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BIOKINETIC AND ARTIFICIAL INTELLIGENCE MODELS FOR THE SIMULATION OF NITROUS OXIDE EMISSIONS FROM WASTEWATER TREATMENT PLANTS

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Abstract

Nitrous oxide (N2O) is considered a potent and very harmful greenhouse gas (GHG), and wastewater treatment plants (WWTPs) are considered a potent source of it. Predicting N2O emissions is a first step in reducing these. One way of doing this is by using a process-based biokinetic model, based on Activated Sludge Models (ASMs) that have been extended to include the N2O production pathways. Alternatively, data-driven Artificial Intelligence (AI) models can be used to predict N2O emissions. In this paper, a biokinetic model has been built and calibrated for the Amsterdam West WWTP (1.1 Million PE; 168 MLD), using the EnviroSim software, BioWin®. A comprehensive monitoring campaign was conducted to characterise the common quality parameters (COD, TKN, TP, TSS, etc.) into their fractions, which were then used as BioWin model inputs. The calibration was conducted in two stages to predict effluent quality followed by model calibration to predict N2O emissions. Additionally, an Artificial Neural Network (ANN) based model was developed using pertinent process parameters, such as the influent flowrate, and NH4 in the aerobic tank as inputs to predict the N2O concentration in the gas phase. Preliminary results demonstrate that the ANN model outperforms the BioWin model in terms of prediction accuracy. Still further work is required to better understand the pros and cons of the two modelling approaches.

Keywords
Nitrous oxide, wastewater treatment, biokinetic modelling, artificial intelligence, artificial neural network.

1 INTRODUCTION

1.1 Background

With the increasing effects of climate change and global warming becoming more apparent, great efforts are being made in reducing the carbon footprint of industries and society in general. Nitrous oxide (N_2O) is considered a potent and very harmful greenhouse gas (GHG); in addition, N_2O has been considered to contribute to the depletion of the ozone layer in the stratosphere [1]. While the global anthropogenic GHG emission contribution from N_2O can be considered minor (6.2% in terms of CO_2eq), the global warming potential of N_2O is very high, 298 times greater than that of CO_2 on a 100-year time scale [2]. In the past decades, wastewater treatment plants (WWTPs) are increasingly considered to be one of the potent sources of N_2O. Therefore, there is a global call for action to invest and investigate in advance wastewater treatment technologies and operational strategies to reduce the generation of the harmful gas [3]. As a result, the quantification of N_2O emissions from full-scale plants have been considered greatly, and monitoring campaigns of varying durations have been conducted. Additionally, biokinetic models, primarily using the widely known activated sludge models (ASMs) have been extended to include the N_2O production pathways. In parallel, like many other domains, more and more data-driven based analytics are being utilised and adopted in the wastewater field, to solve complex process challenges. Artificial Intelligence (AI) models also have been used in the prediction of key

wastewater parameters including N_2O in data-rich systems. In this study, a biokinetic model was calibrated using long-term (1 year) N_2O emissions data from a full-scale WWTP and its predictive capabilities were assessed. To acquire specific data on the raw influent wastewater that is necessary as input into the model, a comprehensive sampling campaign was also conducted. Finally, initial investigations of training AI models to predict the N_2O emissions were conducted. Preliminary comparison of the performance with the biokinetic model predictions have been discussed.

1.2 Biokinetic Modelling of N_2O Emissions

Activated sludge models (ASMs) are widely and successfully used for process modelling, subsequentially supporting in finding solutions to process design and operational problems [4]. The production of N_2O emissions in WWTPs has been associated with the process of biological nitrogen removal, where three production pathways are prominent, of which two are attributed to the ammonia oxidising bacteria (AOB), i.e., hydroxylamine oxidation and nitrifier denitrification; and one is attributed to incomplete heterotrophic denitrification. Over the past decade, such biokinetic models have been extended to also include the production pathways of N_2O, for its prediction and to test control and mitigation strategies. While the current N_2O biokinetic models have been able to predict the general trend of the observed N_2O emissions, the prediction accuracies are still unsatisfactory [5, 6]. Furthermore, when a calibrated model is confronted with unseen data for validation, the prediction accuracy has been reported to be much lower, thereby questioning the capabilities of the models to future data [4, 5, 6, 7, 8].

