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Original Article

Modeling Greenhouse Gas Emissions in a Full-Scale Activated Sludge Unit Based on Benchmark Simulation Model – A Case Study of Isfahan Wastewater Treatment Plant

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Abstract
Background: The objective of this study was to establish a facility-level modeling tool to assess the performance of internal operational strategies and external emissions.
Methods: The biological process model in Benchmark Simulation Model No. 2 (BSM2) was upgraded to include two-stage and four-stage nitrification, as well as denitrification processes, to effectively simulate nitrous oxide (N_2O) production. Emissions of carbon dioxide (CO_2), methane (CH_4), and N_2O were also incorporated, taking into account digestion, cogeneration, and sludge storage processes. The refined model was utilized in a case study at the Isfahan Wastewater Treatment Plant (WWTP) in Iran to assess various operational strategies and explore potential challenges related to emission management.
Results: The simulation results, based on the model's structural assumptions, indicate a negative impact on greenhouse gas (GHG) emissions associated with regional energy upgrades in the ventilation system and activated sludge sector. For example, variations in the biogenic and non-biogenic CO_2 proportions were observed when the total suspended solids (TSS) removal efficiency was altered, decreasing or increasing to 30/70 and 20/80, respectively. While off-site CO_2 emissions can be mitigated, this reduction is offset by a significant rise in N_2O emissions. This is particularly concerning given that N_2O exhibits a greenhouse effect nearly 300 times greater than that of CO_2.
Conclusion: It should be pointed out that numerous studies are needed to evaluate plant-wide control strategies in WWTPs for informed and effective decision-making regarding performance optimization.
Keywords: GHG emissions, Modeling, N_2O, WWTP

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Introduction
Treatment objectives have expanded and regulations have become more stringent after the introduction of wastewater treatment plants (WWTPs).[1,2] Today, WWTPs not only eliminate disease, but also prevent harmful emissions in developed countries.[3] On the other hand, it is recommended to reuse resources, enhance effectiveness of energy, as well as decrease greenhouse gas (GHG) emissions through maintaining adequate water flow.[4]

Improving the performance of treatment plants is a challenging task. First, the incoming cargo exhibits continuous variability in both flow and concentration, making it inherently uncontrollable and arriving consistently at all hours throughout the year.[5,6] WWTPs cannot be shut down for inspection or maintenance. Moreover, the design, which integrates sequential processes with multiple feedback streams, introduces numerous feedback effects, resulting in complex interconnections among the processes.[7,8]

In such cases, mathematical modeling is a good tool to evaluate WWTP performance. The model describes the processes and their relationships in detail, taking into account the surrounding conditions.[9] Thus, the adverse effects of the plant can be identified and analyzed to facilitate investigation and the prevention of common issues.[10] Simulation studies enable not only the assessment of current operations but also the analysis of potential future scenarios, such as forecasting demand, planning company expansion, or evaluating other business strategies.[11] Modeling and simulation provide a solid foundation for decision support in evaluating business processes.[12]

The research on GHG emissions has advanced alongside the growing understanding of GHG production in wastewater treatment. Numerous research teams have contributed to this field, developing various models to enhance our knowledge and approach to GHG emissions in such systems. Biological GHG production includes carbon dioxide (CO_2) emissions, through chemical oxygen demand (COD) respiration and methane (CH_4) and CO_2 emissions from anaerobic digesters estimated using different models.[13] However, the development of nitrous oxide (N_2O) production processes is important and complex. All the models proposed in the literature attempt to explain the observed phenomena by proposing one or more methods of production. For example, Blomberg et al presented a simple two-step extension of the activated sludge model no. 3 (ASM3) model to include N_2O.[14] On the other hand, Li et al suggested that four-step denitrification involving electron competition requires a complex model system to describe N_2O production under COD-limited conditions.[15]

