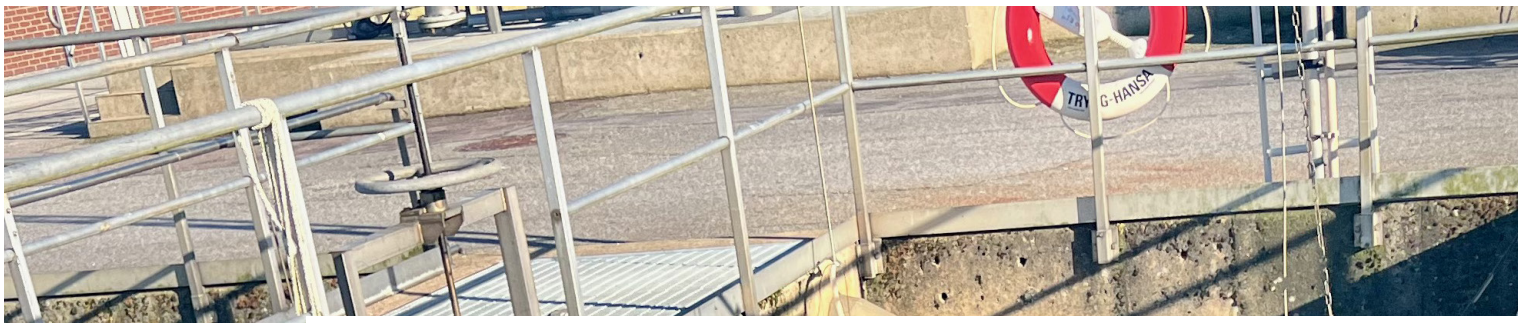

Modelling the full-scale N2O emissions from wastewater treatment plants for identifying mitigation strategies

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by

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The picture on the front page: Photo from Klagshamn wastewater treatment plant. Foto: Naga Deepika Peddamudium

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Preface

With this project, I completed my master's degree in water resources engineering at Lund University, Faculty of Engineering. It was great with a lot of experiences with many new friends. The degree project is very educational and since it is performed in collaboration with Industrial Electrical Engineering and Automation (IEA), LTH, VA SYD, and the Klagshamn treatment plant, it helped me to meet professional people to get valuable suggestions to improve the project.

I am able to finish my degree project and it is possible because of my supervisor, Ramesh Saagi, who guided me throughout the project with his numerous knowledge of modelling the wastewater treatment process and also for providing a nice room with a system to work for my thesis. I have learnt so many things from you during my degree project with all your feedback and you have always been so cooperative and a big thank you for that. I would like to also thank Ulf Jeppsson, head of the department, IEA, LTH for accepting me to do the project at the department and following up on the progress of the project. Thanks to Ivelina Dimitrova, Sara Ekström and David Gustavsson at VA SYD for the Klagshamn treatment plant visit and for explaining the details of the treatment process and providing valuable measurement data to perform the study and guiding the project with progress meetings. Thanks to my examiner Åsa Davidsson for helping me with good tips and suggestions and you have been so supportive during the study. I appreciate people in the VA technology: Michael Cimbritz and Åsa Davidsson who have encouraged me to do a degree project. Thanks to Adnan for being an opponent of my thesis and for giving me comments.

Thanks to DHI for providing a licence to access WEST software along with tutorials, which is the key to doing the modelling studies of my project. Special thanks to Fabio for giving me tricks in the software which helped me for performing modelling study.

Lastly, I am grateful to my friends and family and special thanks to Srinivas, my partner for the care and support.

Popular Scientific Summary

Traditional operation of wastewater treatment plants is solely focused on efficient pollutant and nutrient removal to protect the health and environment of society. Recently, a new aspect came into consideration with respect to mitigating greenhouse gas specifically N_2O emissions and energy demands for the sustainability of WWTPs. Klagshamn WWTP, located in southern Malmö is discharging high N_2O emissions from the treatment process and for this reason, VA SYD wants to explore different operating strategies to mitigate nitrous oxide emissions from the biologically activated sludge treatment process, using the N_2O measured data from floating hoods arranged at the treatment plant. Modelling a mechanistic model is a cost-efficient way to investigate different strategies for mitigating N_2O emissions.

A model of Klagshamn wastewater treatment plant process is developed in the WEST software with the ASM2dISS model. The model includes two pathways of N_2O emissions (ie., Nitrifier denitrification pathway by AOBs and heterotrophic denitrification pathway by OHOs). Full-scale measurement data is carefully preprocessed and subjected to flow balances and linear regressions to eliminate outliners and select suitable simulation periods. The steady-state and dynamic model simulation results are calibrated and validated against measurements with showing a reasonable fit, considering parameters such as solids content, nitrogen species, and N_2O by adjusting the kinetic parameters. Despite the limitations in the available production pathways within the model, the dominant pathway for N_2O emissions is determined to be heterotrophic denitrification. Based on the simulation results, several strategies for mitigating N_2O emissions are evaluated, and two particularly effective strategies are proposed in this study. The first strategy involves modifying the retention time of solids in the process, while the second strategy focuses on implementing internal recirculation within the treatment process. The second strategy is further explored through four different cases, considering variations in recirculate flow rates and the number of anoxic zones. Both proposed strategies yield positive outcomes, but the second strategy demonstrates a higher reduction in the N_2O emission factor compared to the first. Among the four cases analysed for the second strategy, it is revealed that the third case, which involves internal recirculation at three times the influent flow rate with one anoxic zone, achieves a substantial 47% reduction in the N_2O emission factor.

Furthermore, the proposed strategies are assessed for their impact on the treatment process, including nitrogen species concentrations, to evaluate their influence on process efficiency and identified to be within acceptable limits. It is recommended to thoroughly consider the advantages and disadvantages of each strategy before implementing the proposed mitigation measures.

Keywords: Modelling, simulation, ASM2dISS, N_2O production pathways, N_2O emission factor, mitigation strategies.

Abstract

Nitrous oxide (N_2O) emissions, which primarily originate from the biological nitrogen removal process, dominate the release of greenhouse gases (GHGs) in wastewater treatment plants (WWTPs). N_2O production occurs through dynamic microbial pathways that have a significant impact on the environment compared with other GHG emissions. Reducing these substantial emissions aligns with the objectives of minimizing the carbon footprint of WWTPs and achieving sustainability. This study aims to investigate the pathways responsible for N_2O production through a comprehensive model-based approach on a full-scale basis to identify effective mitigation strategies.

To model N_2O emissions, this study employs the activated sludge model (ASM), specifically ASM2dISS, which incorporates two N_2O production pathways: nitrifier denitrification and heterotrophic denitrification pathways. The collected measurements are pre-processed in MATLAB by filling in the missing values and removing the outlier values using flow balances and the data is analysed for obtaining clean data for modelling the treatment plant and for choosing the periods for model simulations. With the available data, the model is constructed in the WEST and firstly, steady-state simulations are calibrated, and then dynamic calibrations are performed using dynamic data of 24-hour daily measurements. Calibrations are executed for solids, nitrogen species and N_2O emissions of the treatment process and the calibrated model is validated for different periods. Kinetic parameters are adjusted in the model and calibration and validation results are compared with the plant measurements. Model simulations generally predicted well with the measured values in most of the simulated days except nitrate content in the activated sludge units which is slightly underestimated than the measurements. It is identified that nitrate concentration is strongly correlated with N_2O emissions and as calibration is focused on N_2O emissions, nitrate calibration is limited considering its effect on N_2O emissions. Model results revealed that N_2O emissions are contributed by both nitrifier denitrification and heterotrophic denitrification pathways with heterotrophic denitrification as a dominant pathway.

The calibrated model is used for implementing the mitigation strategies in the activated sludge process. Two approaches have been proposed as mitigation strategies, one is to vary the SRT of the system and another approach is to introduce internal recirculation in the secondary treatment process. The second approach is evaluated with four cases, by varying recirculation flow rates and the number of anoxic zones in the process. Results are compared with calibrated values as a reference, in which results from both approaches showed a good reduction of N_2O emissions. When results from all the strategies are compared, 3 times the internal recirculation with 1 anoxic zone showed good possibilities for lowering N_2O emissions from the treatment process. Each strategy comes with certain positives and negatives in terms of process modifications and energy demands, therefore every aspect needs to be considered for implementing the proposed mitigation strategies.

Abbreviations

GHG, Green House Gas; CF, Carbon Footprint; BNR, Biological Nitrogen Removal; AOB, Ammonia-Oxidizing Bacteria; NLR, Nitrogen Loading Rate; ASMs, Activated Sludge Models; IWA, International Water Association; EF, Emission Factor; IPCC, Intergovernmental Panel on Climate Change; CAS, Conventional Activated Sludge; ASP, Activated Sludge Process; MBBR, Moving Bed Biofilm Reactor; ANAMMOX, Anaerobic Ammonium Oxidation; WAS, Waste Activated Sludge; RAS, Return Activated Sludge; BOD_7, Biological Oxygen Demand at 7 days; COD, Chemical Oxygen Demand; TOC, Total Organic Carbon; TSS, Total Suspended Solids; VSS, Volatile Suspended Solids; pH, potential of Hydrogen; P_{tot}, Total Phosphorous; N_{tot}, Total Nitrogen; DHI, Danish Hydrological Institute; ISS, Inorganic Suspended Solids; VFA, Volatile Fatty Acid; OHO, Ordinary Heterotrophic Organisms; PAO, Phosphorous Accumulating Organisms; SS, Suspended Solids; COD_{filt}, Filtered COD; PI controller, Proportional-Integral controller; MLSS, Mixed Liquor Solids Concentration; SRT, Sludge Retention Time; PO, Orthophosphate; ALK, Alkalinity; NOB, Nitrite-Oxidizing Bacteria; DO, Dissolved Oxygen; IR, Internal Recirculation; WWTP, Waste Water Treatment Plant.

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1 Introduction

The environment is acknowledged as an essential factor that can be associated with almost every activity. Regarding this, wastewater treatment plants (WWTPs) which are provided for sanitary purposes impact the environment due to their energy consumption, chemical usage, greenhouse gas (GHG) emissions into the atmosphere, sludge production, and disposal etc. Specifically, GHG emissions in the form of nitrous oxide (N_2O), carbon dioxide (CO_2), and methane (CH_4) during different treatment processes immensely influence the environment and climate change. Therefore, it is of particular interest to analyze and identify the generation of GHGs within WWTPs. CH_4 and N_2O hold a global warming potential (GWP) of 28 and 265 times respectively, compared with CO_2 in a 100-year period (Massara et al., 2017; Solís et al., 2022). N_2O generation from WWTPs contributes to about 26% of the total GHG emissions from water and wastewater systems (Kampschreur et al., 2009; Massara et al., 2017). In this study, an investigation is performed to primarily analyze the N_2O emissions from a full-scale WWTP in Malmö, Sweden using process models to identify mitigation strategies.

The impact of climate change drives Swedish water and wastewater organizations to take great responsibility to achieve a net zero climate footprint by 2030 (Swedish Water, 2023). This degree project is framed by the project, Identification of operating strategies to minimize nitrous oxide emissions from activated sludge in wastewater treatment – case study Klagshamns WWTP, running from 2022 to 2023. The project is funded by Svenskt Vatten Utveckling and VA SYD (utility managing water and wastewater for several regions in Skåne). The average nitrous oxide emissions from WWTPs according to Intergovernmental Panel on Climate Change (IPCC) guidelines corresponds to approximately 1.6% of the incoming nitrogen. VA SYD has identified that Klagshamn WWTP has high nitrous oxide emissions - approximately 3% of the total incoming nitrogen. The aim of this project is to develop a dynamic process model that can describe the current operation and eventually evaluate operational scenarios to reduce N_2O emissions using the simulated model. Proposed strategies will be evaluated for implementation at the treatment plant after the completion of this study. The underlying goal is to reduce nitrous oxide emissions from wastewater treatment plants.

1.1 The need for computing the N_2O emissions from WWTPs

The sustainability of wastewater treatment plants in terms of carbon footprint (CF) is highly important for the environment. Awareness of N_2O emissions from WWTPs is substantially increasing among water authorities (Law et al., 2012). Nitrous oxide (N_2O), a GHG that is produced during the biological nitrogen removal (BNR) process, contributes a high share of the overall CF from WWTPs (Maktabifard et al., 2022). Considering the influence of N_2O emissions, it should be included as part of making the decisions for performance improvements. Hence, research has been performed over the past few years to identify the N_2O emissions activity to suggest mitigation strategies (Law et al., 2012; Vasilaki et al., 2019). Also, N_2O emissions indicate the environmental protection and sustainability of the WWTPs in the long run (Vasilaki et al., 2019; Mehrani et al., 2022).