The modelling investigations were mostly carried out using datasets obtained from a controlled environment as a lab-scale or pilot-scale setup, barring a handful of cases that used data from full-scale systems [5, 6, 7, 9, 10]. Therefore, the applicability of such biokinetic N_2O models in a full-scale WWTP can be questioned given the controlled operating and process conditions that are administered in lab/pilot scale setups. Furthermore, in the cases of full-scale based investigations, the duration of data used for the calibration and validation purposes can be considered short-term (< 1 month) or medium-term (< 1 year). In the prediction of N_2O emissions using biokinetic models, there is a clear requirement to analyse the performance of the models when calibrated on long-term data containing seasonal variations and under full-scale operating conditions.

1.3 Data-driven Modelling of N_2O Emissions

The use of data-driven based analytics or AI models to predict N_2O emissions in WWTPs is still sparse. Even though advanced information extraction methods and dimensionality reduction techniques have been used on WWTP data, a handful of investigations have used these methods to analyse data from N_2O monitoring campaigns [11]. For example in the investigation in [12], a Random Forest (RF) analysis, a machine learning method, was used to identify the primary effecters of N_2O emissions from a full-scale BNR system. In [13], Support Vector Machine (SVM) classifiers were trained to predict, with high accuracy (95% - 99%), whether the dissolved N_2O will be consumed during the anoxic and anaerobic phases and subsequently, used the information from the classifiers to predict the average dissolved N_2O concentration in the anaerobic and aerobic phases by training a Support Vector Regression (SVR) model for each. The SVR models were reported to predict with good accuracy with R^2 values ranging from 0.85 – 0.94 on the training dataset and 0.75 – 0.82 in the test dataset. The use of Deep Learning (DL) models for N_2O predictions is still a novelty, with only a handful of studies being conducted [14, 15]. A Deep Neural Network (DNN) model was developed to predict the N_2O in the liquid phase using over a year of operational data from a WWTP, while using the influent flowrate, DO, NH_4, NO_3, air flowrate and temperature as inputs. While using a trailing moving average to smoothen the data, a significantly high R^2 value of 0.9 was achieved. Furthermore, the DNN model was compared with a Long Short Term Memory (LSTM) based Recurrent Neural Network (RNN) model, that utilised historical N_2O data to predict future values. The two models were assessed for their forecasting capabilities over

a 1-day prediction horizon. It was seen that the DNN model's performance was limited (R^2 = 0.76), while the LSTM model achieved better results (R^2 = 0.94). Accordingly, the application of data-driven models could present a suitable alternative to biokinetic modelling, especially to overcome the latter's limitations.

2 METHODOLOGY

2.1 Brief Description of WWTP

The case study for this investigation is the Amsterdam West WWTP (**¡Error! No se encuentra el origen de la referencia.**) that is operated by the water company Waternet. Amsterdam West WWTP has a capacity of 1.1 million population equivalent (168 MLD) and serves the Amsterdam city and its neighbouring regions. The raw influent wastewater, post the grit chambers and primarily settlers, is distributed to 7 treatment lanes to conduct the activated sludge (AS) process for biological nitrogen and phosphorus removal. The process configuration applied for the AS is the modified University of Cape Town (mUCT) process.

Figure 1: Amsterdam West WWTP

For this study, data from legacy online sensors measuring key process parameters of the influent flow, wastewater quality parameters in the bioreactor, recirculation flowrates, sludge flowrates, and effluent flowrates, were used. Most importantly, time series online sensor data of the N_2O emissions measured in one treatment lane is also available. A distinctive condition in Amsterdam West is that the bioreactor units are covered, which allows for the accurate capture of the off-gas emissions from the AS processes, providing direct measurements of the N_2O in the gaseous phase. All signals have a time resolution of 1 minute. Furthermore, historical laboratory measurements are also available for TKN, TN, Total P, BOD, COD for all stages in the wastewater treatment process.

2.2 Biokinetic Modelling to Predict N_2O Emissions

A comprehensive sampling campaign was conducted to characterise the influent as well as to obtain additional effluent data to calibrate the biokinetic model. Flow proportional daily composite samples and diurnal sampling were taken for the raw influent and effluent wastewater, where the following parameters were monitored: COD_{total}, $COD_{filtered}$, BOD_{total}, $BOD_{filtered}$, TKN, NH_4, NO_3, Total P, Ortho-PO_4, ISS and TSS. Numerous samples were also taken at various locations including the anaerobic, anoxic, and aerobic zones of the bioreactor, sludge treatment lines and return streams.

For this investigation, a biokinetic model using the ASDM model coupled with a N_2O model was calibrated for 1 treatment lane of the Amsterdam West WWTP. The simulation software by EnviroSim, BioWin® was used to conduct the research. Initially, the process configuration (Figure 2) of the WWTP was set up in BioWin using the plant design and operating parameters.

