Mathematical modelling of Corleone (Italy) full-scale wastewater treatment plant for estimating the greenhouse gas emissions: a sensitivity analysis

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Abstract: This study summarises the sensitivity analysis results using a novel mathematical model. The mathematical model already published represents the modification of the activated sludge model no. 1 (ASM1) in view of including the nitrous oxide (N_2O) emission (namely ASM1+N_2O model). The ASM1+N_2O model was applied to a full-scale wastewater treatment plant in Corleone (Italy). Sensitivity analysis was performed by applying a local approach. In view of comparing results obtained for the model outputs taken into account (mixed liquor suspended solids - MLSS, effluent total COD, and effluent NH_4-N - S_{NH} concentrations) a normalised sensitivity index (SI) was assessed. Calculated normalised SI for model outputs highlight specific influential parameters, notably Y_H, fp, μ_H, b_H, and those related to ammonia-oxidizing bacteria (AOBs). For the MLSS model output, only two model parameters were found influential, but 8 significant model parameters (4 for each) were identified for effluent total COD and S_{NH} concentrations. This study provides insights for a more efficient calibration process, laying the groundwork for future research on the ASM1+N_2O model.

Keywords: Activated sludge models; ammonia-oxidizing bacteria; nitrous oxide

1. INTRODUCTION

Greenhouse gas (GHG) emissions from wastewater treatment plants, including nitrous oxide (N_2O), methane (CH_4), and carbon dioxide (CO_2), contribute to climate change. N_2O has the highest global warming potential among wastewater treatment plant (WWTP) emissions, warranting special attention for mitigation efforts. N_2O production in biological nutrient removal systems is linked to denitrification and nitrification processes involving ammonia-oxidizing bacteria (AOB). The solubility of N_2O gas and oxygen levels influence its emissions during these processes (Mannina et al., 2019).

Mathematical models are crucial for WWTP design and optimisation. N_2O emissions from WWTPs can be accurately predicted using dynamic mechanistic models considering operational parameters (Mannina et al., 2019). While various studies have adapted activated sludge models (ASMs) for N_2O analysis, focusing on different aspects (among others, Zaborowska et al., 2019; Abulimiti et al., 2022), none have comprehensively addressed GHG emissions, energy consumption, and biological processes under long-term dynamic conditions until Gulhan et al. (2023). Their modification of activated sludge model no. 1 (ASM1) provides a plant-wide approach for simulating N_2O emissions, revealing trade-offs among effluent quality, energy consumption, and GHG emissions in the water-energy-carbon nexus. Nevertheless, Gulhan et al. (2023) established the importance of each model parameter based on their previously acquired knowledge without performing an accurate sensitivity analysis. Sensitivity analysis is essential for pinpointing the most influential model parameters, simplifying the calibration process and providing more accurate results (Mannina et al., 2018). This study employs explicitly sensitivity analysis on the ASM1+N_2O model proposed by Gulhan et al. (2023) to identify the parameters most influencing the model response.

2. MATERIALS AND METHODS

2.1 Model Description

The ASM1 + N_2O model (Gulhan et al., 2023), comprising 19 processes, includes biomass categories for heterotrophic, ammonia-oxidizing, and nitrite-oxidizing organisms. The transition of dissolved N_2O gas to the model was represented using the N_2O stripping model for both anoxic and aerobic conditions. The stoichiometric and kinetic model parameters are defined in Table 1. The model matrix can be found in Gulhan et al. (2023).