1.2 Aim and objective

The purpose of this project is to perform a model-based analysis of N_2O emissions in the secondary treatment process at the Klagshamn WWTP Malmö, Sweden. The model results can be used to evaluate and identify mitigation strategies to reduce N_2O emissions.

Research questions include:

- Can the measured emissions be simulated well with the model with a limited set of pathways (i.e., Nitrifier denitrification and heterotrophic denitrification pathways) available in WEST simulation software?
- Can the developed dynamic model be used to evaluate the strategies to mitigate N_2O emissions from the secondary treatment process?
- What would be the limitations and uncertainties of the proposed strategies?
- Do the proposed strategies influence the treatment process and efficiency?

1.3 Limitations of Study

Considering the scope of the thesis, the following limitations are made:

- A model with only two N_2O pathways is chosen to perform the model studies, as the used simulation software has a limited set of pathways for N_2O production from the biological treatment process.
- Due to the scope of the project, the model is limited for not modelling the post-denitrification, post-precipitation, and sludge treatment processes of the treatment plant.
- The developed model is focused only on N_2O emissions from the secondary treatment process and other elements like secondary clarifier is not considered for capturing the N_2O emissions in the process.

2 Literature review

2.1 Mechanism and operating parameters for N_2O production

To compute N_2O emissions from WWTPs, it is crucial to investigate its generation mechanism and triggering operational conditions. About 90% of N_2O is produced in the biological steps of the secondary treatment process through nitrification and denitrification processes (Campos et al., 2016). The conversion of nitrogen to gaseous form involves different bacterial populations and process conditions, leading to different emission levels. There are three major microbial pathways attributed to N_2O production:

- NH_2OH oxidation pathway, where Ammonia-oxidizing bacteria (AOB) oxidizes ammonia (NH_3) to nitrite (NO_2^-) through hydroxylamine (NH_2OH) by firstly oxidizing NH_3 to NH_2OH and then to NO_2^-. N_2O is formed as a by-product due to the insufficient oxidation of NH_2OH to NO_2^-, which is termed as the NH_2OH oxidation pathway.
- Nitrifier or ammonia-oxidizing bacteria (AOB) denitrification pathway, in which, NO_2^- and NO reduction to N_2O as a final product is carried out during the AOB denitrification process, typically referred to as nitrifier or AOB denitrification pathway.
- Heterotrophic denitrification pathway, where NO_2^- and/or NO_3^- formed from autotrophic nitrification is converted to Nitrogen gas (N_2) by heterotrophic denitrification during which N_2O is formed as an intermediate (Law et al., 2012; Ni & Yuan, 2015).

N_2O production is associated with two steps ie., autotrophic nitrification and heterotrophic denitrification. As shown in Figure 2.1, N_2O is produced from the intermediates of the oxidation of hydroxylamine related to the imbalance activity of AOB. NH_4^+ oxidation to NO_2^- occurs in two steps and in the first step ie., the hydroxylamine pathway, the unstable conversion of NH_2OH to NO_2^- produces N_2O. In the second step as nitrifier denitrification, AOB reduces NO_2^- to NO by forming N_2O as the end product with ammonium as an electron donor. Under denitrifying conditions in the process, the reduction of NO_3^- to N_2 takes place in four steps as shown in Figure 2.1. Coupled with the oxidation of organic substrates, NO_3^- is first converted to NO_2^- and then to NO. The reduction of NO to N_2 forms N_2O as an intermediate product.

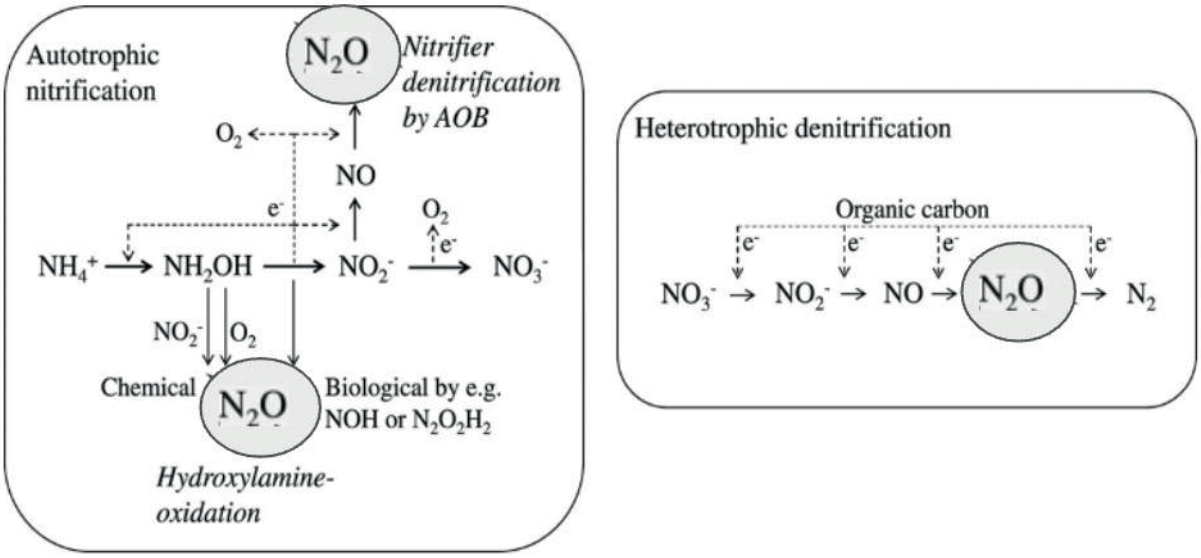


Figure 2.1. Schematic representation of relevant N_2O production pathways in the wastewater treatment process. The left figure represents the autotrophic nitrification and denitrification pathway, and the right figure represents the heterotrophic denitrification pathway.

The specific conditions determine the dominant pathways for N_2O production. Many factors are linked that affect the nitrification and denitrification processes thus impacting N_2O production. These include bioreactor configuration, nitrogen loading rate (NLR), BNR process (advanced or conventional), pH, carbon source, temperature, seasonal variations, etc (Massara et al., 2018; Vasilaki et al., 2019; Law et al., 2012). The factors that majorly contribute to N_2O production from the nitrification step are insufficient dissolved oxygen (DO) levels, high nitrite (NO_2^-) concentration in nitrification and denitrification along with less chemical oxygen demand (COD) to nitrogen ratio (COD/N) at denitrification (Massara et al., 2018).

2.2 Modelling approaches for N_2O emissions

Computer modelling is an appealing approach to achieving knowledge of the operating mechanisms of WWTPs. Modelling and simulation of the treatment process involve several assumptions, precautions, and limitations. More details of the literature review and different modelling approaches for analyzing the N_2O emissions from previous studies are discussed briefly in this section.

Model studies are useful to estimate N_2O emissions from WWTPs, specifically, mechanistic models are powerful tools for investigating the dominant emission pathways (Sun et al., 2017; Maktabifard et al., 2022). Activated Sludge Models (ASMs) (Henze, 2006) developed by the International Water Association (IWA) task group (Henze, 2006) are popularly used mechanistic models for describing the BNR processes in the WWTPs (Massara et al., 2017; 2018; Mehrani et al., 2022). Various extensions have been made to these models to determine N_2O production. There are many successful studies with the application of mechanistic models for N_2O predictions (Massara et al., 2018; Su et al., 2019; Zaborowska et al., 2019). However, there are still various challenges and limitations due to its sensitivity to variations in the process and operating conditions, over-parameterization, and

comprehensive efforts for calibration and validation (Hwangbo et al., 2021; Mehrani et al., 2022).

Several studies have highlighted N_2O models to describe the dominant pathways for N_2O production during nitrification and denitrification processes. Models of N_2O production by AOB are of two categories, single pathway (either AOB denitrification or hydroxylamine oxidation) and two pathway models integrating both AOB pathways (B.-J. Ni et al., 2013; Pocquet et al., 2016). Mampaey et al. (2013) developed a single pathway model for ammonium oxidation of AOB as a one-step process (ammonia to nitrate). Models are extended to include the heterotrophic denitrification pathway incorporating four-step denitrification (Hiatt & Grady, 2008) along with the AOB pathways (B. J. Ni et al., 2013; Peng et al., 2014; Duan et al., 2020; Domingo-Félez & Smets, 2020; Massara et al., 2018). Most findings according to the literature reviews of all the above mentioned are, the NH_2OH oxidation pathway is dominant for N_2O production when subjected to too low/high NO_2^- concentration along with high levels (>2.5 mg/l) of DO; Nitrifier denitrification pathway is dominated at low DO levels (approx. 1 mg/l) and with moderate NO_2^- accumulation; Ammonium (NH_4^+) accumulation during aeration leads to an increment in the production of by-products like NH_2OH; Higher external carbon source i.e., COD/N ratio (>1) availability increases the N_2O reduction rates; Controlled pH around 7 and with an approximate temperature of 20°C conditions ensure the safe completion of nitrification and consumption of N_2O through denitrification. The inclusion of all pathways resulted in complex models with over parameterized for calibration and validation. A single pathway model for N_2O production by AOB simplified the structure with few parameters and is convenient for calibration (Maktabifard et al., 2022).

To get deeper insight, B. J. Ni & Yuan. (2015) considered all three pathways for a full-scale study where production from the AOB denitrification pathway decreased and increased production from NH_2OH pathways occurred with the increased DO. Blomberg et al. (2018) extended the ASM3 N_2O model and included N_2O stripping to investigate full-scale emission predictions. Zaborowska et al. (2019) analyzed the full-scale study of the combined N-P activated sludge system by extending ASM 2d with all N_2O pathways and N_2O liquid-gas transfers, where heterotrophic denitrification is identified to be the predominant pathway. Maktabifard et al. (2022) experimented with the confirmation of the applicability of an existing N_2O model to another full-scale WWTP and identified heterotrophic denitrification as the main N_2O production pathway.

2.3 N_2O emission factor

Emission factor (EF) quantification is essential to assess the environmental impacts and to reduce them. N_2O emission factor is generally represented as the ratio between emitted N_2O-N (Kg-N d^{-1}) and influent N-load (Kg-N d^{-1}), some cases use nitrogen removal amount with nitrification and denitrification instead of influent nitrogen load (Law et al., 2012). The theoretical calculation methods of N_2O emissions rely on country specific EFs which underestimate the actual emissions (Ye et al., n.d.). Intergovernmental Panel on Climate Change (IPCC) Guidelines recommended an EF of 0.016 kg N_2O-N/kg N load in 2019 (Ye et al., n.d.). EFs are influenced by various factors like process configuration, operational and environmental conditions, monitoring campaigns etc (Vasilaki et al., 2019; Vasilaki et al., 2020). Long-term data over 1-year monitoring campaign is needed to assess the process-based N_2O EFs in WWTPs. A review of the literature study overviewed a range of (0.01 – 2 % of the N-load) and

in some cases >10%. Vasilaki et al. (2019) demonstrated the impact of the duration of a monitoring campaign over a range of 0.3% of N-load for a less than 1-month campaign to 1.7% of N-load for 1 year campaign period. The study also overviewed the seasonal variation impacts of EFs and Zhu et al. (2019) identified higher EF in winter (5.9%) than in the summer periods (2.9%). Conventional activated sludge (CAS) systems with aerobic reactors attributed to an average EF of 0.27% of N-load (Chen et al., 2016). The N_2O EF reported by Massara et al. (2018) is 10% of the removed NH_4-N.

3 Wastewater treatment plant description

3.1 Process configuration

Klagshamn treatment plant is located in the south of Malmö, and it is operated by VA SYD. The sewage network of Malmö is distributed into seven areas of which, two areas are connected to the Klagshamn treatment plant and the remaining to the Sjölunda treatment plant. The Klagshamn treatment plant process is split into two parallel lines. The configuration and the process operations of the treatment plant are described in detail in the following paragraphs.