Monteith et al[16] were the first to develop a plant-level model that integrated GHG emissions. The model relies on uniform factors at the unit process level while allowing for the incorporation of specific conditions and data tailored to each case. Subsequent researchers further developed this approach.[17,18] However, in the first attempt to estimate plant-level GHG emissions, only CO_2 and CH_4 were calculated and N_2O was not considered.[19,20] Once the N_2O value was obtained, it was incorporated into the modeling process. The first plant-wide models incorporated N_2O emissions, along with other emissions, using available dynamic modeling tools. These models were based on either mechanical or static measurements of the components contributing to N_2O emissions.[21-23] This development highlighted the importance of monitoring the key factors driving N_2O production.[24] Therefore, recent studies have focused on the mechanistic model of N_2O and made additional contributions.[25,26]

Dynamic activated sludge models (ASMs) are widely used in wastewater engineering for purposes such as benchmarking, diagnosis, education, and optimization, in addition to evaluating control and operational strategies before full-scale implementation. Recent advancements in understanding the chemical and biochemical pathways of GHG production have led to efforts to integrate the generation and emission of CO_2, CH_4, and N_2O into conventional ASMs. Despite this progress, few studies have investigated the benefits of including GHG production and emissions as a complementary dimension to traditional effluent quality in performance evaluations. This study introduces an innovative approach by evaluating plant-level control and operational strategies using an integrated GHG modeling framework. This framework captures the primary pathways significantly influencing the carbon footprint across all plants. The strategies explored include adjustments to key process parameters, such as: (1) the dissolved oxygen (DO) fraction in the aeration system within the activated sludge section; (2) the total suspended solids (TSS) removal efficiency in the primary clarifier; (3) the temperature settings of the anaerobic digestion (AD) process; and (4) the management of streams in the anaerobic digester stemming from sludge treatment processes. Besides, this work examines the critical interactions between water and sludge dynamics. The analysis delves into variations in the effluent quality index (EQI), operating cost index (OCI), and emissions of CO_2, CH_4, and N_2O, presented through a comprehensive 3D perspective. Consequently, this study provides an in-depth examination of the interactions and trade-offs between localized energy efficiency and overall GHG emissions.

Materials and Methods

Isfahan WWTP

The second phase of the North Wastewater Treatment Plant (NTP) in Isfahan began operations in 2008, processing around 45% of the city's wastewater. In contrast, the South WWTP exclusively serves Isfahan's southern region, while several nearby communities are connected to the North WWTP. The facility is designed for biological treatment, handling an average flow of 2 m^3/s and a maximum dry weather flow of 2.8 m^3/s. Initially, NTP focused on carbon removal to meet Iranian national effluent standards. However, a few years after its commissioning, discussions emerged regarding the addition of nutrient removal and excess sludge reduction processes to enhance river water quality. Consequently, an extension of the Isfahan WWTP was proposed. Additionally, upgrades to the carbon removal system are necessary to incorporate nutrient removal, with existing plant units being repurposed without requiring significant modifications as an initial step.

Benchmark Simulation Model No. 2 Greenhouse Gas (BSM2G) Description

The BSM2G is an advanced version of the standard Benchmark Simulation Model No. 2 (BSM2) model. It adapts the six core components of the BSM platform—facility design, sample location, input load, sensors and actuators, simulation method, and analysis process—by modifying sample flow, input load, and the analysis process. The finalized BSM2G model was developed and implemented with significant contributions from Barbu et al and Santín et al.[27,28] Figure 1 illustrates the BSM2G unit, which incorporates both direct on-site manufacturing and indirect off-site manufacturing processes.

BSM2G Library Model

Activated Sludge Reactor Unit

The ASM1 bioremediation model used in BSM2 was improved by adding a reactive framework to simulate the biological production of nitric oxide. Two major

