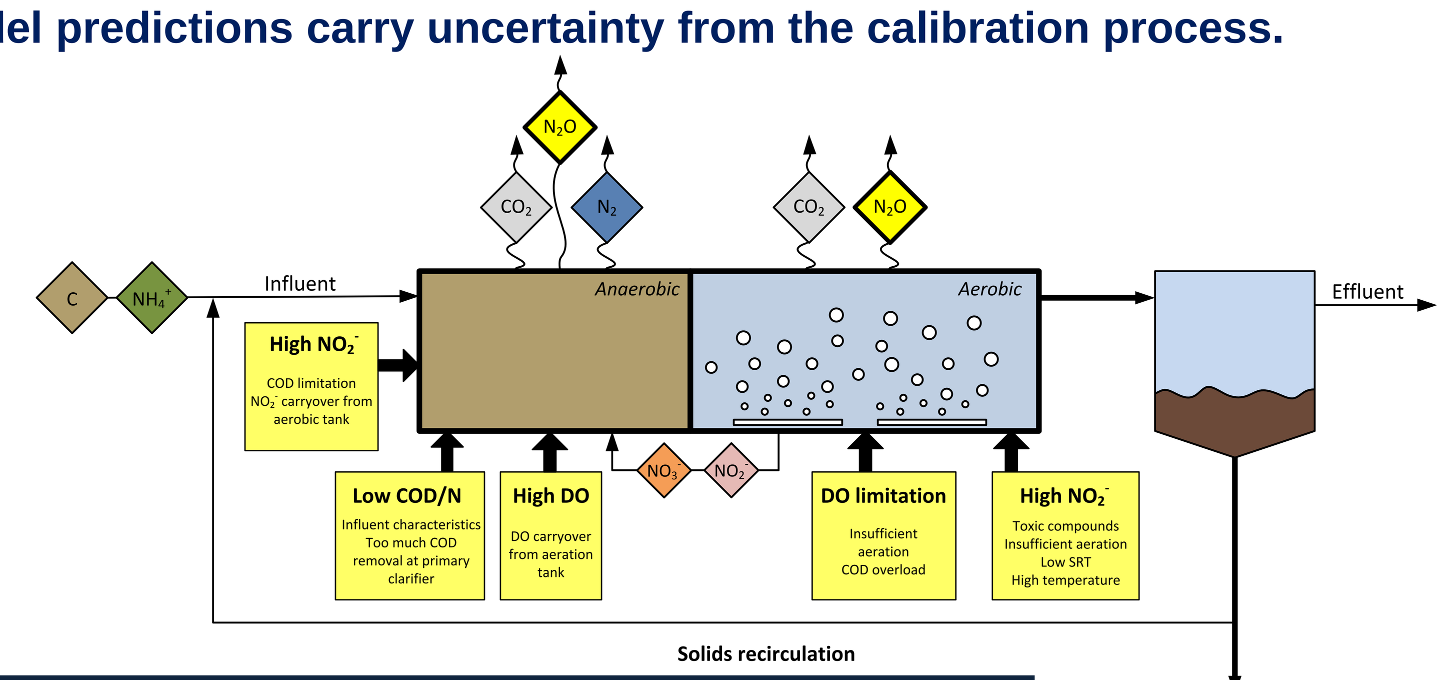
1. Introduction and research questions

Nitrous oxide emissions during nitrogen removal in wastewater treatment operations can compromise the environmental impact of the process.

The carbon footprint of a WWTP is highly sensitive to N_2O emissions.

Model predictions carry uncertainty from the calibration process.

