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Towards an optimal experimental design for N_2O model calibration during biological nitrogen removal

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Abstract
Process models describing nitrous oxide (N_2O) production during biological nitrogen removal allow for the development of mitigation strategies of this potent greenhouse gas. N_2O is an intermediate of nitrogen removal, hence its prediction is negatively affected by the uncertainty associated to its substrates. Improving experimental designs for model calibration reduces prediction uncertainties. Moreover, the individual analysis of autotrophic and heterotrophic contribution to the total NO and N_2O pool was assessed for already proposed model structures under different experimental scenarios. The results show the need for information-rich experiemental designs to assess the predicting capabilities of N_2O models. This work represents a step further in understanding the N_2O production and emissions associated to conventional wastewater treatment. Moreovere, it will facilitate the development of strategies to minimize the carbon footprint of wastewater treatment plants.

Keywords
Modelling; N_2O; uncertainty; production pathway; experimental design

INTRODUCTION

Nitrous oxide (N_2O) is a by-product of biological nitrogen removal (BNR) with a strong environmental impact as a greenhouse gas. Research has focused on conceptualizing our understanding of the complex interrelationships governing BNR to lastly develop mitigation strategies. However, the wide range of N_2O-associated parameter values and model structures reported indicate a lack of understanding of the underlying biological process. The development of accurate process models has therefore been proven challenging.

N_2O can be produced biologically by autotrophic and heterotrophic bacteria under different operating conditions. Thus, the desired N_2O mitigation strategies are specific to the main producing pathway. However, a high parameter uncertainty difficults accurately elucidating whether autotrophic or heterotrophic microbial processes contribute more to the total N_2O pool. Experimental design for parameter estimation becomes essential to decrease the uncertainty of estimates. Here we assess how model predictions propagate parameter uncertainty into the model output under different scenarios and studied the identifiability of top-sensitive parameters.

MATERIALS AND METHODS

Model structures

Heterotrophic contribution has been shown to play an important role in the total N_2O production pool even in systems with high autotrophic activity (Wang, Jiang, et al., 2014). Hence, all the model structures considered combined an autotrophic and heterotrophic N_2O production pathway from

literature (Spérandio, Pocquet, et al., 2014). Parameters from autotrophic models which do not affect nitrite production were considered as N_2O-associated (η_{AOB}, K_{NO}^{AOB}, K_{NO2}^{AOB} and $K_{i,O2}^{AOB}$) (Ni, Ruscalleda, et al., 2011).

Uncertainty analysis

Parameter uncertainty was ranked based on literature values (5-25-50%). Values were randomly sampled (LHS = 500 samples) and Monte Carlo simulations were performed to map parameter uncertainty into model outputs.

Also, the individual contribution of each production pathway to the total NO and N_2O pool was calculated for each scenario.

Experimental data

Experimental data from different experimental designs was used to compare model predictions. Mixed liquor and nitritating biomasses were used to assess the impact of biomass composition in both batch and continuous systems.

RESULTS AND DISCUSSION

The impact of parameter uncertainty on model predictions was assessed to compare the influence of model structures on the uncertainty (Fig. 1). Mapping the uncertainty of the model parameters showed a higher uncertainty in the N_2O predictions compared to other better described nitrogenous species such as ammonium, nitrite or nitrate. N_2O predictions carry a high uncertainty even if N_2O-associated parameters were fixed (0.1% variation). Moreover, parameter values are usually reported with no uncertainty associated, which wrongly decreases the apparent prediction uncertainty. These results indicate the need for a combination of N-removal and N_2O calibration, or conversely, the need to include the uncertainty of fixed values during N_2O calibration. Hence, the confidence regions of the new parameter estimates might be commonly underestimated.