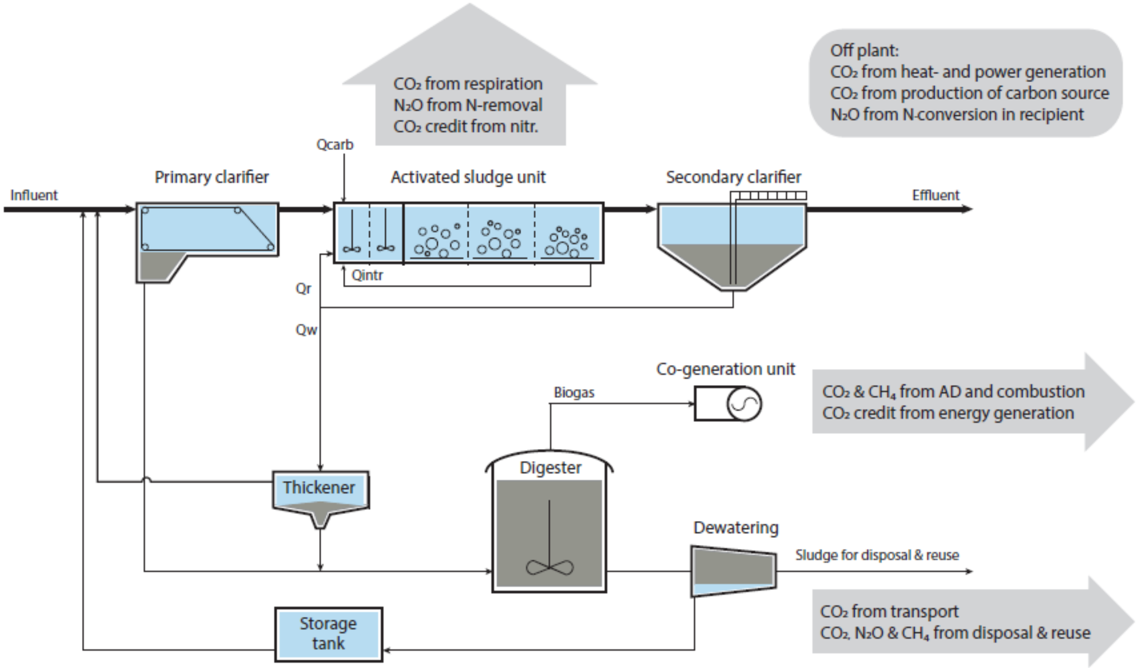

Figure 1. Main WWTP Design in BSM2G With Considering to GHG Emissions (grey boxes)

improvements have been made to the model. The two-stage and four-stage nitrification theories described by Barbu et al suggest a variety of N_2O production.[27] Specific reaction type parameters were used for each of the four denitrification processes. In addition, denitrification by ammonium oxidizing bacteria (AOB) was included according to Santín et al,[28] where AOB is able to reduce NO_2 to NO and N_2O. The kinetic Haldane expression proposed by Massara et al (Equation 1) was introduced to limit AOB denitrification under anoxic conditions.[29]

$$DO_{Haldane} = \frac{S_O}{K_{SO,AOBden} + \eta_{Haldane}.S_O + S_O^2 / K_{IO,IOBden}} \quad (1)$$

where, kinetic parameters are as follows: $KSO,_{AOBden}$ [g O^2/m^3], ŋHaldane [-] and $K_{IO,AOBden}$ [g O_2/m^3] .

Table 1 provides a comprehensive list of all variables applied in the fitted model (ASM1G).[30] CO_2 emissions resulting from biomass combustion were estimated using COD values, while nitrogen balance was determined according to biomass growth, applying a value of 0.31 kg/kg for nitrified nitrogen.

Sludge Train

Effluents from anaerobic digesters and cogeneration units were considered. For digestion, a review of the literature indicated that raw gas deviations of 1%–2% are achievable; therefore, a 1% deviation was adopted in BSM2G.[27] The amount of slippage is calculated from GHG emissions and subtracted from the total gas generated. The remaining gas is directed to a combined heat and power plant. In gas engines, it is estimated that 1.7% of untreated gas is vaporized instead of being combusted.[26] Dissolved CH_4 in sewage sludge (SCH_4) is assumed to be fully separated from the sludge during the discharge stage and released into the atmosphere. This value is automatically calculated based on the comparison and reset to zero once SCH4 is disconnected. During biosolids processing, the sludge must be stored indoors for a period of 12 months before being transported for final disposal or reuse. Nguyen et al based on discharge measurements from sludge storage, estimated that decomposition processes in dried sludge release CH_4 at a rate of 8.68 kg/ton VS and nitrous oxide (N_2O-N) equivalent to 1.1% of total nitrogen (TN) in the sludge.[13] Consequently, the concentrations of COD and TN in the sludge are fixed accordingly.

