Key parameters for modelling Anammox process with N_2O emissions

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Abstract

In this study, a sensitivity analysis and a calibration were applied to a recent published model (Lindblom et al., 2015) used to replicate nitrous oxide (N_2O) emissions in an one-stage nitritation-Anammox process using a moving-bed biofilm reactor (MBBR) at Hammarby-Sjstad pilot plant (Stockholm, Sweden), which treats anaerobic digestion liquor. Results indicate that the biofilm porosity, biofilm density, maximum biofilm thickness and boundary layer thickness were the most sensitive parameters of the model.

The case study

The process is a one-stage nitritation-Anammox process implemented in a MBBR, see biofilm sketch in Figure 1. The influent was mainly formed by

76 $gCOD/m^3$	readily biodeg. substrate
110 $gCOD/m^3$	slowly biodeg. substrate
769 gN/m^3	dissolved NH_4
19 gN/m^3	soluble biodeg. organic N
16 gN/m^3	particulate biodeg. organic N
280 $gCOD/m^3$	inert soluble matter
200 $gCOD/m^3$	inert particulate matter
25 gN/m^3	dissolved nitric oxide

- Intermittent aeration of 45/15 minutes on/off.
- PI controller of dissolved oxygen (DO) concentration at 1.5 mg/L.
- pH (7.1) and temperature (25 °C) were relatively constant.
- Measurements of dissolved ammonium (NH_4) and nitrous oxide gas (N_2O) were obtained.

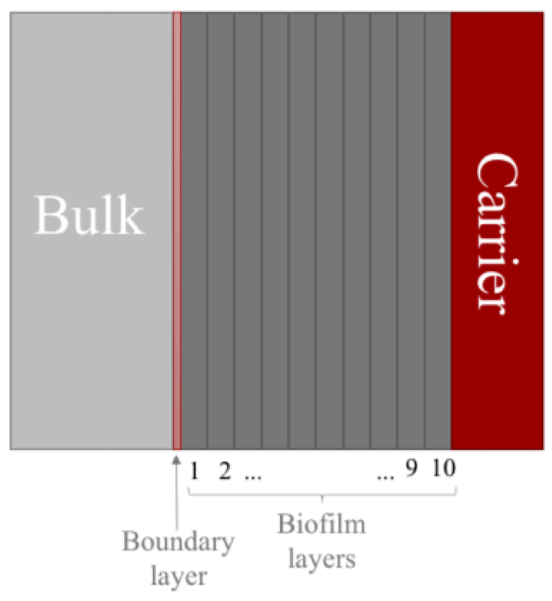

Figure 1: Sketch of the biofilm model.

The model

- Based on the Activated Sludge Model for Nitrogen (ASMN) (Hiatt & Grady, 2008), which extends the Activated Sludge Model 1 (ASM1) with two nitrifyers: ammonia and nitrite oxidizing bacteria. In total: 20 model components and 70 model parameters.
- Autotrophic denitrification was included according to Mampaey et al. (2013).
- Growth and decay of Anammox bacteria were included according to Hao, Heijnen, and van Loosdrecht (2002).
- A model for the stripping of N_2O gas was implemented as suggested by Foley et al. (2015).
- The surface mass transfer coefficient for oxygen (K_La $[d^{-1}]$) was used as input variable to the PI controller of the DO.

Sensitivity analysis and model calibration

- A sensitivity analysis was performed to identify the most sensitive parameters of the model. It was done via the one-at-a-time method.
- The model calibration involved: the definition of the parameter uncertainty, the sampling of the parameter space, and the optimization of parameters.

See Table 1 for details of these steps.

Table 1: Expressions used for the sensitivity analysis and model calibration.

Sensitivity analysis

$$\sigma_{\hat{y}_j}^{\Delta p_i} = \frac{1}{T_s}\int_0^{T_s} \frac{\hat{y}(p_i+\Delta p_i, t) - \hat{y}(p_i, t)}{\hat{y}(p_i, t)} dt,$$

$i = 1, ..., N;\ j = 1, ..., M$

where:
$\hat{y}$: vector of model value, p_i: nominal i^{th} parameter value, Δp_i: change in i^{th} parameter, t: time variable, T_s: time interval, N: total of parameters, M: total of model outputs.

