Sources and propagation of uncertainty in N2O model predictions

Domingo-Felez, Carlos; Valverde Pérez, Borja; Plósz, Benedek G.; Sin, Gürkan; Smets, Barth F.

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DTU Environment
Department of Environmental Engineering

Carlos Domingo-Félez[1], Borja Valverde-Pérez[1], Benedek Gy. Plósz[1], Gürkan Sin[2], Barth F. Smets[1].

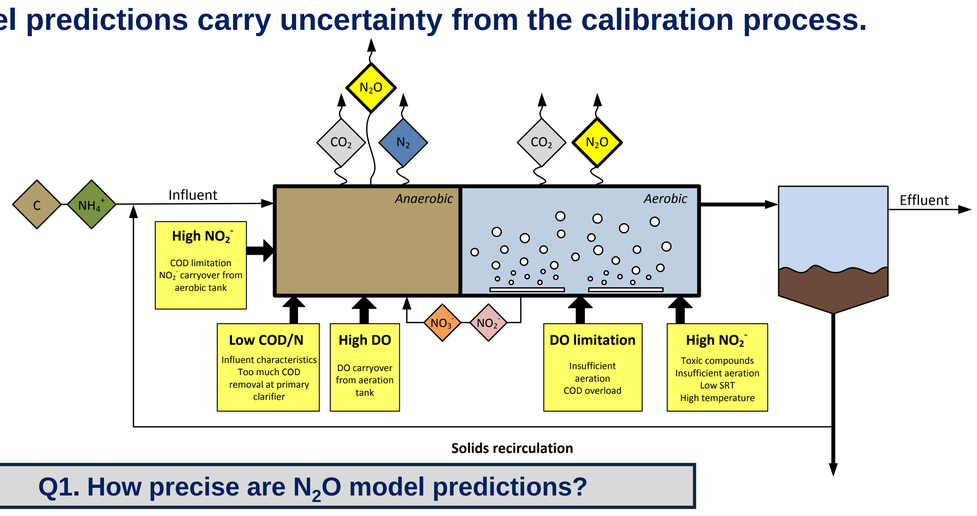
[1] *Department of Environmental Engineering, Technical University of Denmark;*
E-mail: cadf@env.dtu.dk

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

Model_A[1]$_{AOB/HB}$ Model_B[2]$_{AOBHB}$ Model_C[3]$_{AOB(x2)HB}$

Matlab

Batch

Spikes NH_3 / NO_2^- , Q_{air} = constant

Mixed liquor biomass

SND

SBR cycle – Nitrification-Denitrification

NH_3 followed by COD load

Constant DO: 0.5 and 2.0 mg/L

Mixed liquor biomass

Uncertainty propagation[4]

Classification of parameter uncertainty

N_2O model parameters: Explicit (η_{AOB}, $K_{AOB,I,O2...}$) Non-explicit (μ_{AOB}, $K_{NH4...}$)

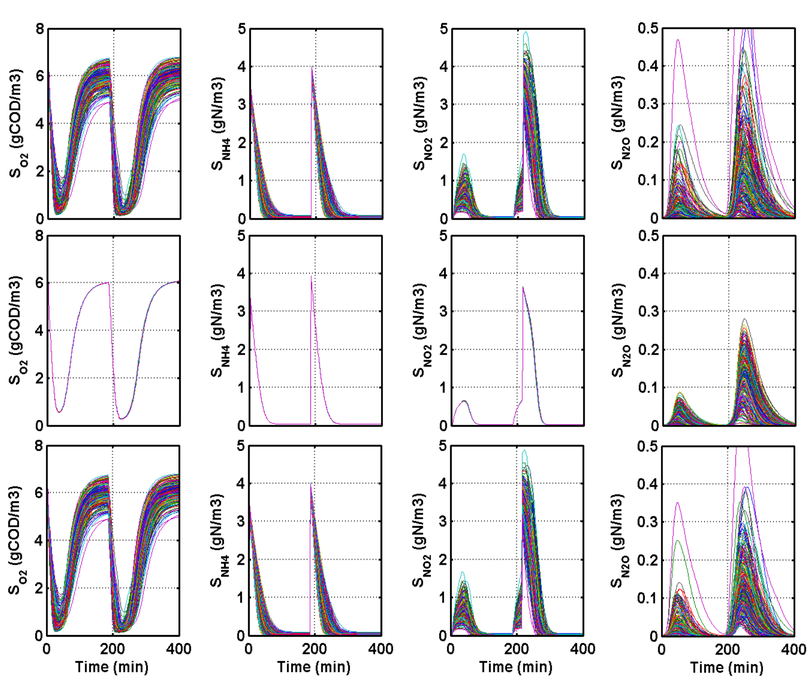
MC simulations (LHS, n = 500)