Indirect and Off-Site Publishing

Various quantities have been employed to remove CO_2 from electricity generation. For BSM2G in general, this value has been updated to the European standard of (0.359 kg/kWh).[9] A value of 0.041 kg/kW related to Iranian electricity production was applied to analyze the situation.[22]

CO_2 emissions from methanol production were added based on the evidence by Yapıcıoğlu and Demir with an emission factor of 1.54 kg/kg methanol.[20] The amount of TN that remains in the stream is partially converted to N_2O in the receiver. N_2O-N emissions from lakes and rivers are included in BSM2G according to an emission factor of 5 g/kg TN emitted from the receiver.[17] The BSM2G standard includes three different waste disposal methods. Santín et al described the principles of increasing CO_2 emissions from sludge mineralization due to COD.[28] To achieve this, additional substances are introduced, resulting in the emission of CH_4 and N_2O under the following conditions:

- 38% agriculture of sludge, transport distance of 150 km, and N_2O-N emission factor of 0.01 kg/kg TN.
- 17% forestry of sludge, transport distance of 144

Table 1. Set of variables for the ASM1G model

Parameter	Explanation	Parameter	Explanation
S_{IC}	Soluble inert COD	DO	Dissolved oxygen
RBC	Readily biodegradable COD	H_B	Heterotrophic biomass
P_{IC}	Particulate inert COD	A_{OB}	Ammonia oxidizing biomass
S_{BC}	Slowly biodegradable COD	N_{OB}	Nitrite oxidizing biomass
SNO_3	Soluble nitrate	P_{ID}	Particulate inert decay
SNO_2	Soluble nitrite	P_{ON}	Particulate organic nitrogen
S_{NO}	Soluble nitric oxide	TSS	Total suspended solids
S_{N2O}	Soluble nitrous oxide	NH	Ammonia nitrogen
S_{N2}	Soluble dinitrogen	ALK	Alkalinity
S_{ON}	Soluble organic nitrogen	F	Flow

km, N_2O-N emission factor of 0.01 kg/kg TN, and CH_4 emission factor of 0.0075 kg/kg of total organic carbon.

- 45% composting of sludge, transport distance of 20 km, and N_2O-N emission factor of 0.01 kg/kg TN.

BSM2G Input Load and Evaluation Graph

The data collection experiment using BSM2 analysis software by Barbu et al revised the exposure profile based on the principles outlined by Qiao et al, incorporating biomass and nitrogen as related effects.[27] In the evaluation methodology, two weighted indices—the EQI and the Operational Cost Index (OCI)—are calculated over the flow violation period, which corresponds to the time of year when effluent quality exceeds regulatory limits. The calibration of EQI should be performed only after integrating GHG production patterns into the analysis. To enhance accuracy, nitrogen oxidation states were incorporated into the estimates for TSS, COD, and BOD, utilizing nitrate weighting factors and accounting for additional biological conditions.

Results and Discussion

GHG Emissions, Wastewater Quality, and Costs Estimation

The modular platform BSM2G was used for its primary objective of benchmarking control strategies. The default control strategy of BSM2 was evaluated against four alternative strategies. The results highlighted components of GHG emissions that overlap with the conventional EQI and OCI. The baseline control strategy in BSM2G consists of two control loops. The first loop regulates the DO concentration in the second aeration reactor using a proportional-integral (PI) controller, which adjusts the airflow to modify the oxygen mass transfer rate (K_{La}). The K_{La} values in the first and third aeration reactors are set to half of the K_{La} in the control reactor. The second control loop employs a PI controller to manage the return flow of nitrates (Q_{intr}) from the fifth reactor to the first reactor, based on the target nitrate concentration in the second anoxic reactor. Additionally, the activated sludge flow rate ($Q_{was,summer}$) varies seasonally with $Q_{was,summer}=450$ m^3/d and $Q_{was,summer}=300$ m^3/d. During the simulation period, activated sludge flow rate (Q_{ras}) and carbon source addition (Q_{carb}) were constant. Four alternative monitoring methods were evaluated for comparative analysis. They were as follows:

1. Control of the DO effect by changing the set point value between 1 and 3 g/m^3. The default value is 2 g/m^3.
2. Changing the pre-cleaning TSS from 33 to 66% (default value of 50%) improved the effect of pre-cleaning.
3. AD mode effect when temperature changed from medium (35 °C) to hot (55 °C) (the default value is 35 °C).
4. Supernatant effect on AD by monitoring reflux rate. This strategy involves storing the drainage solution during the day, when the system load is high, and releasing it at night, when the system load is low. The standard BSM2 strategy does not implement this control method and only returns the solution after the drug has been created.