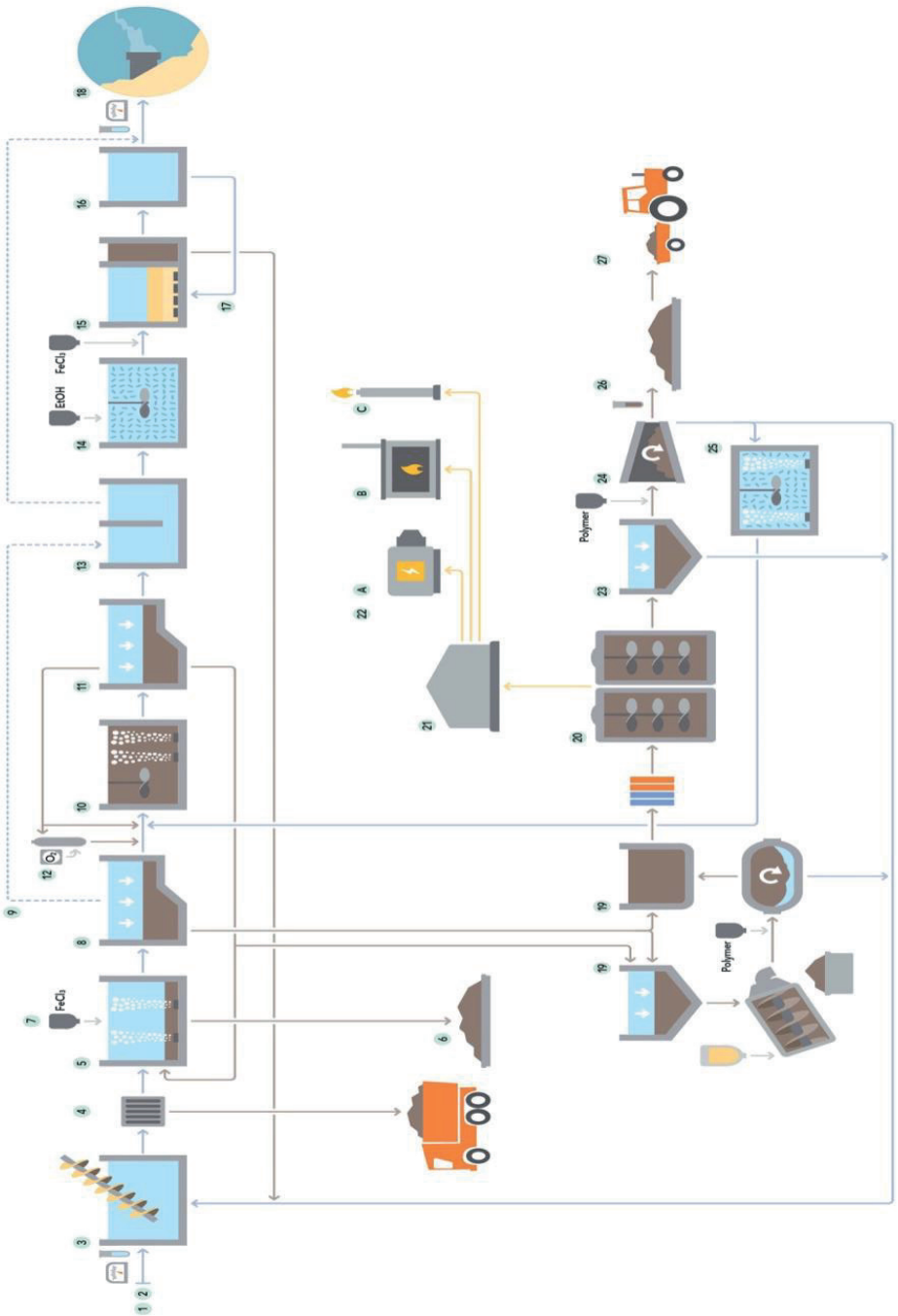


Figure 3.1. Graphical representation of the processes at the Klagshamn treatment plant. Numbers are related to the description of the process (*VA SYD)*

The inlet pumping station (3) in Figure 3.1 consists of 3 speed-controlled screw pumps. Normal inflow is handled with one pump and three pumps are used when the inflow is at maximum load or in the event of breakdown. Wastewater is passed through screens (4 in Figure 3.1) where particles larger than 3mm size are removed. The separation particles are transported for incineration after undergoing washing and dewatering. Aerated grit (5) removes sand and heavier particles and is pumped to sand deposits (6) after dewatering and the lighter particles follow the wastewater. Dosing of iron chloride (7) occurs at the inlet of the aerated grit for the pre-precipitation of dissolved phosphorous and organic matter. Separation of chemical flocs along with primary sludge takes place in the 4 parallel pre-sedimentation basins (8) and the sludge is pumped to the sludge treatment process. During heavy flow conditions that exceed the treatment capacity, primary clarification flow is diverted (9) to a sump (13) past the biological treatment to prevent the washout of microorganisms.

The activated sludge process (10) is a biological stage with high amounts of microorganisms to break down the organic matter and for the nitrification process which converts ammonium into nitrate under aerobic (oxygen) conditions. The process is divided into 8 separate zones in each of the 2 parallel processing lines and zone 8 is divided into two small zones. All the zones can be run either aerobically or anoxically and the air flow is regulated based on dissolved oxygen setpoint. A portion of the separated activated sludge from the secondary clarification (11) is returned to the activated sludge process as return sludge and the remaining portion which is waste sludge is led to the primary clarifiers and then it is taken out for sludge treatment as sludge from the primary clarifier. Ozone plant (12) treats the return sludge before it is sent back to the process due to the prevailing conditions at the plant for the growth of filamentous bacteria which deteriorates the sedimentation properties. Treated water from activated sludge and bypass water from primary clarifiers are mixed in the sump (13) and then pumped to the post-denitrification and filtration.

Post-denitrification of the wastewater is performed in MBBR (Moving Bed Biofilm Reactor) basins (14) loaded with plastic materials with constant motion and acts as carriers for the biofilm to grow. The biofilm-containing bacteria are used to convert the formed nitrate in the activated sludge process into nitrogen gas to release to the atmosphere using ethanol as an external carbon source of energy which is added at the inlet of each line. The final stage of the treatment process is filtration (15). 5 filters which are designed as two-media filters containing sand and anthracite are used for filtration. Iron chloride as a precipitation chemical can be dosed to the process if there is insufficient phosphorous removal from the pre-precipitation process. The collected filtered water (16) is used to wash the filters (17) periodically and the washed water is led back to the plant inlet as backwash and the remaining filtered water is led to the plant outlet (18). Samples are collected and flow is measured at the outlet of the plant for analysis before releasing into the sea (Öresund).

Separated raw sludge from primary clarifiers and secondary clarifiers is treated by gravity thickeners (19) where water content is removed with the addition of polymer. Anaerobic digesters (20) are fed with the thickened sludge to break down parts of the organic matter under anaerobic conditions at 37°C temperature. Produced biogas, consisting of mainly methane and carbon dioxide is collected and stored in gas holders (21). The centrifuges (24) are used for dewatering the stored digested sludge (23) with the addition of polymer for efficient separation. Reject water from the dewatering process with high levels of ammonium is treated separately

in an Anaerobic ammonium Oxidation (ANAMMOX) process reactor (25) using moving carriers to grow microorganisms by aeration and the treated water is led back to the activated sludge process. Reject water is sent to either inlet of the plant or to the first aerated zone of the activated sludge system in line 1. This is controlled according to the height of the flow in the stored tank and the treated reject water from anammox reactors is passed into the first aerated zone and untreated water goes back to the inlet to mix with the incoming water. The dewatered sludge is stored on concrete slabs (26) temporarily and is later used in different ways like fertilizer.

Table 3.1. Plant dimensions data of Klagshamn treatment plant (VA SYD)

Units	Number	Total Volume (m^3)	Total Area (m^3)
Primary treatment			
Grit removal basin	2	200	-
Primary clarifier	4	550	250
Secondary treatment			
Activated sludge basin	2	2200	-
Secondary clarifier	8	612	170
Tertiary treatment			
MBBR	4	275	-
Sand filter	5	-	44
Sludge treatment			
Thickener	2	133	493
Anaerobic digester	2	1750	-
Centrifuge	-	-	-

3.2 Full-scale data availability

This section details the collection of the available full-scale measurement data at the Klagshamn treatment plant.

Flow measurement samplings are available before and after each purification step in the primary and secondary treatment process for the periods of 2022-01-01 to 2023-01-31. Lab sampling on a regular basis, as well as continuous online measurements (for some pollutants), are available. Flow proportional daily, monthly, and random samples are carried out at various sites in the WWTP. The sampling locations and the measured pollutants are shown in Figure

3.2 and listed in Table 3.2 and the available data at each sampling location are listed in Table 3.2. (I).

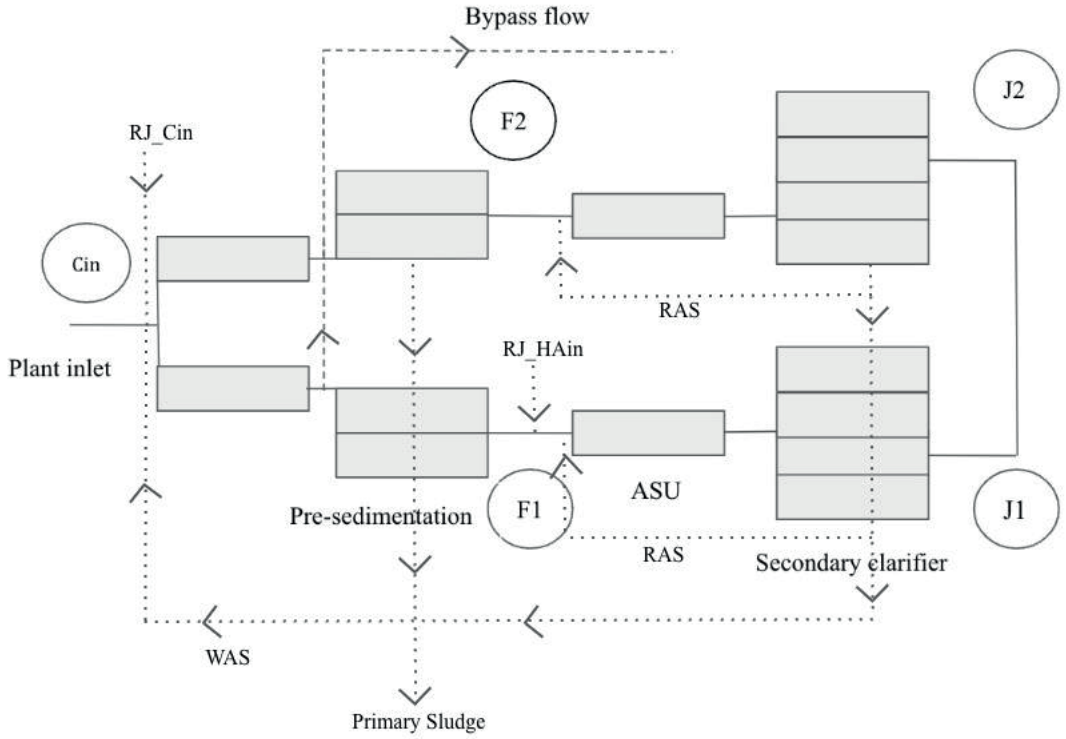


Figure 3.2. Sampling locations for wastewater flow and pollutants measurements at the Klagshamn treatment plant.

Incoming water to the treatment plant is sampled online and calculated at the screwed pumps. For the modelling study, wastewater at the location (C_{in}, as shown in Figure 3.2) is considered as the first sampling point with lab measurements collected after the inlet screw pumps which also includes reject water (RJ_Cin). As shown in Figure 3.2, outflow from primary clarifiers in line 1 (F1) and line 2 (F2) is the second sampling point with online flow measurements and lab samples for pollutant concentrations that are coming out from the primary clarifiers for the biological secondary treatment process. From the pre-sedimentation underflow, sludge flowrate and TSS concentrations are sampled. Outflow from post sedimentation in line 1 (J1) and line 2 (J2) is the third sampling point where all the measurements are of lab samples except flow measurements which are online samples and solids measurements include both lab and online. Return sludge from post-sedimentation is measured online for solids and flow rates. The remaining portion of flow as waste sludge is measured online for flow rate and lab measurements for various pollutant concentrations. The bypass flow measuring sampling point is before the secondary treatment process with online flow rates and lab measurements for the pollutants. The flows from the two bypass pumps are combined and the flows less than 50 m^3/h are removed from the measured data. In the activated sludge unit, the first zone is sampled with online concentrations and the last zone has lab measurements for solids. Reject water samples are collected at the incoming water (RJ_C_{in}) and at the first zone of the activated sludge unit (RJ_HA_{in}).

Table 3.2. Description of the sampling points in the wastewater treatment process at the Klagshamn treatment plant.