Sensitivity analysis

Standardised regression coefficients (SRC, β_i) (convergence for n = 1000, $R^2 > 0.7$, $\beta_i > 0.1$)

3. Uncertainty in model predictions

Model predictions if uncertainty is considered for Model_A, Batch:



All parameters

Parameters specific to N_2O models

Parameters not specific to N_2O models

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

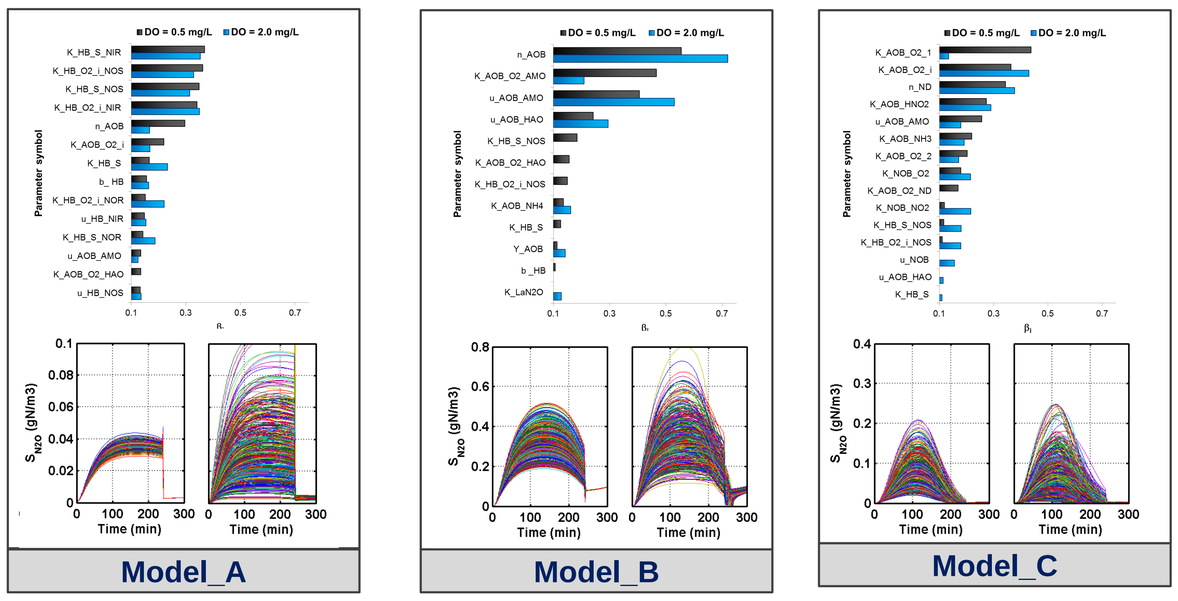
4. Identifying sources of uncertainty

Model evaluation with reported parameter values, scenario SND

	DO = 0.5 mg/L			DO = 2.0mg/L		
	Model_A	Model_B	Model_C	Model_A	Model_B	Model_C
ΔNH4 (mgN/L)	29	26	25	35	38	39
$N_2O_{\_emitted/removed}$	2.1%	2.3%	4.8%	0.4%	3.6%	0.5%
$N_2O_{\_prod}$ NN	-	95%	1%	-	99%	4%
$N_2O_{\_prod}$ ND	58%	-	91%	67%	-	82%
$N_2O_{\_prod}$ HD	42%	5%	8%	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).

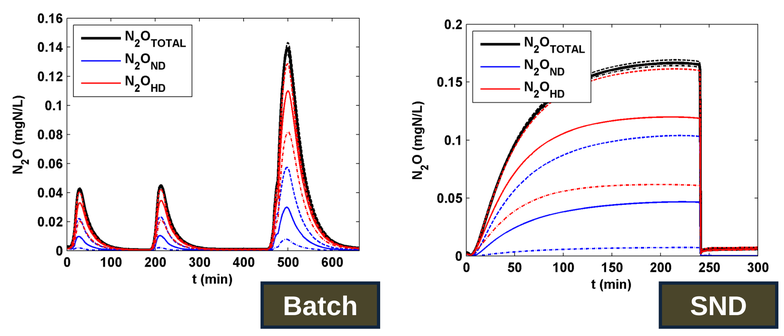
SND

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.**

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[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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LaGaS