Figure 2 summarizes the EQI, OCI, and GHG emissions resulting from a typical control strategy

The findings indicated that altering the target value of the DO strategy had the most significant effect on GHG emissions among the strategies tested. Lowering the DO set point in the activated sludge (AS) resulted in an increase in SNO_2 concentration, which promoted AOB denitrification and subsequently leads to N_2O production in the model (Figure 3).

The SNO_2 profiles exhibit clear seasonal variations, emphasizing the importance of accounting for dynamic changes in NE formation. Simultaneously, reducing flights lowers indirect CO_2 emissions from power generation but increases overall CO_2 emissions. The study concluded that while the extent of TSS removal has little effect on emissions, enhancing TSS removal significantly improves wastewater quality and reduces operational costs. The slight rise in emissions is attributed to higher gas efficiency from increased N_2O production, which offsets the impact of elevated biogas production.[15] Furthermore, the findings suggest that transitioning to

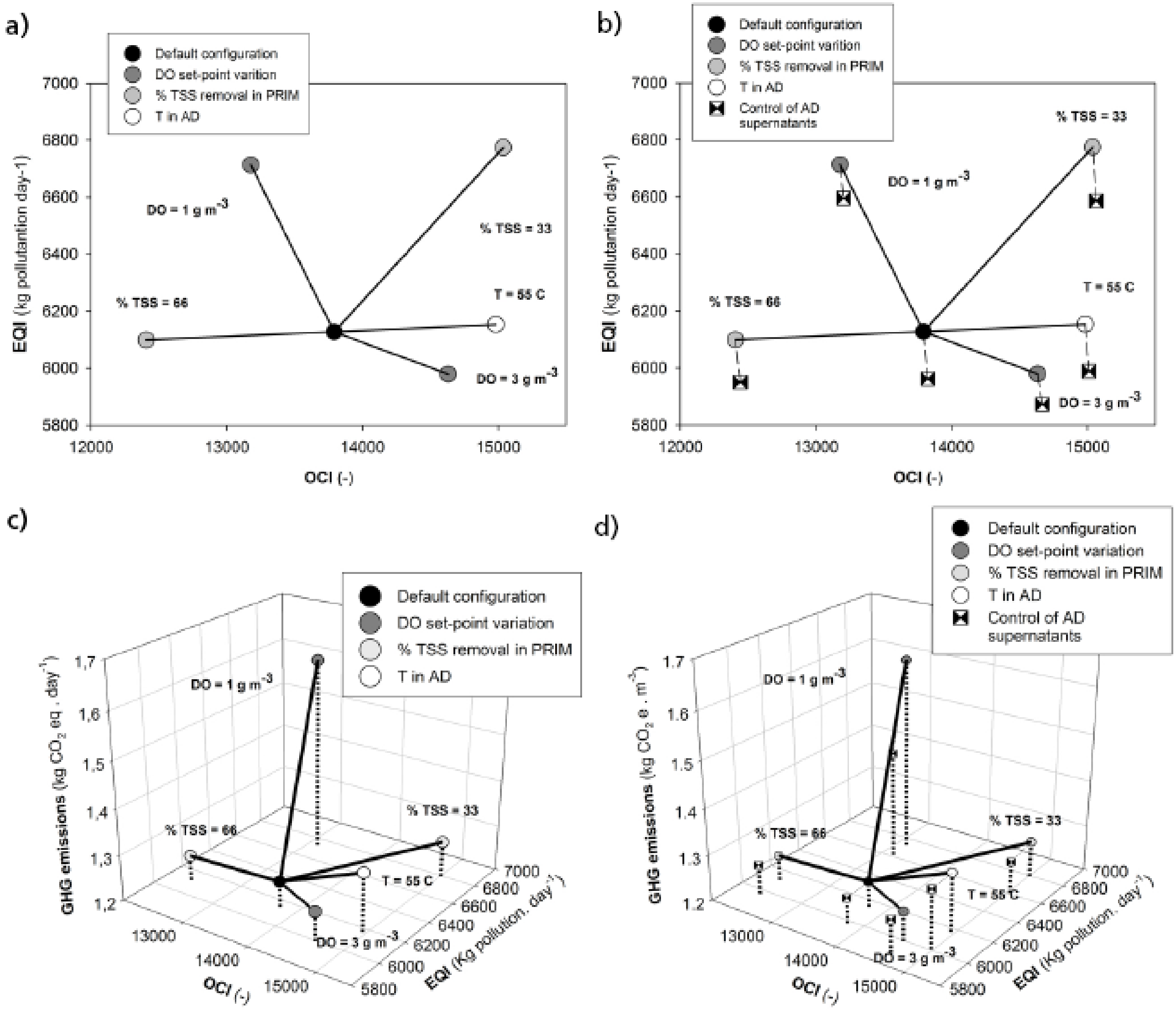

Figure 2. EQI, OCI, and GHG Emissions for The Simulated Strategies

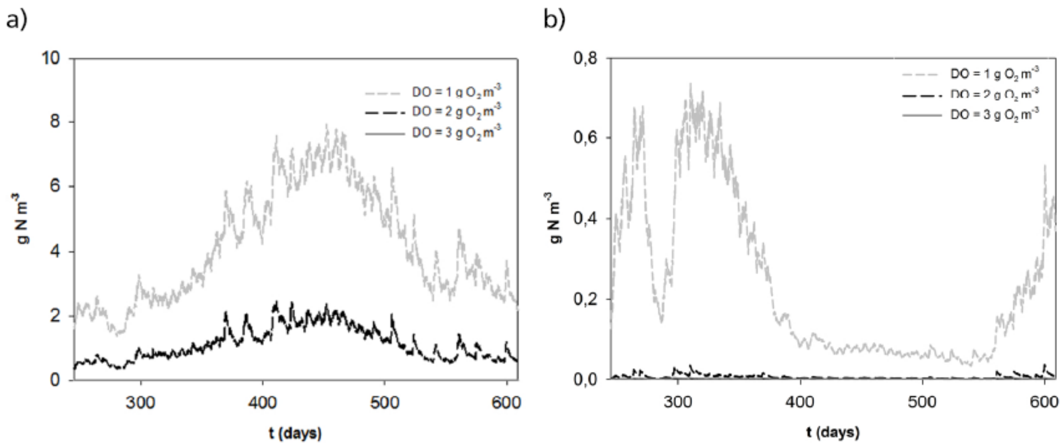

Figure 3. Dynamic Outlines of (a) Ammonium Nitrogen and (b) Nitrite Nitrogen Within the DO Changes. In both graphs, the concentrations at DO=3 g/m^3 is zero or close to zero

a thermophilic digestion process with consistent and adequate digestion offers benefits for AD treatment. However, this approach increases operating costs and GHG emissions due to higher heat requirements. Finally, the fourth strategy, controlling the sludge return pump, proved effective across all scenarios. This strategy slightly enhanced emission quality by reducing SNH_4^+ peaks, though it had minimal impact on emissions in most cases.

Emission reductions were primarily driven by lower N_2O levels, as low DO and high ammonia concentrations are linked to a greater risk of N_2O production.[23]

Adjusted N_2O Generation Within a Full-Scale Activated Sludge System

In a case study at the Isfahan Wastewater Treatment Plant in Iran, N_2O measurements were conducted in one of five identical rooms corresponding to the plant's AS units. Over approximately 100 days, the samples were collected in both liquid and gas phases. A sensor placed inside the tank measured N_2O concentrations and was repositioned twice during the measurement period to capture the reactor's full performance, providing data from three different locations. The concentration data are illustrated in Figure 4. Since the system operates within an enclosed room, gas is pumped into the ventilation system, which collects it via a direct AS barrier. Ventilation measurements were subsequently used to calculate N_2O concentrations.