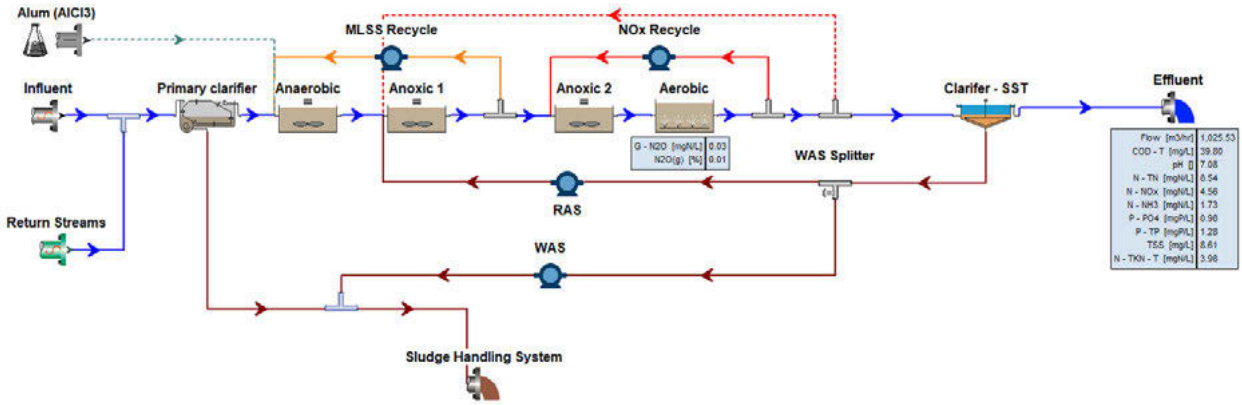

Figure 2: Process Configuration of 1 treatment lane in Amsterdam West WWTP, as setup in the simulation software BioWin.

Subsequently, the calibration procedure was conducted in two stages. In the first stage, the model was calibrated using the wastewater characteristics and fractions obtained from the sampling campaign as well as historical datasets. Subsequently, steady-state and dynamic simulations were performed using the N_2O model default values in BioWin. In the second stage, further calibration was conducted with a goal to match the observed plant N_2O emission data. The N_2O model provided in BioWin includes the description of all three N_2O production pathways. The kinetic parameters specific to N_2O production from the nitrification and denitrification processes were then fine-tuned to be able to match the observed N_2O emissions from the gaseous phase. During the calibration of the N_2O specific kinetic parameters, it was ensured that the effluent quality is matched at all times with the observed data which served as a strict boundary to adhere to.

The calibration of the model for dynamic simulations was conducted using a variety of datasets as acquired from the sampling campaign, historical laboratory measurements and from online sensors. Simulations were performed by inputting the flowrate and quality parameters for the influent wastewater and return streams from laboratory measurements. Daily values of duration 1 year from 11/2020 – 10/2021, covering all 4 seasons, were used.

2.3 Preliminary AI Modelling Investigations

As an alternative to biokinetic modelling of N_2O emissions, preliminary investigations were also made to assess the predictive capabilities of AI models. An Artificial Neural Network (ANN) model was developed. As input to the model, 3 parameters were used, namely the raw influent flowrate to 1 treatment lane, NH_4 concentration levels in the aerobic tank of the bioreactor and the N_2O concentration levels (in ppmv). The target variable is the N_2O concentration levels. The data was resampled to a resolution of 15 minutes. The model structure included 1 hidden layer containing 64 units. The model was trained to take a certain amount of historical input of the variables to make a one-step ahead prediction of the target. As a result, the data was prepared into sequences where data amounting to 2 days (192 values) of all input variables was used as historical input into the model. The data of the target variable were prepared accordingly to also facilitate the training of the ANN model to perform a one-step-ahead prediction. The model was trained on 1 year of data (11/2020 – 10/2021), and 3 months of data was used for testing.