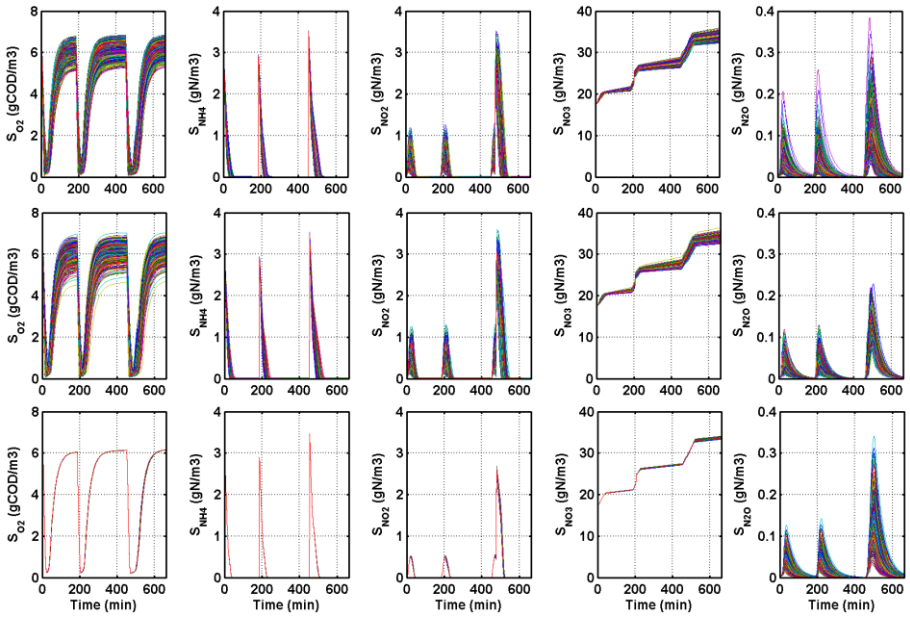

Fig 1. Uncertainty propagation on simulated results during continuously aerated batch experiments on mixed liquor biomass. Uncertainty is associated to all model parameters (Top panel). All, but N_2O-related, parameters are uncertain (Middle panel). Only N_2O-related parameters are uncertain (Bottom panel).

The information associated to each experimental scenario was evaluated to rank model structures based on goodness-of-fit and identifiability of the most sensitive parameters. Improving the quality

of experimental designs will decrease prediction uncertainties which will yield in a better process understanding.

The contribution of each N_2O-producing pathway was evaluated for different scenarios, which will allow testing future mitigation strategies (Fig. 2). The sensitivity of a model output during an experiment helps develop information rich experimental designs. Here we also studied the contribution of each process during experiments to the net mass balance of NO and N_2O. This procedure adds valuable information to previous sensitivity analysis studies on N_2O emissions.

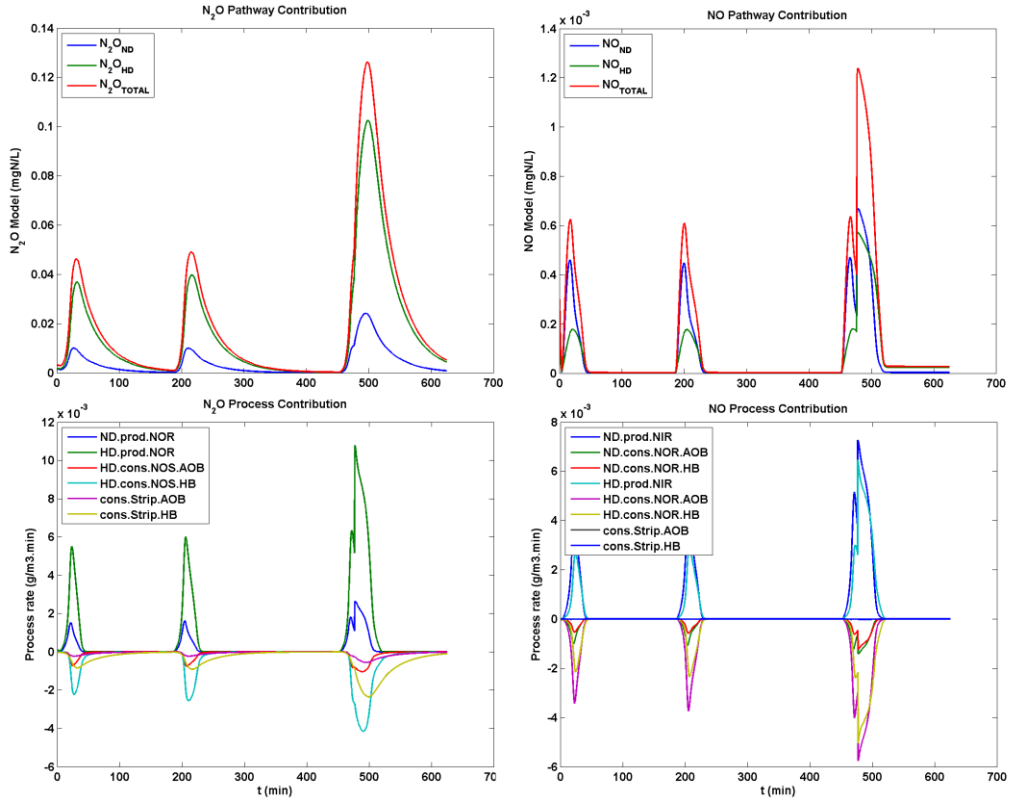

Fig 2. Modelling results for the total (red) and specific ND (blue) and HD (green) pathway production of N_2O (left) and NO (right) during experiments from Fig. 1 (Top). Evaluation of the individual process contribution to the N_2O and NO total production pool (Bottom).

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