The N_2O concentrations measured in the reactor suggest that N_2O formation does not occur in the hypoxic zone (Figure 5). At the end of the final anoxic zone, dissolved N_2O concentrations are minimal. However, N_2O levels are higher in the ventilation zone and continue to increase throughout the reactor. Given the stripping effect caused by ventilation, it can be concluded that most N_2O production and emissions originate in the ventilation zone. This is likely due to the relatively high concentration of N_2O -N, measured at approximately 0.3 g/m³. As illustrated in Figure 6, the average emission levels align with the measured values, though the model does not fully capture the dynamic behavior of the emissions. The model estimates baseline N_2O emissions at approximately 30 kg/day, while measured emissions significantly decrease by day 425 (Figure 6). The model's predictions follow the general denitrification equation but could be improved by integrating hydroxylamine oxidation and AOB dissociation under dynamic conditions.[29] N_2O production is primarily driven by nitrite oxidation rates and is more closely linked to AOB activity than to DO levels. Although this enhanced dual model is not applied in the Isfahan WWTP case study, the findings emphasize the need to consider additional interaction pathways in future research. To reduce atmospheric emissions, one critical factor is calibrating aqueous-phase N_2O concentrations to values lower than those measured in the aeration zones.[10]

Conclusion

Incorporating GHG emissions as an evaluation criterion adds valuable insight into the management and operational strategies of a WWTP, providing additional information about the plant's overall "sustainability." Simulation results of various control strategies reveal potential trade-offs, such as the benefits of energy recovery technologies (e.g., active energy recovery from AD) versus the negative impact of N_2O emissions on the WWTP's GHG profile.

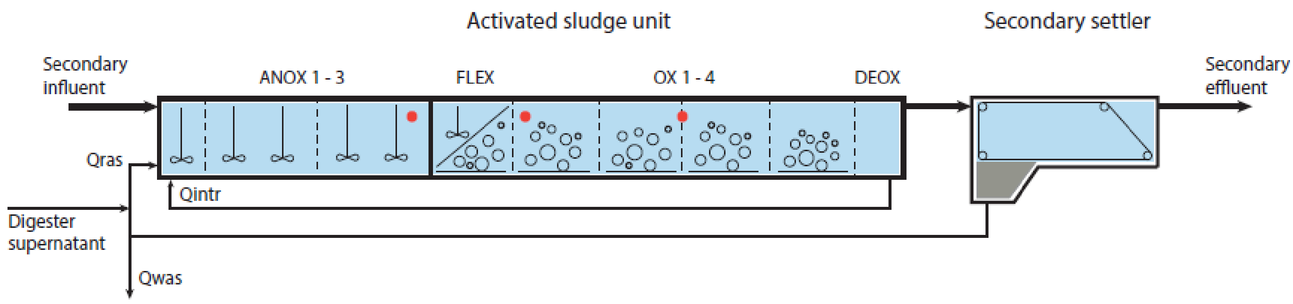

Figure 4. Schematic Diagram of the AS Reactors at the Isfahan WWTP (N_2O measurement points are shown with red markers.)