3 RESULTS AND DISCUSSIONS

The results of the N_2O emission predictions from the biokinetic model (black line) compared with the observed data (blue dots) are depicted in Figure 3, where a seasonal N_2O peak is distinctive. To simulate this peak in the biokinetic model (in BioWin), season-specific fine-tuning of the N_2O related parameters was necessary. Specifically, the parameters related to the nitrifier

denitrification production pathway were adjusted along with the free nitrous acid inhibition parameter to allow for more production of N_2O due to incomplete denitrification. Furthermore, the Arrhenius value related to the mass transfer (Kl) of N_2O was also changed (reduced by half) to allow for more stripping of N_2O from the liquid to gaseous phase. While these changes resulted in successfully and accurately predicting the N_2O seasonal peak, as shown in Figure 3, there are currently no proper scientific justification for these changes in the model. For such a justification, extended research and investigation on these kinetic and temperature dependent parameters are required, which is beyond the scope of this study. Moreover, the occurrence of the N_2O seasonal peak could point in the direction that there are still a lot of uncertainties with regard to the biokinetic processes related to the N_2O production pathways currently in the model. In the seasons where low N_2O emissions were observed, the default parameters available in BioWin were sufficient to accurately predict the N_2O emissions, except for the Arrhenius value for the NOB maximum specific growth rate. Such a result would be expected as the default values available in BioWin were calibrated on datasets obtained from bench-scale studies during summer-like conditions [16, 17]. Adjusting some of the N_2O biokinetic model parameters without scientific justification in order to satisfactorily predict the seasonal peak implies the limitation of the biokinetic model.

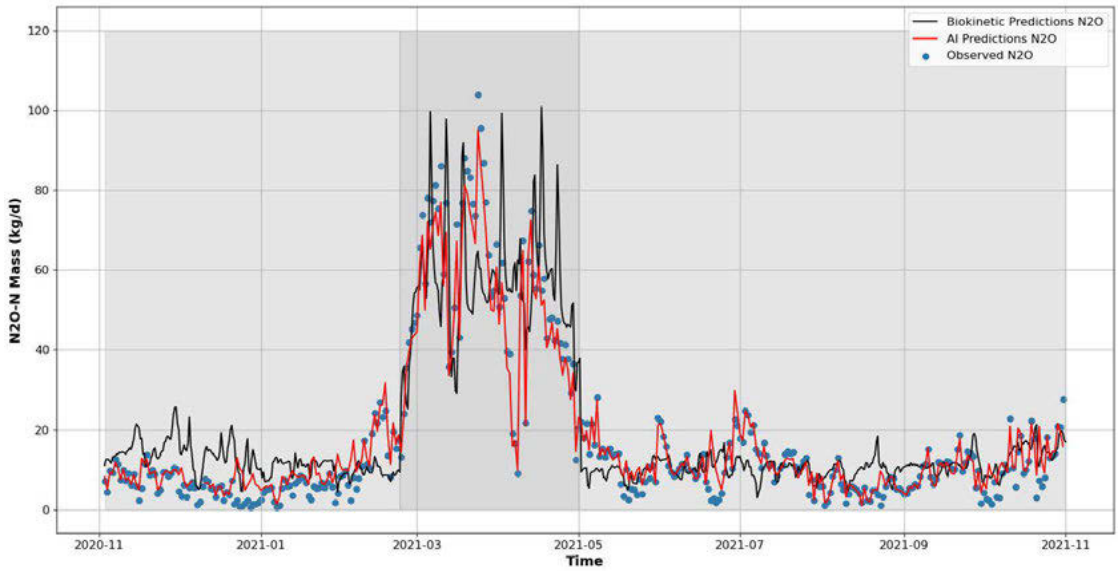

Figure 3: Comparing the Biokinetic Model N_2O Emissions Predictions (black line) and AI Model Predictions (red line) with Observed N_2O Emissions (blue dots) for a Period of 1 Year. The dark grey area signifies the seasonal N_2O emissions peak that was observed.

A similar simulation exercise was conducted using the developed AI model in order to compare with the biokinetic model predictions. From the initial results illustrated in Figure 3, the predictions from the AI model (red line) resulted in a good fit to the observed data, suggesting that the AI model outperforms the biokinetic model. This positive and encouraging outcome from the AI model presents a suitable alternative to overcome the limitations of the biokinetic model in satisfactorily predicting N_2O emissions for all seasonal conditions.

4 CONCLUSIONS

In this study, a biokinetic model was developed first using the BioWin software. This model was calibrated on 1 year of data from a real-life WWTP. Additional data were collected during a comprehensive sampling campaign conducted to characterise the raw influent into its fractions. During the calibration of the biokinetic model, it was established that the default values of the physical and kinetic parameters were unable to adequately predict the seasonal variations

observed in the N_2O emissions. As a result, an AI based model in the form of an Artificial Neural Network was developed and trained on the same data set as an alternative. Preliminary results show that the AI model is outperforming the biokinetic model in terms of prediction accuracy. Therefore, further research on developing data-driven and possibly hybrid models should be pursued. An improved N_2O prediction model can then be used for the development of (near) real-time control strategies to mitigate the production of N_2O emissions from WWTPs.

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