⋆ Counting all the model parameters and outputs results in a $N \times M$ matrix for $\sigma_{\hat{y}_j}^{\Delta p_i}$.
⋆ This analysis was performed with $\Delta p = 10\%$.
⋆ The most sensitive parameters were used in the model calibration.

Model calibration

$$FIT = 1 - \frac{\text{norm}(y - \hat{y})}{\text{norm}(y - \text{mean}(y))},$$

where:
y: vector of experimental values. FIT equal to 1 means perfect match between the model and the experimental values.

⋆ $\pm 50\%$ uniform distribution was assumed in uncertainty of nominal parameters.
⋆ Latin Hypercube Sampling was used for parameter sampling.
⋆ The optimization of parameters was done via Monte Carlo runs.

Results

Figure 2 shows the results of the sensitivity analysis. See that mainly four parameters are the most sensitive ones: the porosity of the biofilm (η $[-]$), the biofilm density (ρ $[gTS/m^3]$), the maximum biofilm thickness (L_{max} $[mm]$), and the boundary layer thickness (L_0 $[\mu m]$).

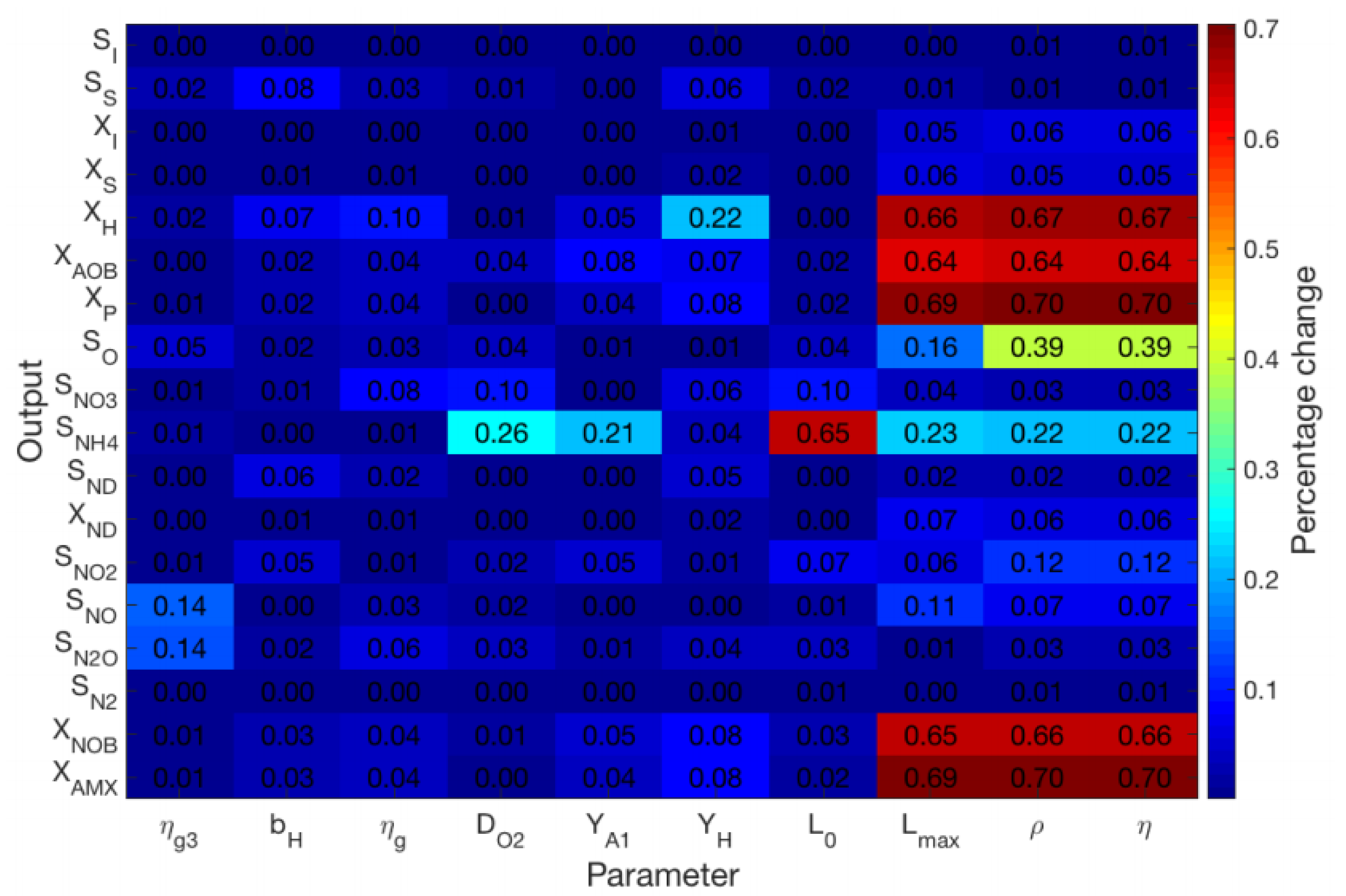

Figure 2: Color plot with sensitivity coefficients for the model output vs. the 10 most sensitive parameters.