Table 1. ASM1+N_2O stoichiometric and kinetic model parameters

Symbol	Definition	Unit
μ_{AOB}	AOB maximum specific growth rate	1/d
μ_H	Heterotrophic maximum specific growth rate	1/d
μ_{NOB}	NOB maximum specific growth rate	1/d
b_{AOB}	AOB decay rate	1/d
b_H	Heterotrophic decay rate	1/d
b_{NOB}	NOB decay rate	1/d
fp	Fraction of biomass leading to particulate products	g COD/g COD
k_a	Ammonification rate	m^3/g COD/d
k_H	Maximum specific hydrolysis rate	1/d
K_{N2O}	Nitrous oxide half saturation coefficient for growth	g N/m^3
K_{N2OHYD}	Nitrous oxide half saturation coefficient for hydrolysis	g N/m^3
K_{NHAOB}	Ammonia half saturation coefficient for AOB growth	g N/m^3
K_{NHH}	Ammonia half saturation coefficient for heterotrophic growth	g N/m^3
K_{NO2}	Nitrite half saturation coefficient for growth	g N/m^3
K_{NO2AOB}	Nitrite half saturation coefficient for AOB	g N/m^3
K_{NO2HYD}	Nitrite half saturation coefficient for hydrolysis	g N/m^3
K_{NO2NOB}	Nitrite half saturation coefficient for NOB	g N/m^3
KN_{O3}	Nitrate half saturation coefficient for growth	g N/m^3
K_{NO3HYD}	Nitrate half saturation coefficient for hydrolysis	g N/m^3
K_{OAOB}	Oxygen half saturation coefficient for AOB growth	g N/m^3
K_{OH}	Oxygen half saturation coefficient for growth	g N/m^3
K_{OHYD}	Oxygen half saturation coefficient for hydrolysis	g N/m^3
K_{ONOB}	Oxygen half-saturation coefficient for NOB growth	g N/m^3
K_S	Readily biodegradable substrate half saturation coefficient	g COD/m^3
K_X	Slowly biodegradable substrate half saturation coefficient	g COD/m^3
Y_{AOB}	AOB yield	g COD/g COD
Y_H	Heterotrophic yield	g COD/g COD
Y_{NOB}	NOB yield	g COD/g COD
η_{1AOB}	Ammonium oxidation pathway factor	-
η_{2AOB}	AOB denitrification pathway factor	-
η_{g1}	Anoxic growth factor (P2)	-
η_{g2}	Anoxic growth factor (P3)	-
η_{g3}	Anoxic growth factor (P4)	-
η_h	Anoxic hydrolysis factor	-
η_{ST}	Stripping reduction factor for aerobic tank	-

2.2 Sensitivity Analysis

Simulations were run in the GPS-X 7.0 software (Hydromantis, Canada) (Fig.1). For the sensitivity analysis, the study followed specific steps to apply local sensitivity analysis (LSA) (Maktabifard et al., 2022). Firstly, the perturbation value was arranged to 10% of the values given in Gulhan et al. (2023). Subsequently, simulations were conducted for each model parameter on-at-a-time using the "Analyze Mode" with "Time Dynamic". Sensitivity indexes (S_I) for each model output were then calculated using the method proposed by Mannina et al. (2011). Likelihood measurements were initially determined for each parameter (Equ.1), and sensitivity indexes (Equ.4) were derived from Equ 2 and 3. To identify influential parameters, sensitivity indexes were normalised and scaled to the maximum sensitivity index value. The results were then sorted in decreasing order, and a parameter was considered influential if its sensitivity index value exceeded 0.20.

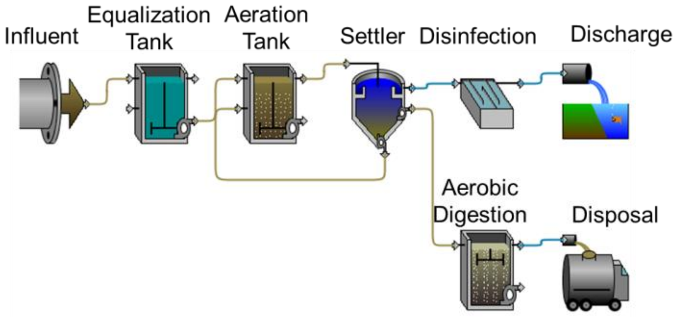

Figure 1. Flow diagram of Corleone WWTP in GPS-X.