Name of the location	Description of the location
C_{in}	Incoming water after passing screw pumps
F1 & F2	Ougoing water from pre-sedimentation in line 1 and 2
J1 & J2	Outgoing water from post-sedimentation in line 1 and 2
RJ_C_{in}	Untreated reject water mixing with the incoming water
RJ_HA_{in}	Treated reject water from anammox reactors going to the first aerated zone of activated sludge system in line1
WAS	Waste activated sludge flow
RAS	Return activated sludge flow

Table 3.2.1. Locations of the sampling points and measured variables at the sampling points

Location	Data availability
Incoming water (C_{in})	Flowrate, N_{tot}, P_{tot}, $NH4^{+}$-N, PO_4^{3-}P, BOD_7, COD, TOC, TSS, pH
Outflow from pre-sedimentation (F1 & F2)	Flowrate, N_{tot}, P_{tot}, $NH4^{+}$-N, NO_2^{-}N, NOx-N, PO_4^{3-}P, BOD_7, COD, TSS
Outflow from post-sedimentation (J1 & J2)	Flowrate, N_{tot}, P_{tot}, $NH4^{+}$-N, NO_2^{-}N, Nox-N, PO_4^{3-}P, BOD_7, COD, TSS
Activated sludge unit	$NH4^{+}$-N, PO_4^{3-}P, TSS, VSS, pH, Temperature, air flowrate, SRT, N_2O
WAS	Flowrate, TSS, VSS, Nox-N
RAS	Flowrate and TSS
Effluent water	Flowrate, N_{tot}, P_{tot}, $NH4^{+}$-N, NO_2^{-}N, Nox-N, PO_4^{3-}P, BOD_7, COD, TSS, TOC, pH
Backwash	Flowrate, BOD_7, COD, P_{tot}, Nox-N, TSS, N_{tot}

Bypass	Flowrate, N_{tot}, P_{tot}, $NH4^{+}$-N, Nox-N, PO_4^{3-}P, BOD_7, COD, TSS
Anammox	Flowrate, P_{tot}, $NH4^{+}$-N, NO_2^{-}N, Nox-N, BOD_7, COD, TSS
Primary sludge	Flowrate, TSS
Rejectflow	Flowrate, reject water tank height

Every alternative zone (ie., Zone 2, 4, 6, and 8) in both lines is equipped with an oxygen meter and floating hood for N_2O measurements, and the final zone is also provided with an ammonium meter. Regulation of oxygen content of the zones is based on the ammonium set value in the final zone and airflow rate data is available for all the zones. Each floating hood covers a dimension of $1m^3$ of the basin surface (See Figure 3.2.1). Zone 2, 4, 6, and 8 in line 1 and line 2 are selected to arrange the floating hoods for the period from 2022-07-22 to 2023-01-31. The exhaust air is collected and a small flow of it is transported to the measuring unit via a hose to pass through a pre-humidifier which cools and filters the air for N_2O measurement.

Figure 3.2.1. Arrangement of floating hood in the activated sludge unit for measuring N_2O emissions at the Klagshamn wastewater treatment plant (Picture taken by me during the plant visit to Klagshamn WWTP).

3.3 Effluent requirements

The WWTP has effluent demands for biological oxygen demand (BOD_7) at 7 days, Total Phosphorous (Ptot), and Total Nitrogen (Ntot), and the values are mentioned in Table 3.3. Emission conditions are changed in 2018 regarding the total nitrogen from 12-10 mg/l.

Table 3.3. Effluent requirements for Klagshamn treatment plant (*VA SYD)*

Parameter	Effluent monthly average (mg/l)	Effluent yearly average (mg/l)
BOD_7	10	10
Total Phosphorous	0.3	0.3
Total Nitrogen	-	10

4 Methodology

4.1 Modelling of N_2O emissions in WEST

Modelling offers to replicate the wastewater treatment plants as a reliable representation of real-world systems (DHI). Several varieties of models have been developed according to the plant-specific process configurations. This made it easier to develop a perfect model of the treatment plant. In the following sections, the process models that are used for the present study are described briefly.

4.1.1 WEST software

WEST simulation software is developed by Danish Hydrological Institute (DHI) which enables organizers, consultants, and engineers to optimize the wastewater treatment processes (WEST Getting Started Report, 2022). Commercial software WEST, which acts as a user-friendly platform for simulating wastewater treatment plants is used for this project. The reactions and equations of the processes are all pre-programmed in the software. The graphical setup of the plant layout can be constructed for executing steady-state and dynamic simulations. Special tools (i.e., Advanced virtual experiments) like parameter estimation, scenario analysis, and sensitivity analysis can be used to upgrade the project. WEST is developed based on the popular ASM models by (Henze, 2006). Different activated sludge models have been built like ASM1, ASM2, ASM2d, ASM3, and ASMG each of which has a specific use and can be used according to the purpose of the project (Henze, 2006). These different models describe different biological processes as some models consider nitrification and denitrification as a single step which indicates that, nitrite is not considered as a state variable, and other models determine the process in detail by considering the intermediate steps. Out of the available models in the WEST, the ASM2dISS model is chosen to be ideal for modelling in this project. The description of the ASM2dISS is in the following section.

4.1.2 ASM2dISS

ASM2dISS model is an extension of the ASM2d model which accounts for carbon removal, nitrification, denitrification, and phosphorous removal, with a balance of volatile suspended solids (VSS) and inorganic suspended solids (ISS).

4.1.2.1 State variables

The biological components of the model are listed in Table 4.1.2.1. The components of the model are separated into two large groups ie., soluble and particulate organic matter. These incoming organic fractions are further divided into biologically available matter which is available as a substrate for microorganisms and biologically inert matter. In this model, the biologically available matter of dissolved or particulate is defined as readily biodegradable (S_F and S_VFA) and slowly biodegradable (XC_B). The inert particulate and dissolved organic matter (S_U and X_U) are not degradable and are passed through the process to the effluent without any change. The microorganisms are expressed in terms of three groups of biomasses i.e., nitrifying autotrophs (X_AOB), ordinary heterotrophs (X_OHO), and phosphate-accumulating organisms (X_PAO). The nitrifying organisms are assumed that the ammonium S_NHx is oxidized to (nitrite and) nitrate expressed as S_NOx. Nitrogen S_N2 is assumed as the only outcome of denitrification by heterotrophic organisms.

Table 4.1.2.1. Biological components of the ASM2dISS model (WEST Model Guide, 2023)

Name	Description of the components	Units
S_F	Fermentable organic matter	g COD/m^3
S_VFA	Fermentation products (as acetate)	g COD/m^3
S_O	Dissolved oxygen	g DOm^3
S_NHx	Ammonium + ammonia nitrogen	g N/m^3
S_NOx	Nitrate + nitrite nitrogen	g N/m^3
S_N2	Dissolved nitrogen gas	g N/m^3
S_PO	Soluble inorganic phosphorous	g P/m^3
X_U	Particulate undegradable organics	g COD/m^3
XC_B	Slowly biodegradable substrates	g COD/m^3
X_U_Ig	Particulate undegradable inorganics	g COD/m^3
S_U_Ig	Soluble undegradable inorganics	g COD/m^3
S_Alk	Alkalinity	mol/m^3
X_AOB	Autotrophic nitrifying organisms	g COD/m^3
X_OHO	Ordinary heterotrophic organisms	g COD/m^3
X_PAO	Phosphorous accumulating organisms	g COD/m^3
X_MEOH	Metal-hydroxides	g TSS/m^3
X_MEP	Metal-phosphates	g TSS/m^3
X_PAO_PP	Stored polyphosphate in PAOs	g P/m^3

4.1.2.2 Dynamic process

Various biological processes involved in the treatment process of the ASM2dISS model are explained in this section to understand the events happening within the model. Four processes were considered: growth of biomass, decay of biomass, ammonification of soluble organic nitrogen, and hydrolysis of organics.

- Growth of biomass: Autotrophic biomass growth is associated with the soluble ammonia nitrogen and oxygen acting as energy sources for the growth which results in producing nitrate. Heterotrophic growth occurs under aerobic and anoxic conditions.

The readily biodegradable substrate is used for the growth of heterotrophic biomass by utilizing oxygen for aerobic growth. Anoxic growth with nitrate nitrogen as an electron acceptor in proportion with readily biodegradable substrates results in nitrogen gas production. Monod kinetics are used for modelling autotrophic and heterotrophic aerobic growths. The anoxic growth rate for heterotrophic adds an empirical coefficient to the Monod kinetics.

- Decay of biomass: The modelling approach for the decay of autotrophic and heterotrophic biomass is on the basis of the death-regression concept (Henze, 2006) Decaying involves the conversion of biomass to the combination of particulate and slowly biodegradable substrate without any electron acceptor.
- Ammonification of soluble nitrogen: The conversion of soluble organic nitrogen to ammonia nitrogen is a simple first-order empirical equation but it is adequate for modelling the entrapped organic nitrogen where the conversion is coupled with the hydrolysis process rate.
- Hydrolysis of organics: Under aerobic and anoxic conditions, the hydrolysis rate of heterotrophic biomass to convert slowly biodegradable substrates to readily biodegradable substrates is a first-order reaction. The hydrolysis rate of the accumulated organic nitrogen is proportional to the hydrolysis of the slowly biodegradable substrate.

In the ASM2dISS model, autotrophic nitrifying organisms are assumed to oxidize ammonium (S_NHx) to (nitrite and) nitrate which are described as the variable S_NOx. Here hydroxylamine pathway which is an intermediate reaction during the ammonium oxidation is not included. Dinitrogen S_N2 is considered to be produced as a product of the denitrification process by heterotrophic organisms. Heterotrophic denitrification occurs in four steps, ie., Nitrate (NO_3) from nitrification is firstly converted to NO_2 and the formed NO_2 is transformed into NO, and in the next step, it is produced as N_2O and as the final step the produced N_2O is converted as N_2. When denitrification is incomplete and N_2 is not completely converted to N_2, N_2O accumulation takes place which increases the N_2O emissions from the process.

As the hydroxylamine pathway is not included in the model for N_2O emissions, only one AOB pathway ie., nitrifier denitrification pathway by AOB and heterotrophic denitrification pathways are available in the ASM2dISS model for modelling N_2O emissions.

4.1.3 Sedimentation

4.1.3.1 Primary clarifier

The point settler model is a simplified version of the actual process developed for primary sedimentation. The settling tank doesn't have a volume and it acts as a perfect phase separator. The model acts as a completely mixed reactor, and it is based on the mass balance over the settling tank for soluble and particulate materials (WEST model guide) and flow balance (see equation 1). The parameters of the model are shown in Table 4.1.3.1 below.

Flow balance equation:

$$Q_{out} = Q_{in} - Q_{under} \quad (1)$$

Where: Q_{in}, Q_{out}, Q_{under} denotes the influent, effluent, and desired underflow rates (m^3/d) respectively.

Table 4.1.3.1: Model Parameters of the point settler model (WEST Model Guide, 2023)

Name	Description	Value	Units
F_TSS_COD	TSS/COD ratio	0.75	--
f_ns	Fraction of non-settleable solids	0.6	--
F_Energy_FlowRate	Conversion factor Energy needed/Pump flow rate	0.04	--

4.1.3.2 Secondary clarifier

The Takács model is developed based on the Vitasovic model (WEST model guide, DHI). The settling tank is modelled consisting of a number of layers and describes the mass solids balances between the layers. A few assumptions made for the model are,

- The incoming solids are homogeneously distributed over the feed layer and the flow is vertical.
- The settling velocity is a non-linear function of the overflow rate.

Above the feed layer, the flux is upwards which results in the overflow rate and below the feed layer, the flux is downwards, therefore, it results in underflow rate. The parameters of the model are shown in Table 4.1.3.2.

Table 4.1.3.2. Model Parameters of the Takács Model (WEST Model Guide, DHI, 2023)

Name	Description	Value	Units
F_TSS_COD	TSS/COD ratio	0.75	--
A	Surface area of the clarifier	1500	m^2
H	Height of the clarifier	4	m
X_T	Threshold suspended solids concentration	3 000	g/m^3
X_Lim	Minimal concentration in sludge blanket	900	g/m^3
r_H	Hinderred settling parameter	0.000576	m^3/g
r_P	Low concentration settling parameter	0.00286	m^3/g
V0	Maximum threshold settling velocity	474	m/d
V00	Maximum practical settling velocity	250	m/d
f_ns	Fraction of non-settleable solids	0.00228	--

F_Energy_FlowRate	Conversion factor Energy needed/Pump flow rate	0.04	--

4.2 Data analysis and pre-processing

4.2.1 Incoming water

To understand the quantity of organic matter and nutrients entering the treatment plant, the incoming wastewater flow rate is examined. Firstly, C_{in} is analyzed which includes the backwash flow from the filters in the final stage of the treatment process, therefore it is not included in pre-processing the data for the model and instead, C_{in} flow measurements are calculated using flow balances. Also that the incoming flow is available as a calculated value in the measurement values and when analyzed with the effluent flow rate, outflow from both lines of pre-sedimentation basins, and backwash flow rates, it has shown a difference in the flow measurements. Therefore, influent flow from the data is not used for modelling and instead, the flow rate at C_{in} is calculated using a flow balance with effluent, backwash, and outflow from pre-sedimentation flow rates. The flow balance for Q_{Cin} is calculated according to the following equation 2.

$$Q_{Cin} = Q_{eff} - Q_{bw} - Q_{pc\_sludge} \quad (2)$$

Where, Q_{in} is the incoming wastewater flowrate, Q_{eff} is the effluent wastewater flowrate, Q_{bw} is the combined backwash flow rate from the filters in the last stage of the purification step in both lines, Q_{pc_sludge} is the total underflow sludge flowrate from the pre-sedimentation basin in both lines.