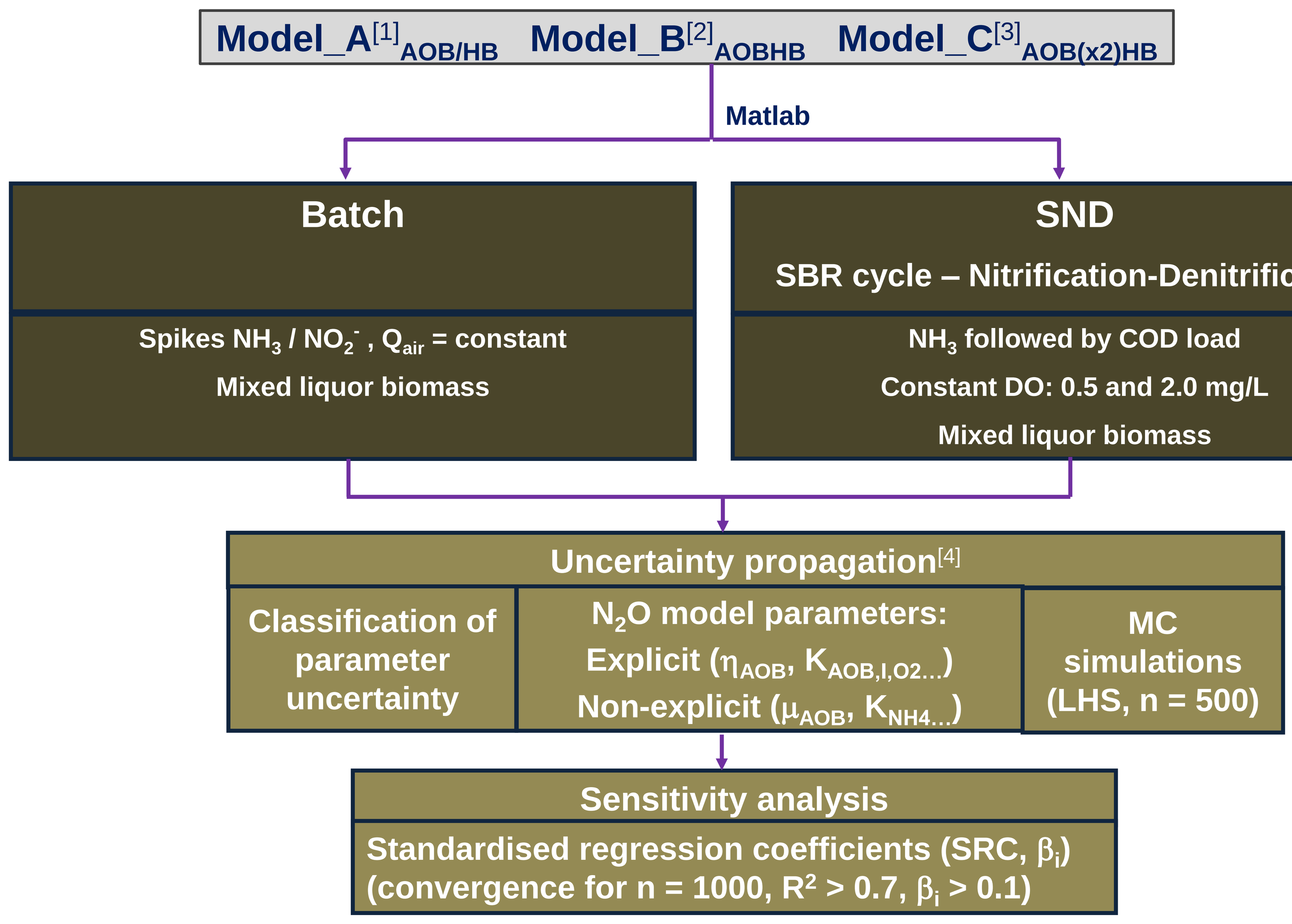


Q1. How precise are N_2O model predictions?

Q2. Are calibration results satisfiable for mitigation strategies?