$$L\left(\theta_i/Y_j\right) = \exp\left(\frac{-\sigma^2_{M_j-O_j}}{\sigma^2_{O_j}}\right) \qquad \text{Equation 1}$$

$$\sigma^2_{M_j-O_j} = \sum_{i}^{K}\left(M_{j,i} - O_{j,i}\right)^2 \qquad \text{Equation 2}$$

$$\sigma^2_{O_j} = \sum_{i}^{K}\left(O_{j,i} - \bar{O}_j\right)^2 \qquad \text{Equation 3}$$

$$S_{i,j} = \left|\frac{\left(L\left(\theta_i/Y_j\right)_{max,j} - L\left(\theta_i/Y_j\right)_{min,j}\right)/L\left(\theta_i/Y_j\right)_j}{\left(K_{max,j} - K_{min,j}\right)/K_j}\right| \qquad \text{Equation 4}$$

2.3 Characteristics of Corleone WWTP and Sampling Campaigns

The full-scale Corleone WWTP (located in Italy) treats an average wastewater flow rate of 140 m^3h^{-1} by using a conventional activated sludge (CAS) process with pre-treatment involving sieving and degritting. The wastewater is pumped from the equalization tank to the aeration tank with fine bubble diffusers. Concentrated sludge in the settler is recirculated to the aeration tank, and waste sludge undergoes stabilisation in an aerobic digester before disposal. Settler effluent undergoes disinfection before discharge. The plant maintains a hydraulic retention time (HRT) of 6–7 hours, and flow rates are precisely measured with flowmeters.

Sampling campaigns were conducted, both long-term (64 days, twice a week) and short-term (24 hours). Samples were collected from the aeration tank influent and effluent and mixed liquor-suspended solid (MLSS) samples. Auto samplers were used in short-term campaigns for the WWTP's influence and effluency. All the analyses were performed according to Standard Methods (APHA, 2012). In the hourly sampling campaign, N_2O samples from liquid and gas phases were collected using a hood on the aeration tank surface, following the method by Caniani et al. (2019). Dissolved and gaseous N_2O concentrations were evaluated using a gas chromatograph (GC) (Agilent 8860) with an electron capture detector (ECD).

3. RESULTS AND DISCUSSION

Figure 2 displays the calculated normalised sensitivity indices (S_I) of model parameters for the model outputs of MLSS, effluent total COD, and effluent NH_4-N (S_{NH}) concentrations. Regarding MLSS, the most influential model parameter was found to be the heterotrophic yield (Y_H) (normalised SI: 1.0), followed by the fraction of biomass leading to particulate products (fp) (normalised SI: 0.22). Other model parameters were below the threshold value. Concerning effluent total COD, the most influential model parameters include the heterotrophic maximum specific growth rate (μ_H) (normalised SI: 1.0), heterotrophic decay rate (b_H)

(normalised SI: 0.86), readily biodegradable substrate half-saturation coefficient for heterotrophs (K_S) (normalised SI: 0.55), and Y_H (normalised SI: 0.26), in decreasing order of importance. The stoichiometric and kinetic parameters associated with heterotrophic biomass significantly affect the effluent total COD, as they consume organic matter as carbon and energy sources. For effluent SNH, the most influential model parameters were those related to AOBs, as they oxidise ammonia to nitrite. These parameters include AOB maximum specific growth rate (μ_{AOB}) (normalised SI: 1.0), AOB decay rate (b_{AOB}) (normalised SI: 0.78), oxygen half-saturation coefficient for AOB growth (K_{OAOB}) (normalised SI: 0.54), and ammonia half-saturation coefficient for AOB growth (K_{NAOB}) (normalised SI: 0.31), listed in decreasing order of importance.