For characterizing the incoming wastewater, variables such as COD, TSS, PO_4^{3-}P, NH_4^+-N, TP, and TN are analyzed from the measurement data to understand how the concentrations are changed with the treatment steps. Pre-processing the data is done in MATLAB software by analyzing the data to remove unnecessary measurements for the model. Missing data are analysed, and gaps are filled with the ratios between the concentrations like total nitrogen to COD (TN/COD), suspended solids to COD (SS/COD), filtered COD to total COD (COD_{fil}/COD), etc. During the analysis, the calculated ratios for different constituents of the incoming water are compared with the maximum and minimum values from a previous study by (*Riger 2013*, n.d.)Rieger et al. (2013). Filling the missing data are explained in more detail in section 4.2.2 below.

4.2.2 Methods and data analysis for simulation

For simulating in WEST, the available daily values are used to calculate the mean values of each month for performing the initial simulations. While analyzing the data for simulation, there have been observed missing data in the measurements which need to be filled to avoid gaps in the predictions. This has been done using the existing data, by estimating the ratios of the available measurement values to fill the missing data with the nearest values. Outliers are also available in the measured data which need to be adjusted as they would affect the simulation process. This has been done by setting percentiles based on the visual inspection of the data. Firstly, COD values are predicted by doing linear regression for total nitrogen and COD to fill the missing COD values and using the predicted COD values other concentration values like COD_{fil}, BOD_7, NH_4^+-N, TP, and TSS are filled. As the data of RAS flow rates are available

with a combined flow rate for RAS and WAS flow rates, data for simulating RAS and WAS flows are also calculated according to equation 3, using sludge flow from the post-sedimentation basin and WAS flow rates.

$$Q_{RAS} = Q_{sc\_sludge} - Q_{was} \quad (3)$$

The amount of wastewater divided between the two lines is calculated based on the flow balance using outflow from the post-sedimentation basin, primary sludge flow, flow diverted as bypass, and waste sludge flow rate. For each line, the balancing is performed which is why half of the primary sludge is considered in the balancing equation 4 as the sludge flow is divided equally to both lines. The mass balance for one of the lines which is the same for another line with respective flow measurements is expressed in Equation 4,

$$Q_{pc} = Q_{sc\_out} + Q_{pc\_sludge} * 0.5 + Q_{bypass} + Q_{was} \quad (4)$$

Where, Q_{pc} is the divided flow rate to the respective lines, Q_{sc_out} is the outflow from the post-sedimentation, Q_{pc_sludge} is the sludge underflow from pre-sedimentation, Q_{bypass} is the bypass flowrate and Q_{was} is the waste activated sludge flow rate.

$FeCl_3$ dosing at the inlet of the aerated sand trap is proportional to the phosphate load and the two phosphate meters present at the inlet and outlet of pre-sedimentation control the dosing. The obtained measured data is the sum of pre & post-precipitation dosage in which post-precipitation dosage is of a small portion. With the given $FeCl_3$ measurements, the dosage is calculated by Equation 5,

$$Q_{FeCl3} = (Q_{in} * C_{FeCl3})/C_{dose} \quad (5)$$

Where, Q_{FeCl3}: The dosed amount of ferric chloride (m^3/d), Q_{in}: Incoming flowrate of wastewater (m^3/d), C_{FeCl3}: Concentration of $FeCl_3$ after mixing with wastewater ($gFeCl_3/m^3$), C_{dose}: Concentration of the solution added (g/m^3)

The range for measurement of N_2O is 0-1000 ppm at 5°C of constant temperature. N_2O emissions are determined in terms of emission factor using equation 6. The N_2O emission factor (EF) in this study is described as the ratio of the total production of N_2O (kg N_2O) to the influent total nitrogen load (kg TN) to the plant.

Emission factor (EF) for N_2O,

$$EF\ (\%) = \frac{N2O\ load\ \left(\frac{kgN}{d}\right)}{Influent\ N\ load\ \left(\frac{kgN}{d}\right)} * 100 \quad (6)$$

Concentrations are also analysed for the collected data, for example, ammonium concentration is observed to be similar in the influent and outflow from the pre-sedimentation basins, which would usually be the case that ammonium removal does not happen at this treatment step. Periods for the model simulations for calibration and validation are selected based on the basis that there should not be heavy or extreme events. For selecting the periods for calibration and validation, the availability of the N_2O measurements is also considered. This has been discussed in detail in section 4.4.

4.3 WEST Model Construction

In the WEST block library, a municipal wastewater unit is used for developing incoming water to the model. Characterization of influent water flow is used from the data analysis and is loaded into the municipal water unit as an input file. Figure 4.3 shows the layout of the constructed model. The incoming water is divided into 2 parallel lines using a percentage of flow divider. The divided lines are provided with the precipitation dosage of $FeCl_3$. For the primary treatment process, an activated sludge unit is used to replicate the aerated sand trap for modelling the precipitation reactions. Each line uses 1 pre-sedimentation basin which includes the combined volume of 2 pre-sedimentation basins in each line at the treatment plant. The biological secondary treatment process is modelled using nine series (Zone 8 is divided as Zone 8a and 8b) of activated sludge units in each line which are completely mixed reactors with the real dimensions. The four actual basins for the post-sedimentation at the treatment plants are demonstrated as one combined volume post-sedimentation basin for each line. Some fraction of flow from the secondary clarifiers from both lines is returned to the activated sludge unit as RAS and the remaining fraction i.e., WAS is transferred back to the incoming water before splitting the flow to 2 lines. Splitting the fractions of RAS and WAS is done using a flow splitter. The bypass from each line before secondary treatment is taken with a flow splitter unit. Input is added to the incoming water as reject water (RJ_C_{in}) and to the first zone of activated sludge in line 1 (RJ_HA1, see Figure 4.3).

Oxygen contents in the activated sludge reactor units in zone 2, 4, 6, and 8b are controlled using PI controllers in both lines. Zone n and zone n-1 are controlled using a set value in zone n. A process calculator is used for calculating the SRT (Solids retention time) values in the process.

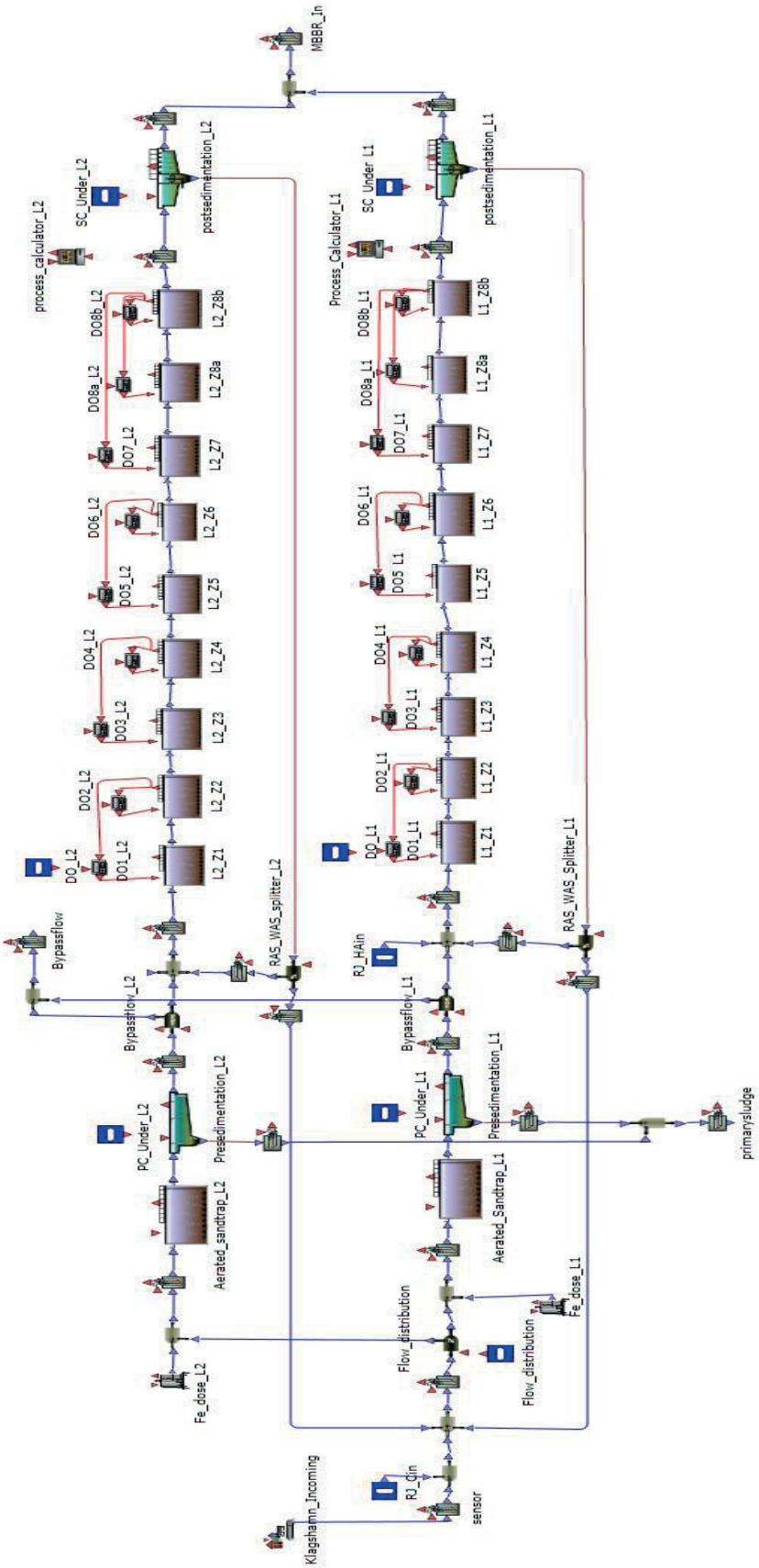


Figure 4.3. Model construction layout of the Klagshamn treatment plant process in the WEST for the primary and secondary treatment processes.

4.4 Calibration and validation

For calibrating the model for N_2O emissions, firstly solids in the treatment process need to be calibrated to match the measured data. For this purpose, sludge content in the activated sludge unit reactors, sludge contents of excess sludge, and return activated sludge along with solids coming out from pre- and post-sedimentation clarifiers are required. These sludge content measurement data can also be used to calibrate the right sludge age of the model. The data of solids content in the treatment process include both online and lab measurements. Solids from pre- and post-sedimentation data are available from online and lab measurements. Mixed liquor solid concentration (MLSS) in the activated sludge and solids in the RAS measurements are from online but measurement for solids content of WAS is from the lab. To calibrate the nitrification in the treatment process, measurements for nitrogen are required. Measurements for nutrient concentrations are available as described earlier in Table 3.2. (I). It is needed to collect data for calibrating the N_2O emissions from the floating hoods arranged in every second alternative of the ASU reactor zones.

4.4.1 Calibration

WEST provides an option to perform steady-state simulations and dynamic simulations. The developed model is imported with dynamic input data, WEST first performs the steady-state simulation by automatically calculating the weighted average values. Then the constant average values of all the parameters are simulated for 100 to 200 days until all the values are reached a constant value and then afterwards the dynamic simulation is performed for 30 days. The dynamic simulation considers the simulated steady-state values of all the variables as the initial values for the simulation. In this project, firstly a steady state simulation is performed and then calibration is performed for dynamic variations. Simulation of the model for calibration and validation is carried out by analyzing the obtained measurement data for the periods of 2022-01-01 to 2023-01-31. The methodology for calibration follows as:

- Firstly, the solids in the process i.e., MLSS (Mixed Liquor Suspended Solids) in the last zone of each line, solid content in primary clarifier sludge, and solids in the outflow from pre- and post-sedimentation are calibrated which also includes the calibration of the sludge age.
- Then the calibration of nitrification takes place for NH_4^+-N, NO_3^-N concentrations in both lines.
- Finally, N_2O production and total emission factors are calibrated for both the lines in zone 2, 4, 6, and 8 where floating hoods are arranged for measuring the N_2O emissions.