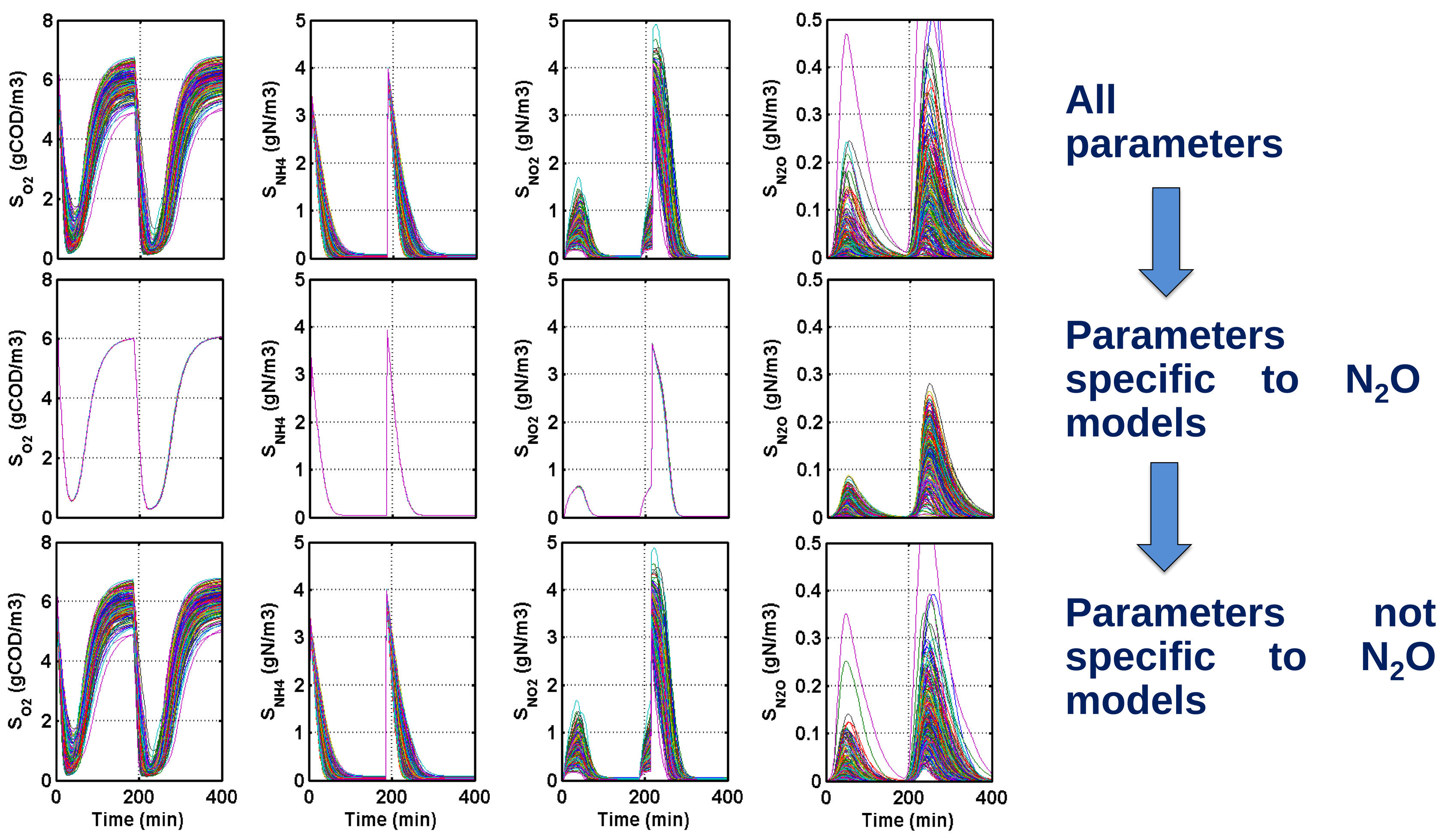
Q3. How can we reduce the uncertainty of model predictions?

2. Computational work performed



3. Uncertainty in model predictions

Model predictions if uncertainty is considered for Model_A, Batch:



Model predictions for N_2O carry higher uncertainty associated to previous processes.

Higher coefficient of variation for N_2O compared to DO, NH_4^+, NO_2^- along the experiment.

What parameters carry most of the uncertainty?