The most sensitive parameters obtained in the sensitivity analysis were used for the model calibration, the results are shown in Figure 3.

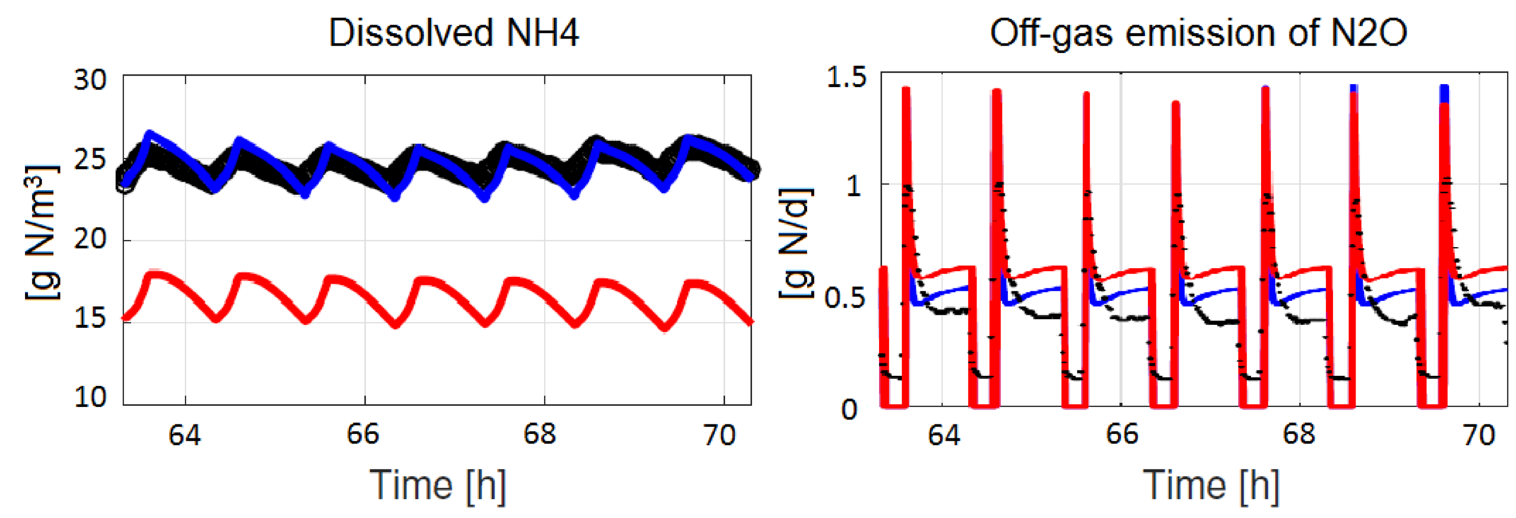

Figure 3: Comparison between experiments and model. Left: dissolved NH_4, Right: off-gas emission of N_2O. Measurements (black dots), model outputs with no-calibrated (red lines) and with calibrated (blue lines) parameters.

The following values correspond to the best fitting of the model to the experiments: $\eta = 0.29$, $\rho = 4.65 \times 10^4$ gTS/m^3, $L_{max} = 1.78$ mm, $L_0 = 71.99$ μm. Detailed results can be found in Jonfelt (2016).

Conclusions

- The procedure followed in this work gave an overall analysis of the most sensitive parameters of a model for one-stage nitritation-Anammox system.
- Biofilm porosity, biofilm density, maximum biofilm thickness and boundary layer thickness of the biofilm were the most sensitive parameters of the model.
- Optimization of these parameters performed the estimation of NH_4 and N_2O gas emissions of a pilot plant implemented using a MBBR.
- A similar analysis might be done for future versions of the current model, it would help in getting a better estimation of the experimental results.

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