Average mean values of the measured data are used for performing steady-state simulation and then the model is run with the dynamic variations with 24-hour daily measurements as input to the model for calibrating against the measured data by following the calibration procedure mentioned above. For calibrating the solids, settling parameters are used and kinetic parameters of the reaction process are used to calibrate the nitrogen species and N_2O emissions. The calibrated parameters are compared with the previous study by Zaborowska et al. (2019).

4.4.2 Validation

For performing the validation, another period is chosen which is not used for calibration. Sludge contents are adjusted to match the solids in the process in the same way as it is done in the

calibration. Other than the calibrated parameters, no other parameters were changed during the validation.

4.5 Mitigation strategies

Once the calibration of the model is completed, the model is simulated for identifying efficient strategies to mitigate N_2O emissions. Calibrated results are used as a reference to compare the results of the mitigation strategies. Various approaches are investigated in order to reduce the N_2O emissions from the treatment plant. For this purpose, two approaches have been identified to be promising to analyze as mitigating strategies. Two strategies are:

- SRT variations: The sludge age of the process is changed by changing the sludge withdrawal from the post-sedimentation and WAS flow in the biological secondary treatment process.
- Implementing internal recirculation: wastewater flow is recirculated to the biological secondary treatment process with anoxic zones. Four cases have been evaluated in this approach to understand the changes happening with this approach in the treatment process.

All the other process parameters are not changed during the analysis of the strategies. In both approaches DO set points are not considered to vary as the values are already high with an average value of 2.5 and 3.5 mg/l in lines 1 and 2 respectively and increasing further can be more energy demanding and decreasing might affect the treatment efficiency. The model is adjusted for the sludge underflow from the post-sedimentation which is fractioned as RAS and WAS flow in the ASP for lines 1 and 2. This has influenced the sludge retention time in the system which can also be explained through equation 7. For the second approach, the process configuration is changed with internal recirculation flow. The flow from the effluent of the ASP process is sent back to the inlet of the ASP process. The recirculation flow rate and the number of anoxic zones has varied to investigate the efficiency of the approaches to identify effective mitigation strategies.

$$\text{Sludge Retention Time, SRT (d)} = \frac{V * X}{Q_W X_W + Q_e X_e}$$

Where: V is the aeration tank volume (m^3), X is concentration of volatile suspended solids in the aeration tank (g/m^3), Q_W is the waste sludge flowrate (m^3/d), X_W is the concentration of volatile suspended solids in the waste sludge (g/m^3), Q_e is the treated effluent flowrate (m^3/d), X_e is the concentration of volatile suspended solids in the treated effluent (g/m^3).

5 Results and discussion

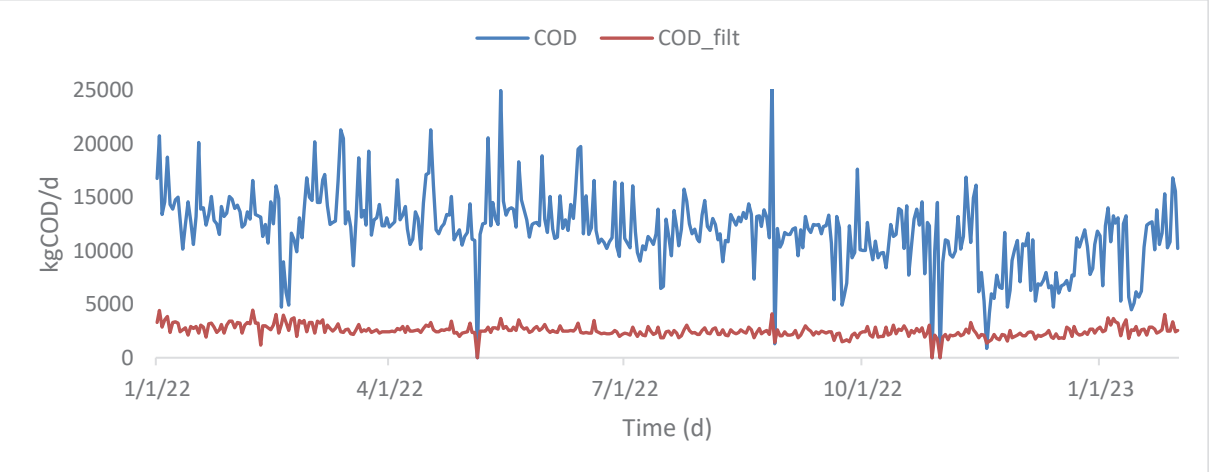
This chapter presents the results of the modelling of the Klagshamn treatment plant. Results from the data analysis are presented and discussed in section 5.1 and calibration and validation results are explained in sections 5.2 and 5.3 respectively. Finally, simulations of mitigation strategies are discussed in section 5.4.

5.1 Data analysis

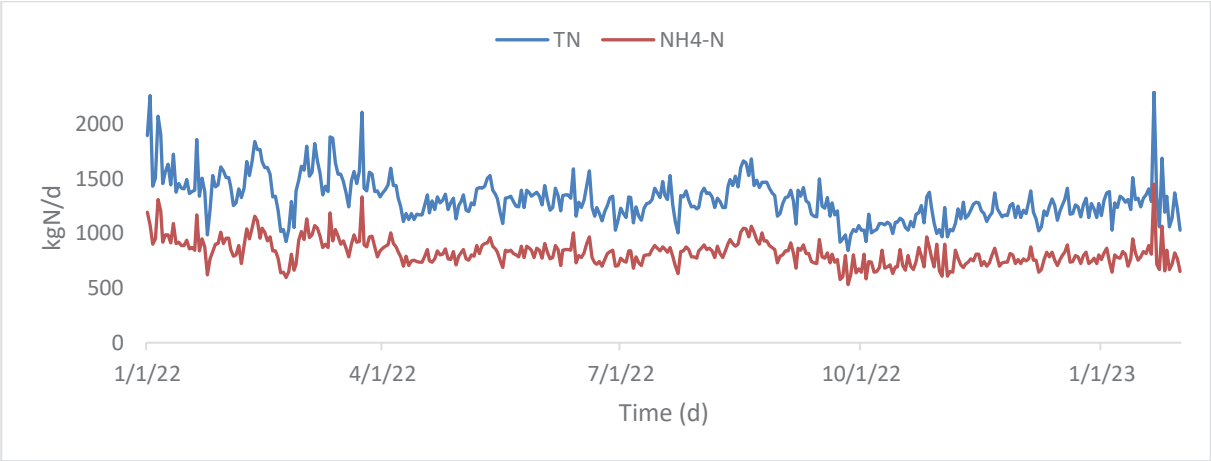
This section elaborates on the results of analyzing the data for incoming water and selecting the periods for calibration and validation.

5.1.1 Incoming water

The results from the preprocessing of the data are presented in Figure 5.1.1 which represents the data after filling the gaps. Analysis revealed that the incoming wastewater concentrations ie., the filtered COD, NH_4^+-N, and PO_4^{3-}P, TN quantities are constantly entering the treatment plant as seen in Figure 5.1.1. There is also observed a spread in the variation pattern for incoming COD and TSS. Figure 5.1.1 determines that there is no specific trend observed for the incoming loads for the measurement periods of 2022-01-01 to 2023-01-31 as the treatment plant is not connected with any large industries with the process water.



(a)



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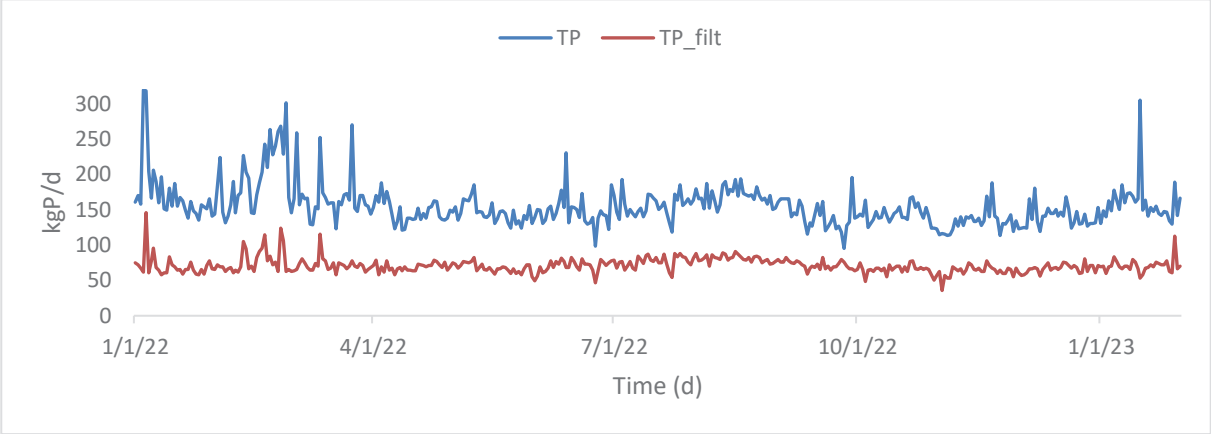
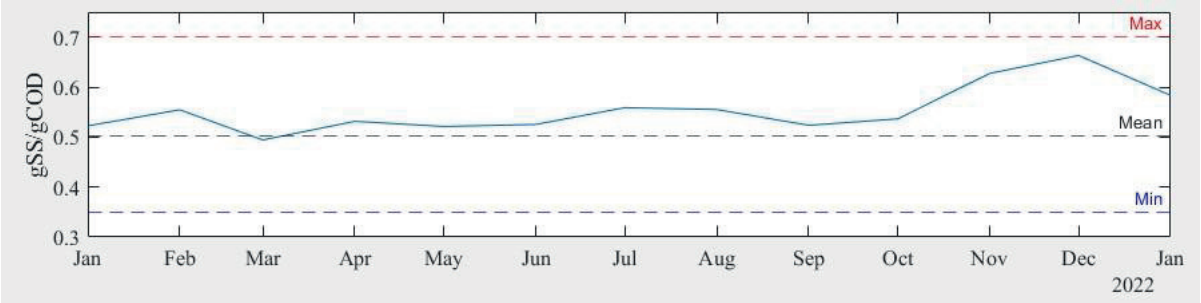


(c)

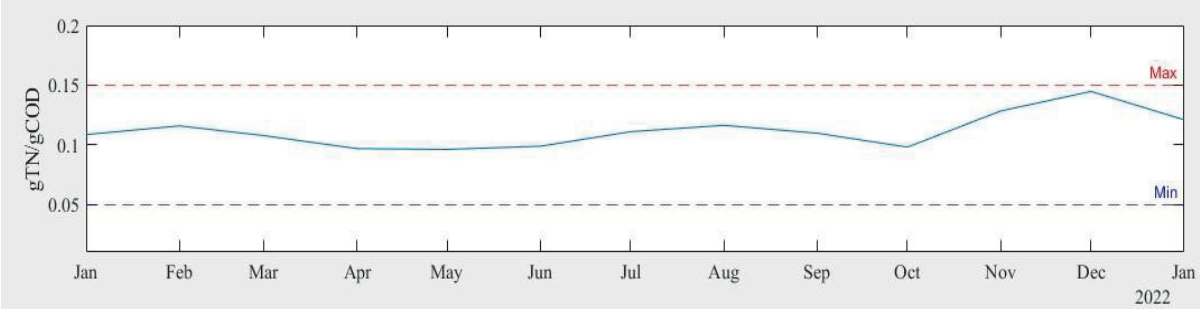
Figure 5.1.1. Incoming load of (a) COD, COD_{filt} , (b) total nitrogen (TN), ammonium nitrogen (NH_4^+-N), (c) total phosphorous (TP) *and TP_{filt} to klagshamn wastewater treatment plant during period 2022-01-01 to 2023-01-01.*

Analysis of the incoming water is performed using the ratios of the measured concentrations. The results of the analysis are shown in Figure 5.1.1.2, where the ratio values for TN/COD, filtered COD to total COD (COD/COD), and SS/COD are compared with the reference maximum and minimum values from *Riger (2013*). The comparison of the values is verified to be within the acceptable limits for municipal wastewater. Most of the values are lower than the reference values as seen in Figure 5.1.1.2. This could be justified, for instance, the reason for lower values of TN/COD would be that either the TN would be low, or COD would be high. When looking at the TN and COD concentrations in Figure 5.1.1.2, it is observed that COD is slightly higher in the influent than the usual standard range. There are two reasons for such high amounts, one could be that the solids that are coming from the backwash which are sent to the inlet to mix with incoming water influence the COD concentration in the influent. Another reason is that the wastewater is collected far from the treatment plant using long pipes in which, the concentrations might have already oxidized during the travelling period inside the pipes due to the availability of sufficient time with the long distant pipes to get oxidized. The analysis has been performed after filling in the missing data using the available measurement data for concentrations with the nearest values. It can be uncertain about filling the missing data with

this method as it cannot be the case every time with the same nearest values. But this method is chosen for filling as it is necessary for doing proper simulations without any gaps.