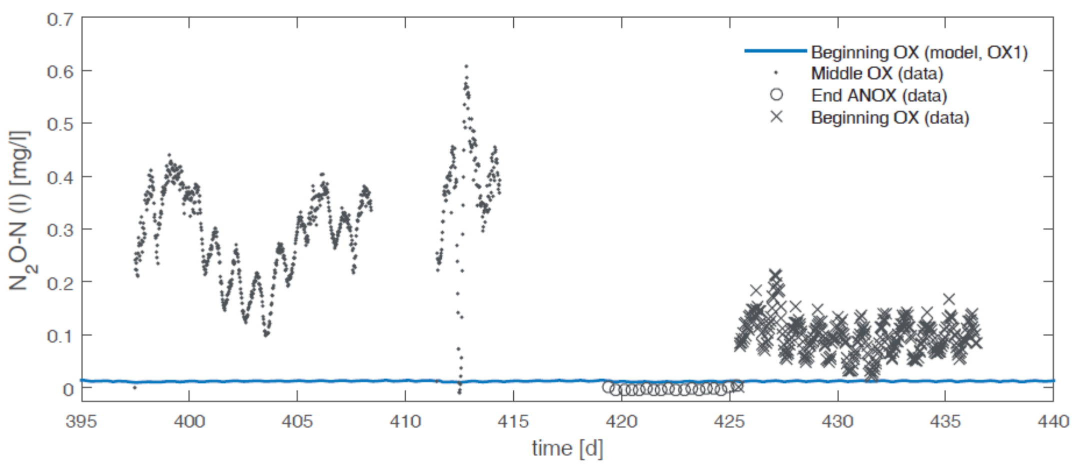

Figure 5. Aqueous N_2O-N at the Isfahan WWTP

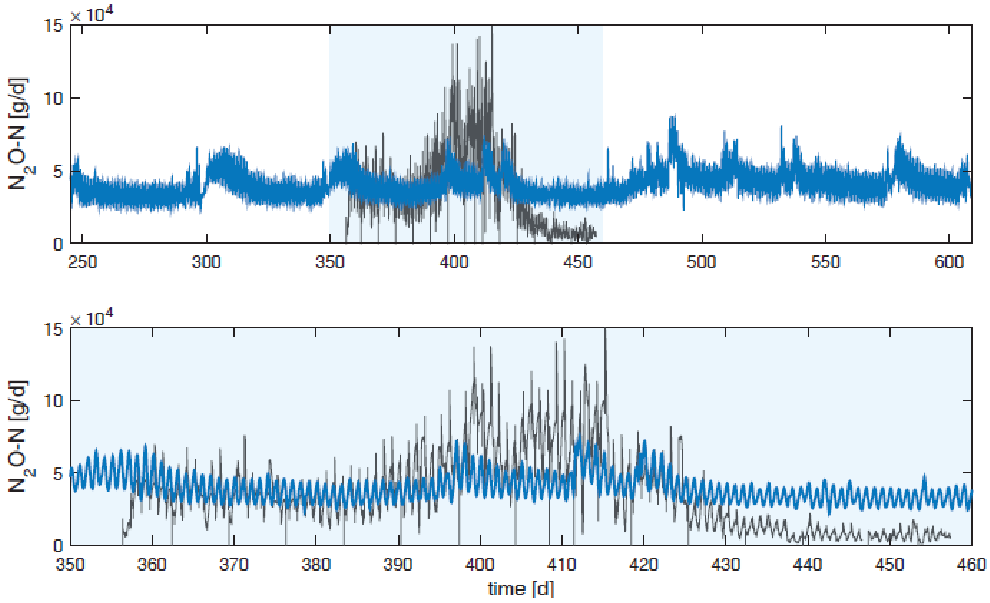

Figure 6. Off-gas N_2O at Isfahan WWTP

The significance of maintaining clean water and sludge channels, along with their combined effects on GHG emissions, is evident in temperature regulation, metabolic cycle optimization, and improvements in primary waste efficiency. The elimination equation can be simplified for practical application, which predicts a maximum N_2O emission that was not observed experimentally. Furthermore, because the removal equation is structured as it is, adjusting the solution concentration and N_2O flux simultaneously is not feasible. For large-scale modeling of N_2O emissions, insights into N_2O formation pathways during gas retention can be derived using advanced instrumentation. The model was calibrated using N_2O emission measurements from the Isfahan WWTP in Iran, and simulations indicate that it is well-suited for typical urban wastewater restoration under current operational conditions. While the findings are specific to the Isfahan WWTP, they highlight the practical applicability of the developed tools. Moreover, the model's framework can be adapted for other contexts, offering valuable insights for broader applications.

Authors' Contribution

Conceptualization: Gholamreza Nabi Bidhendi.
Data curation: Hamidreza Shiran.
Formal analysis: Hamidreza Shiran.
Investigation: Hamidreza Shiran.
Methodology: Nasser Mehrdadi.
Project administration: Gholamreza Nabi Bidhendi.
Supervision: Gholamreza Nabi Bidhendi.
Validation: Nasser Mehrdadi.
Writing-original draft: Hamidreza Shiran, Gholamreza Nabi Bidhendi, Nasser Mehrdadi.

Competing Interests

The authors declare no conflict of interest.

Ethical Approval

All ethical principles were considered in this article.

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