Batch

4. Identifying sources of uncertainty

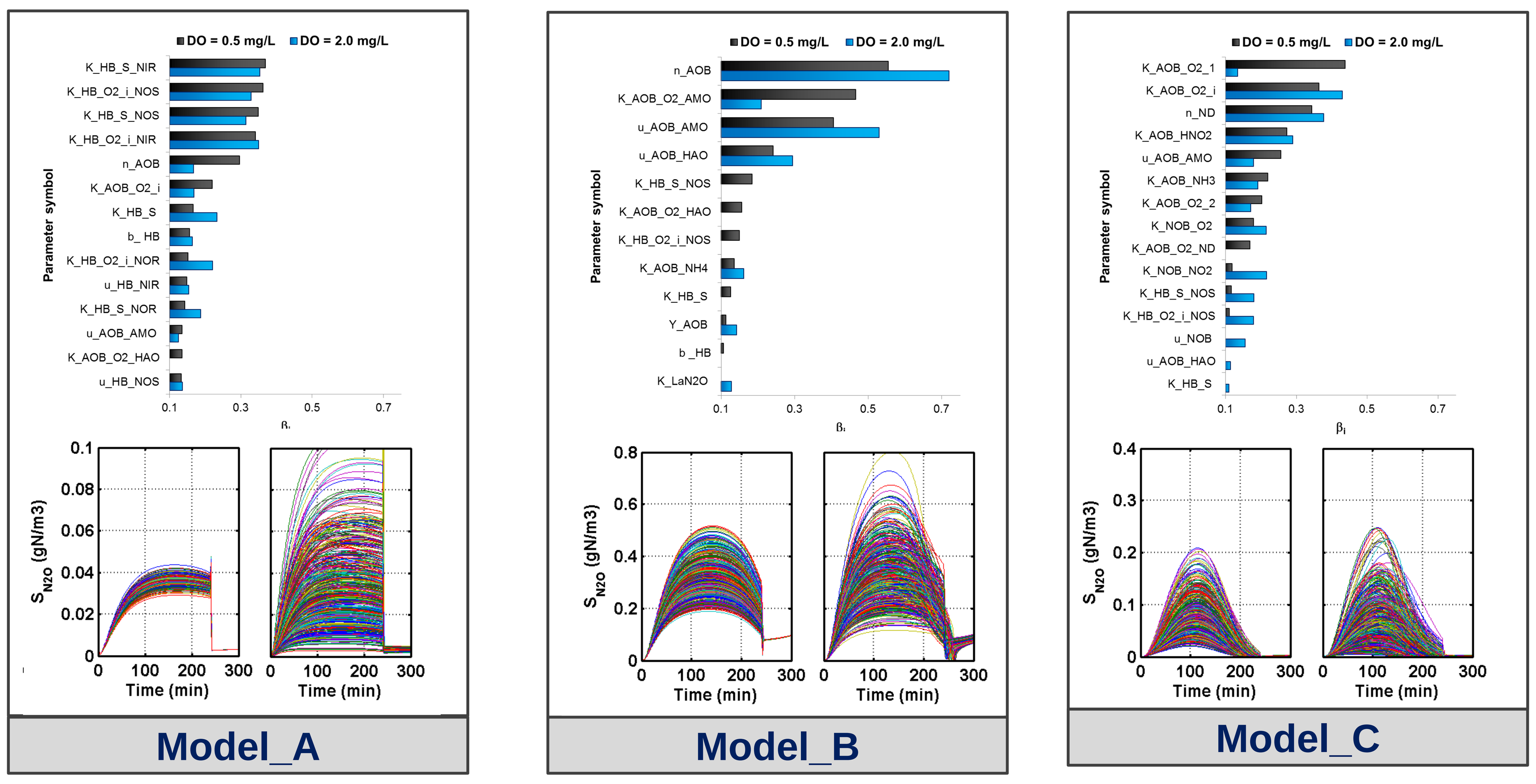
Model evaluation with reported parameter values, scenario SND

DO = 0.5 mg/L	Model_A	Model_B	Model_C
ΔNH4 (mgN/L)	29	26	25
$N_2O_{\_emitted/removed}$	2.1%	2.3%	4.8%
$N_2O_{\_prod}$ NN	-	95%	1%
$N_2O_{\_prod}$ ND	58%	-	91%
$N_2O_{\_prod}$ HD	42%	5%	8%