(a)



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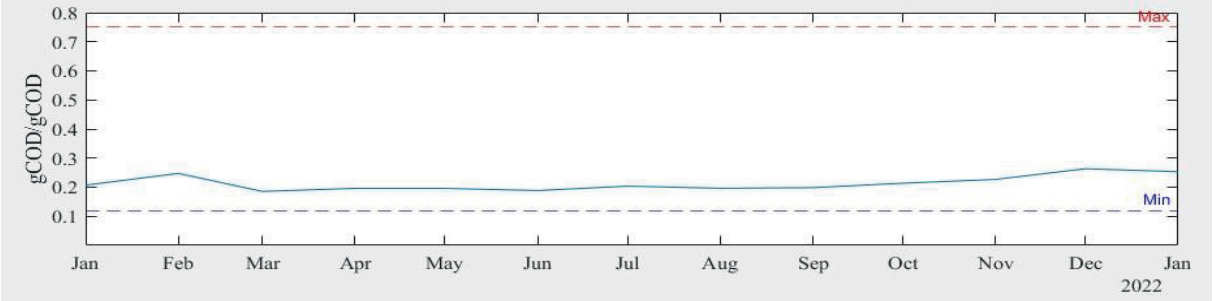
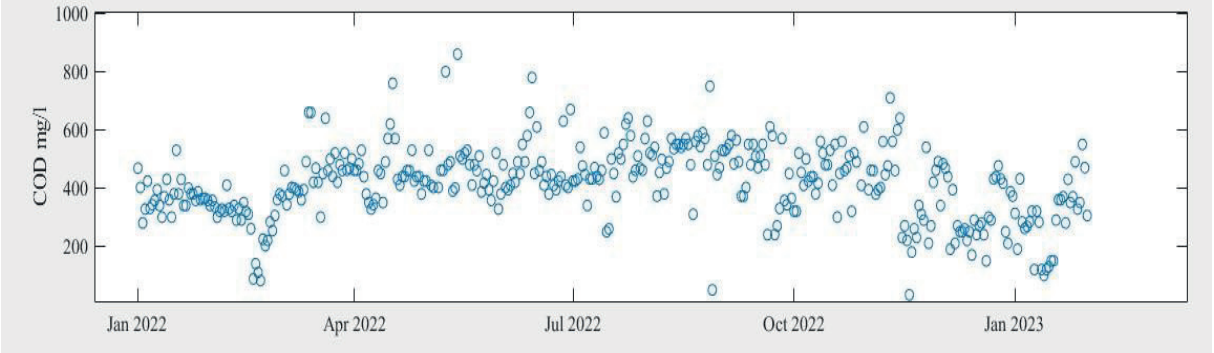
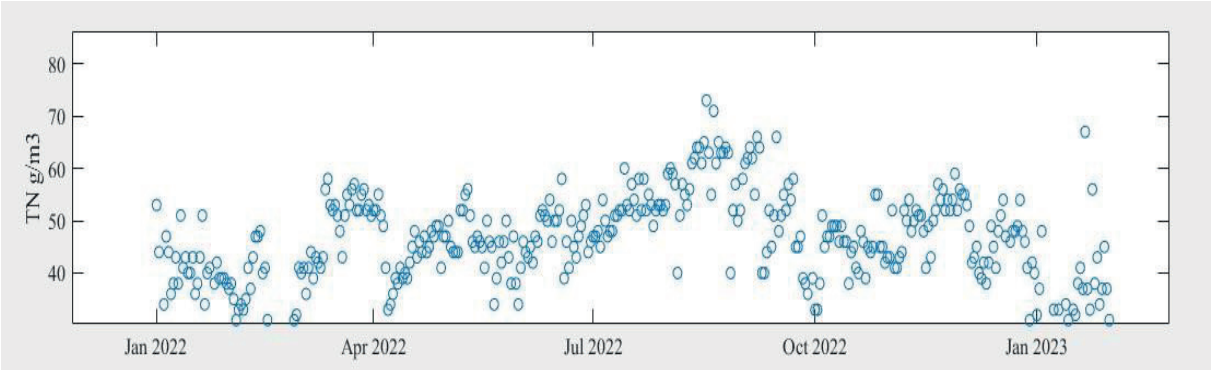


(c)



(d)



(e)

Figure 5.1.1.2. Calculated ratios for incoming water for the Klagshamn treatment plant, compared with values as a reference from (*Riger 2013*, n.d.) *. (a) TSS/COD, (b) TN/COD, (c) COD_{filt}/COD, (d) COD, (e) TN. Light blue lines in a, b and c indicate calculated values, and red and dark blue dotted line is the maximum and minimum value respectively from reference.*

5.1.2 Data analysis for simulation:

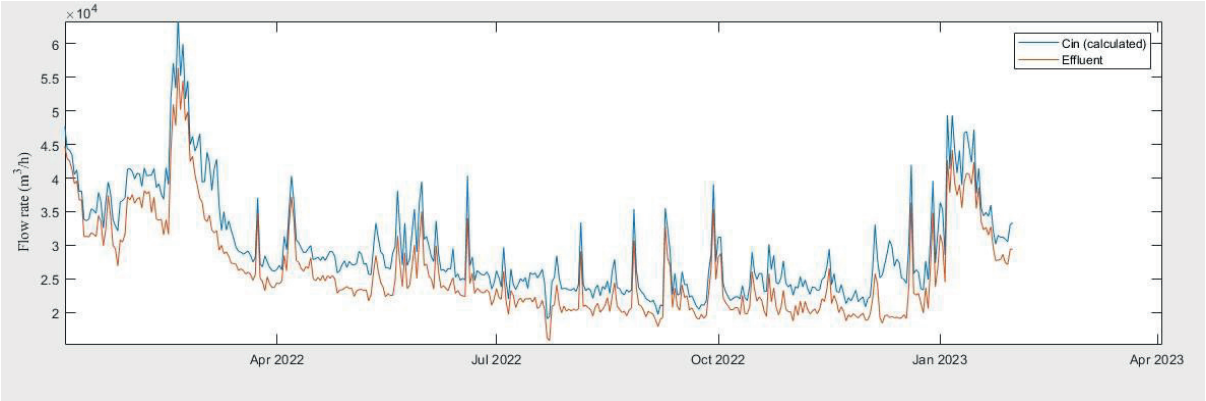
Measured values of incoming water are fractioned to import them as the input variables to the model before starting the simulation. The fractionation results which are obtained for the model are presented in Table 5.1.2. Fractionation is done for COD, TSS, total nitrogen, and phosphorous. The measurement data of COD and COD_{filt} is fractioned into readily biodegradable soluble substrates (i.e., S_VFA, S_F), slowly biodegradable particulate substrate (XC_B), Unbiodegradable soluble and particulate substrates (S_U, X_U), heterotrophic (X_OHO) in the WEST software. Readily biodegradable can be easily consumed by microorganisms but slowly degradable matter consists of particulate materials which can't be easily consumed by the microorganisms. After a certain time, the particulate matter is hydrolyzed, and it is available for the microorganisms to consume. TSS fractionation is carried out for Inorganic suspended solids (X_ISS). Measured data of total nitrogen and total phosphorous is fractioned into ammonium concentration (S_NH) and orthophosphate (S_PO) respectively based on the measured data for ammonium and orthophosphate. It is observed from the measurement data that the pH is mostly constant in the incoming and effluent water, therefore (S_ALK) is assumed to be 15 g/m^3. All the other concentrations of metal hydroxide, metal phosphate, nitrogen, and oxygen are assumed as negligible.

Table 5.1.2: Fractionation results for the model parameters using the data.

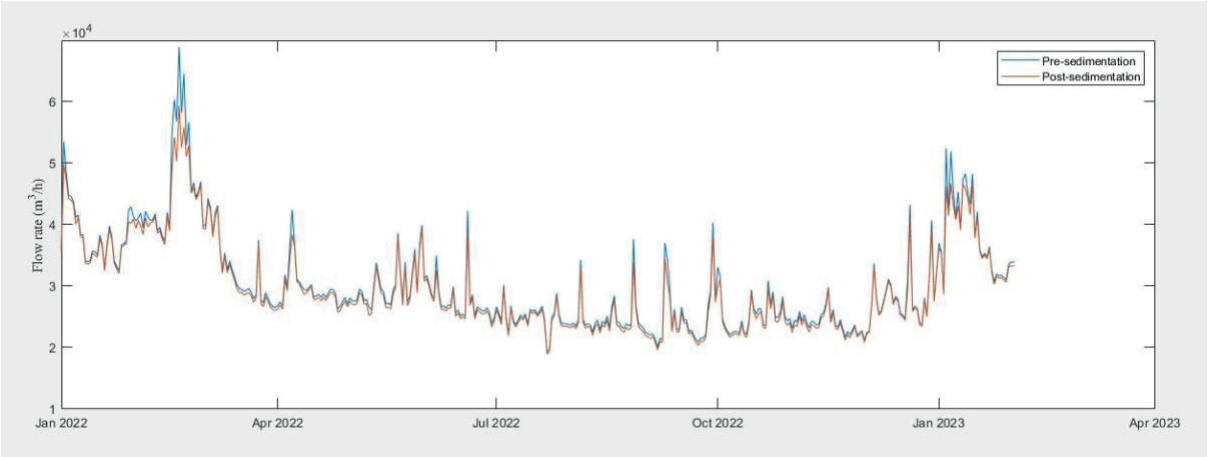
parameter	Description of the parameter	Value
f_S_VFA	VFA fraction of soluble COD	0.23
f_S_F	S_F fraction of soluble COD	0.41
f_S_NH	Total nitrogen to ammonia ratio	0.61
f_S_PO	Total phosphorous to PO ratio	0.41
f_X_OHO	Particulate COD to X_OHO ratio	0.06

f_XC_B	Particulate COD to XC_B ratio	0.76
i_COD/VSS	COD to VSS ratio	2.24
i_TSS/ISS	TSS to ISS ratio	6.65

The model is simulated first with the mean average values of each month which are calculated from daily measured values. Data is analyzed to identify the appropriate periods to perform the simulations. The analysis resulted that, 2022-10-01 to 2022-10-31 can be selected for calibration and 2022-11-01 to 2022-11-30 is selected for validation. Analysis of the incoming, effluent, pre-, and post-sedimentation flows is observed in Figure 5.1.2 where October and November months are identified to have more stable flow measurements than all the other periods. The stable conditions could be that there might not have been any extreme event conditions during that period. This is the best way to select the periods for simulation as it extreme events are significant to consider as it will affect the model simulation. Another major consideration for selecting the periods for calibration and validation is the N_2O measurement data. Even though the measurements for N_2O are available for the whole period (periods are mentioned in section 5.1.1), measurements are not available for some periods due to malfunctioning and replacing the equipment and loss of data for some periods. The arrangement of floating hoods is also changed for some time within the zones in both lines. By considering all these and analyzing the data, suitable periods are selected for calibration and validation.



(a)



(b)

Figure 5.1.2. Flowrates of wastewater in the Klagshamn treatment process, (a) Incoming and effluent flowrates, (b) Outflow rates from pre- and post-sedimentation basins.

5.2 Calibration

Calibration results of the model for solids, nitrogen species, and N_2O production of the treatment process are presented and discussed in this section along with the description of calibrated parameters.

5.2.1 Parameters

For calibrating the solids in the process, f_ns, the fraction of non-settleable solids for both pre and post sedimentation are adjusted which describes the separation efficiency of particulates. The separation fraction is adjusted in both the lines with different values to match well with the measured data. The parameter is reduced to 0.3 in line 1 and 0.35 in line 2 as line 1 has an additional amount of waste flow rate from line 2 which needs to be considered for maintaining the correct solids in both lines. The reduction of this value from the default value of the model is justified in that when decreasing the non-settleable solids, more solids can be captured as sludge from the pre-sedimentation basins. This adjustment also assisted in calibrating the correct sludge age of the process. For calibrating the nitrate and ammonium concentrations, K_F1, S_F saturation coefficient for aerobic growth rate is adjusted which determines that it affects the growth rate of the aerobic microorganisms while converting the ammonium to nitrate. This value is adjusted in such a way that it doesn't affect N_2O production as the nitrate concentration is correlated with the N_2O emissions (See figure 5.2.1). Correlation analysis gave an R^2 (coefficient of determination) of 0.7798 which indicates a strong correlation.