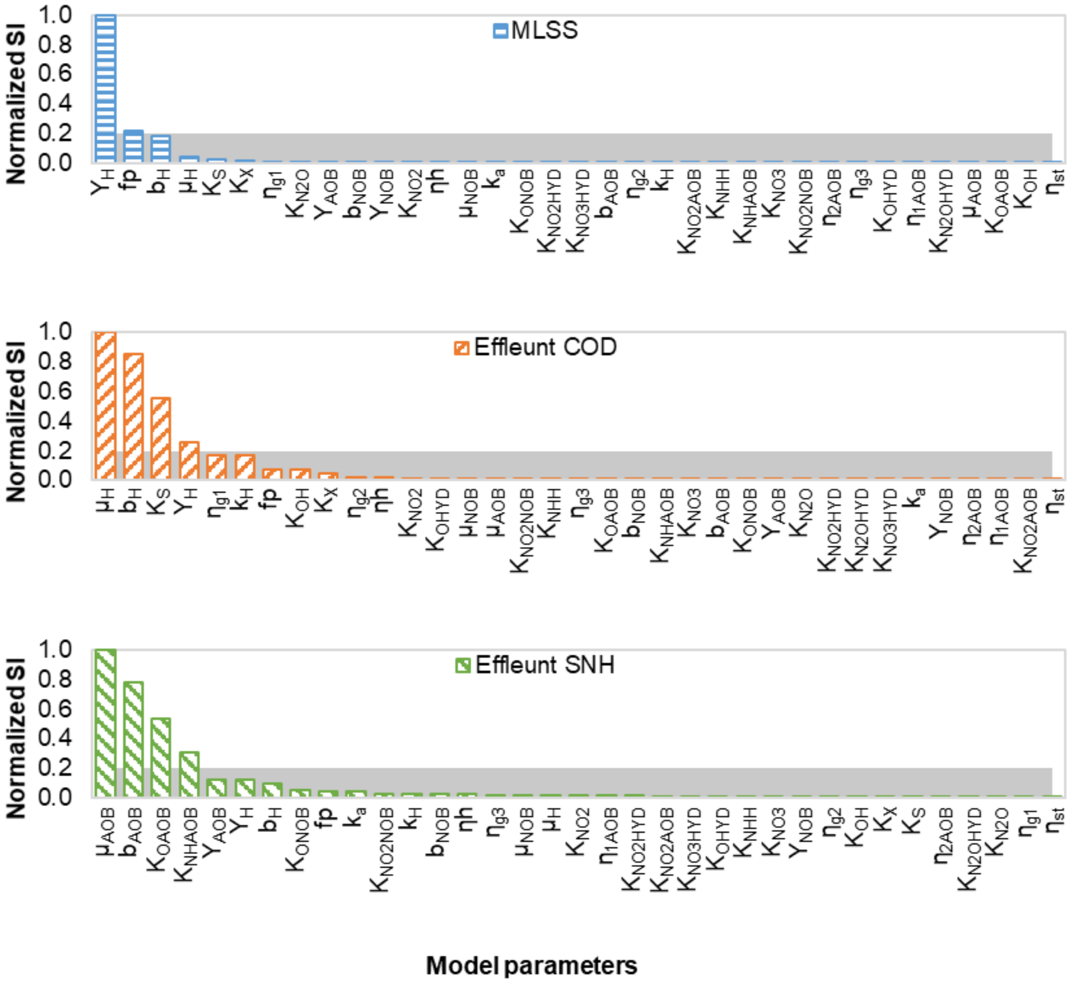

Figure 2. Normalised SI of model parameters for model outputs of MLSS, effluent COD, and effluent SNH.

This study highlights the crucial model parameters essential for calibrating the ASM1+N_2O model, specifically focusing on model outputs such as MLSS, COD, and SNH. Emphasising these significant parameters streamlines the calibration process, reducing the time required for this crucial step. The full paper will elaborate on the sensitivity of model parameters for N2O concentration in the liquid and gas phases.

CONCLUSIONS

Gulhan et al. (2023) addressed the absence of comprehensive studies on GHG emissions, energy consumption, and biological processes under long-term dynamic conditions by modifying ASM1 for N_2O emission simulation at the Corleone WWTP. However, it is important to note the absence of sensitivity analysis in their model calibration process. As demonstrated in this study, sensitivity analysis is indispensable for identifying key model parameters, thereby simplifying the complexity of calibration. The calculated normalised sensitivity indices for MLSS, effluent COD, and effluent NH_4-N concentrations revealed specific influential parameters for each output, focusing on yh, fu, muh, bh, and parameters related to AOBs. This study contributes to a more efficient and targeted calibration process for the ASM1+N_2O model, laying the groundwork for future research in this domain. The full paper will elaborate on the sensitivity of model parameters for N2O concentration in the liquid and gas phases.

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