DO = 2.0mg/L	Model_A	Model_B	Model_C
ΔNH4 (mgN/L)	35	38	39
$N_2O_{\_emitted/removed}$	0.4%	3.6%	0.5%
$N_2O_{\_prod}$ NN	-	99%	4%
$N_2O_{\_prod}$ ND	67%	-	82%
$N_2O_{\_prod}$ HD	33%	1%	14%

Ranking of the most sensitive parameters for each model/scenario

Propagation of uncertainty for: reported parameters (bottom left), and reported + sensitive non-calibrated parameters (bottom right)



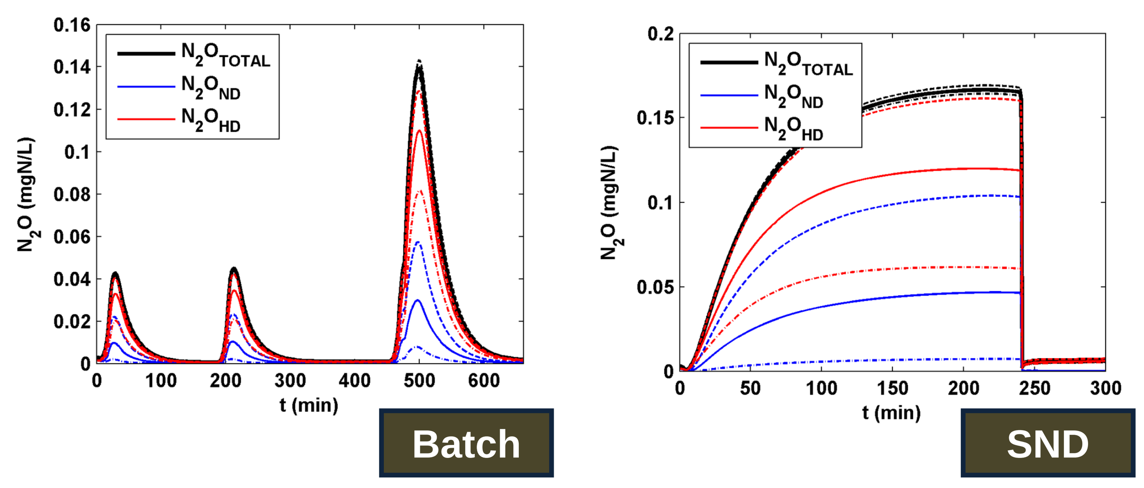
For the 3 models considered N_2O emissions were sensitive to non-explicit N_2O parameters from AOB and HB.

Calibration efforts for sensitive parameters can reduce the prediction uncertainty (Calibrated parameters: Model_C = 11, Model_A = 5).

SND

5. Total vs Individual pathway contribution

Strategies to mitigate N_2O emissions are pathway-dependent.
Are individual N_2O production pathways sensitive to the same parameters as total N_2O?
Uncertainty in non-sensitive parameters to total N_2O revealed poor identifiability of individual pathway contributions.



Effect of varying non-sensitive parameters to N_2O predictions (black) and to individual pathway contributions (red, blue) (95% CI dashed lines. $K_{HB,NO}$, $K_{AOB,NO}$: 0.02 mgN/L ± 90%)

6. Conclusions – Outlook

- **Uncertainty of N_2O emissions is related to both explicit and non-explicit N_2O model parameters.**
- **N_2O model calibrations should systematically address sensitivity and identifiability problems due to uncertainty propagation from previous processes.**
- **Adequate experimental design for model calibration can significantly reduce uncertainty of parameter estimates and therefore prediction uncertainty.**
- **Precise N_2O predictions might underestimate uncertainty of individual pathway contributions.**

WWTmod 2016

[1] 10.1021/es201489n
[2] 10.1021/es4005398
[3] 10.1016/j.watres.2015.11.029
[4] 10.1016/j.watres.2010.08.025

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