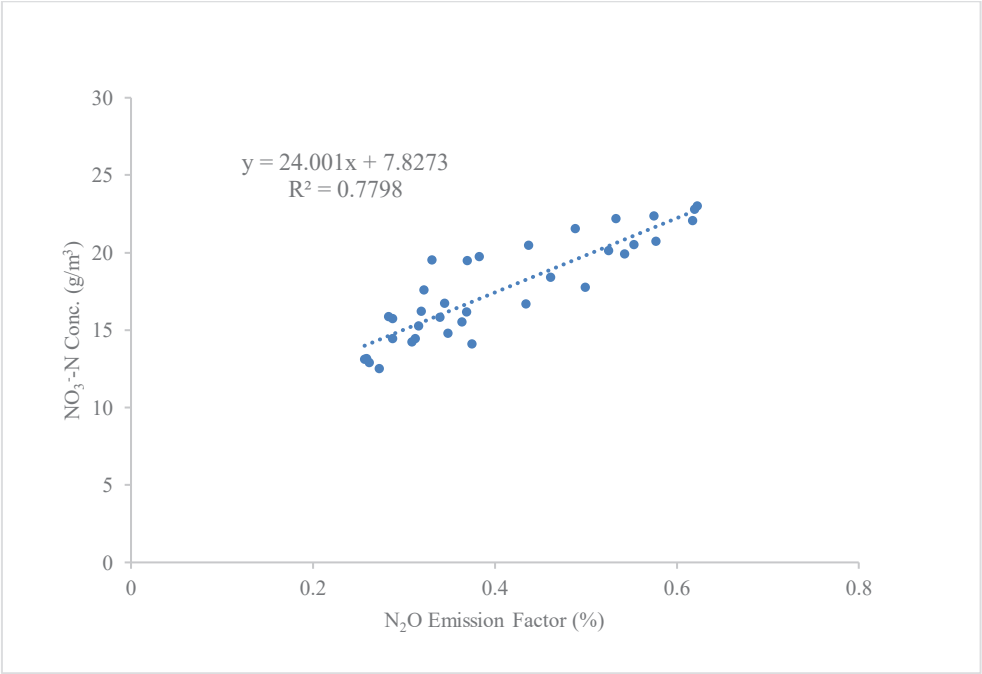


Figure 5.2.1: Calculated correlation between Nitrate concentrations and N2O emission factor for line 1

N_2O production is calibrated using kinetic parameters for OHOs which are listed in Table 5.2.1 along with the calibrated values from the previous study by Zaborowska et al. (2019). For denitrification of the heterotrophic denitrifies, correction factors associated with anoxic conditions are important and are used for accounting for a fraction of biomass to get denitrified. Depending on the steps involved in the N_2O production, correction factors are adjusted. n2_g_OHO is the parameter associated with the growth rate of OHOs which is increased to 0.6 from the default value of 0.3 which indicated the increase in the anoxic growth rate for converting nitrate to nitrite. This increment increased the conversion and production of nitrite available for the next step in the heterotrophic denitrification process. n5_g_OHO is decreased from the default value of 0.8 to 0.4, which is associated with a slowdown in the anoxic growth rate for converting N_2O to N_2 which increased the production of the N_2O. The N_2O saturation coefficient of OHOs is calibrated with higher values than the default and reference values.

Table 5.2.1. Set of calibrated parameters and their values along with default and reference values from Zaborowska et al. (2019).

Parameter	Description	Default value	Calibrated value	Reference values from Zaborowska et al. (2019)	Units
K_F1	S_F saturation coefficient for aerobic growth rate	4	2	4	g/m^3
K_F5	S_F saturation coefficient for OHO growth, N_2O to N_2	4	8	4	g/m^3
K_N2O_OHO	N_2O saturation coefficient for OHOs	0.02	0.06	0.35	g/m^3
n2_g_OHO	Correction factor for anoxic growth of OHOs, NO_3 to NO_2	0.3	0.6	0.4	-
n5_g_OHO	Correction factor for anoxic growth of OHOs, N_2O to N_2	0.8	0.4	0.4	-
f_ns	Fraction of non-settleable solids from the pre-sedimentation clarifier	0.6	Line 1: 0.35; Line 2: 0.3	-	-
f_ns	Fraction of non-settleable solids from the post-sedimentation clarifier	0.00228	Line 1: 0.0015; Line 2: 0.002	-	-

5.2.2 Calibration results:

The first thing calibrated in the model is for solids in the treatment process. The measurement values from pre-processed data are used to compare the calibrated results. The results from this comparison can be seen in Figure 5.2.2, where solids are calibrated for the outflow from pre-

and post-sedimentation, and sludge underflow from the pre-and post-sedimentation process. Figure 5.2.2 (a) represents solid content in the outflow from the pre-sedimentation from both lines 1 and 2 which showed a higher estimation than the measured data. TSS in the model is calculated based on the volatile and inorganic suspended solids, in which the VSS is calculated based on its ratio to particulate COD, (1.6 gCOD/gVSS) but the ISS fraction is depending on the biomass contents of AOB, NOB, and PAO and metal compounds. These fraction calculations for ISS might have influenced the high TSS estimation in the model. It has also been observed variation for the TSS in the incoming flow in the model when compared with the incoming measured data. This has also affected the solids content in the sludge flow from the pre-sedimentation basin which can be seen in Figure 5.2.2 (b). The solid contents from underflow from the pre-sedimentation are underestimated as more solids are going out of the basin for the secondary treatment process. The calibration results of the MLSS in the activated sludge unit reactors in lines 1 and 2 are presented in Figure 5.2.2 (c and d), which shows an estimation compared with the data. The simulated model results are compared with the lab measurements which are available for only a few days for the simulation period in the last zone of the activated sludge unit process. It is difficult to estimate the dynamic patterns with such less measured data, but the mean values of the simulated values seem to fit correctly for both the lines i.e., 4000 and 3900 g/m^3 of MLSS for lines 1 and 2 respectively. Sludge flow from post-sedimentation clarifiers is given in Figure 5.2.2 (e and f), which showed an overestimation of solids compared with the measured data. It is difficult to match with the measured data as calibrating the solids in the sludge is affecting the MLSS in the ASP units as the model is not performing as it is at the treatment plant. Compared with line 2, line 1 is estimated to match the solids in most of the days except the last few days. Also, the measured data is available for both online and lab measurements, the simulated results are compared with the lab measurements, and it is observed that a few values in line 1 have slightly higher measurements than the online measurements unlike in line 2. This could be the reason for the better fit with line 1. Calibrating the solids in turn resulted in getting a correct sludge age of the process which are obtained as mean values of 8 and 11 days for lines 1 and 2 respectively which matches well with the measured data. The simulated results for SRT are not presented to compare with the data as there are no lab measurements available for the simulated period.

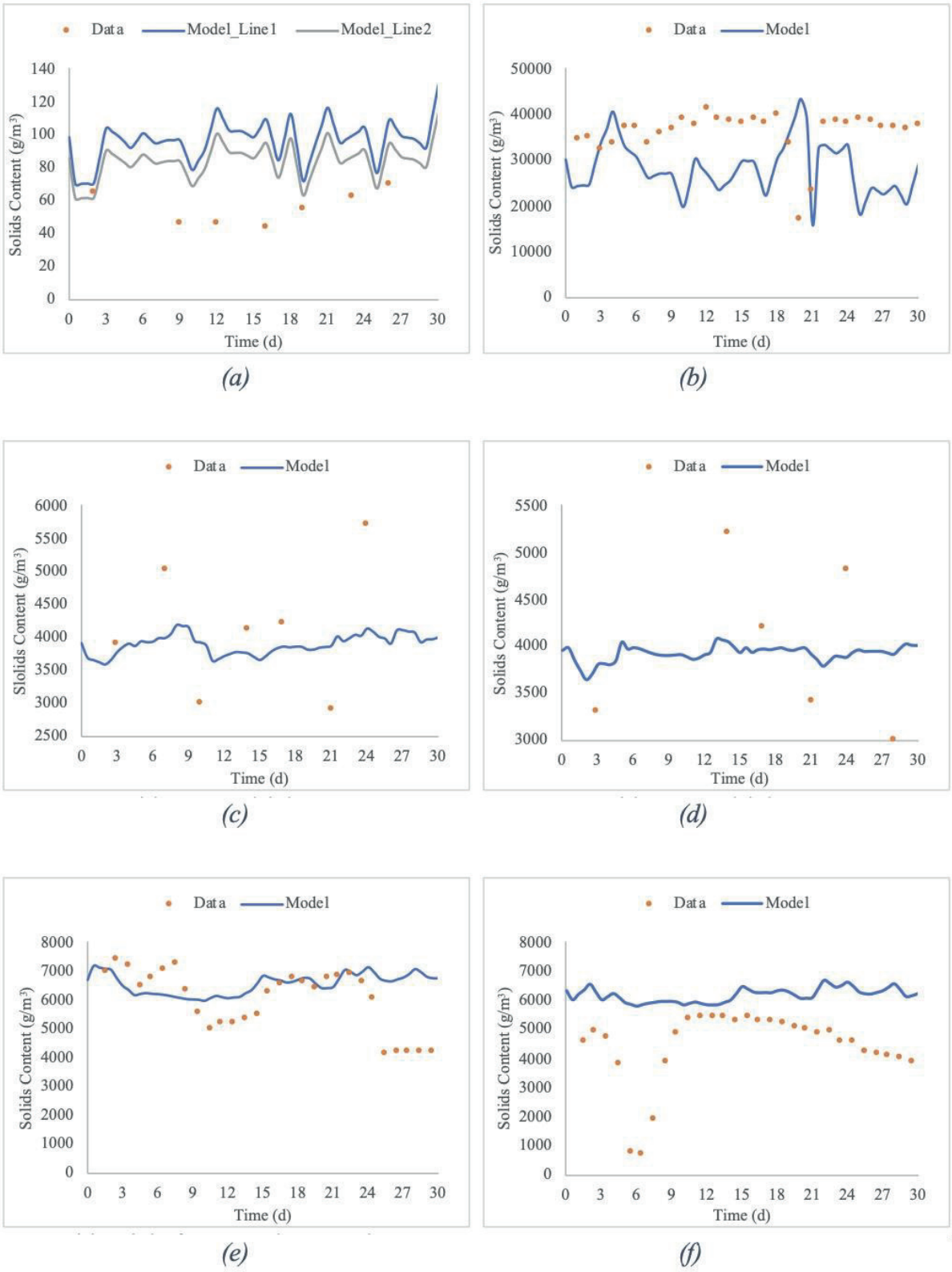


Figure 5.2.2. Calibrated results of the solids in the treatment process. (a) solids content in the outflow from the pre-sedimentation basin in lines 1 (Blue line) and 2 (Grey line), (b) combined solids in the underflow sludge from pre-sedimentation basin, (c) MLSS in activated sludge unit reactors in zone 8b for line1, (d) MLSS in activated sludge unit reactors in line 2, (e) Solids content in the underflow sludge from post-sedimentation for line 1, (f) Solids content in the

underflow sludge from post-sedimentation in line 2. Blue lines represent the calibrated model results and red dots are measured data.

Figure 5.2.3 shows the results from the calibration of nitrification concentrations of N species in the model. Nitrogen species calibrated include NH_4^+-N and NO_3^-N concentrations which are coming out from post-sedimentation from both the lines. The initial goal is to calibrate the nitrogen species in the last zone of the activated sludge unit process, but instead, it is calibrated for the outflow from post-sedimentation as the data is available with lab measurements to compare the simulated results, and also that there will not be much difference in both the values as no nitrification happens at that stage Firstly, ammonium concentration is calibrated using growth rates of autotrophic parameters, and then eventually while calibrating the N_2O production, growth rates have changed back to the default values as the parameter calibrated for N_2O emissions affected the ammonium oxidation in the process. Thus, without any change in the kinetic parameters, ammonium concentration is being calibrated. With the availability of less measured data, it is difficult to predict if the simulation results captured the dynamic variation patterns. From the graphs a and b in Figure 5.2.3, it is visualized that line 1 simulations are within the range of the measured data but line 2 underestimated the ammonium content. Nitrate concentrations in the process are simulated and the results are presented in Figure 5.2.3 c and d, which can be seen that the calibration of the nitrate concentration is not well reproduced as the measured data., it can be justified that the values of the model and data are low, and it can be considered as satisfactory as both show similar results with low values.

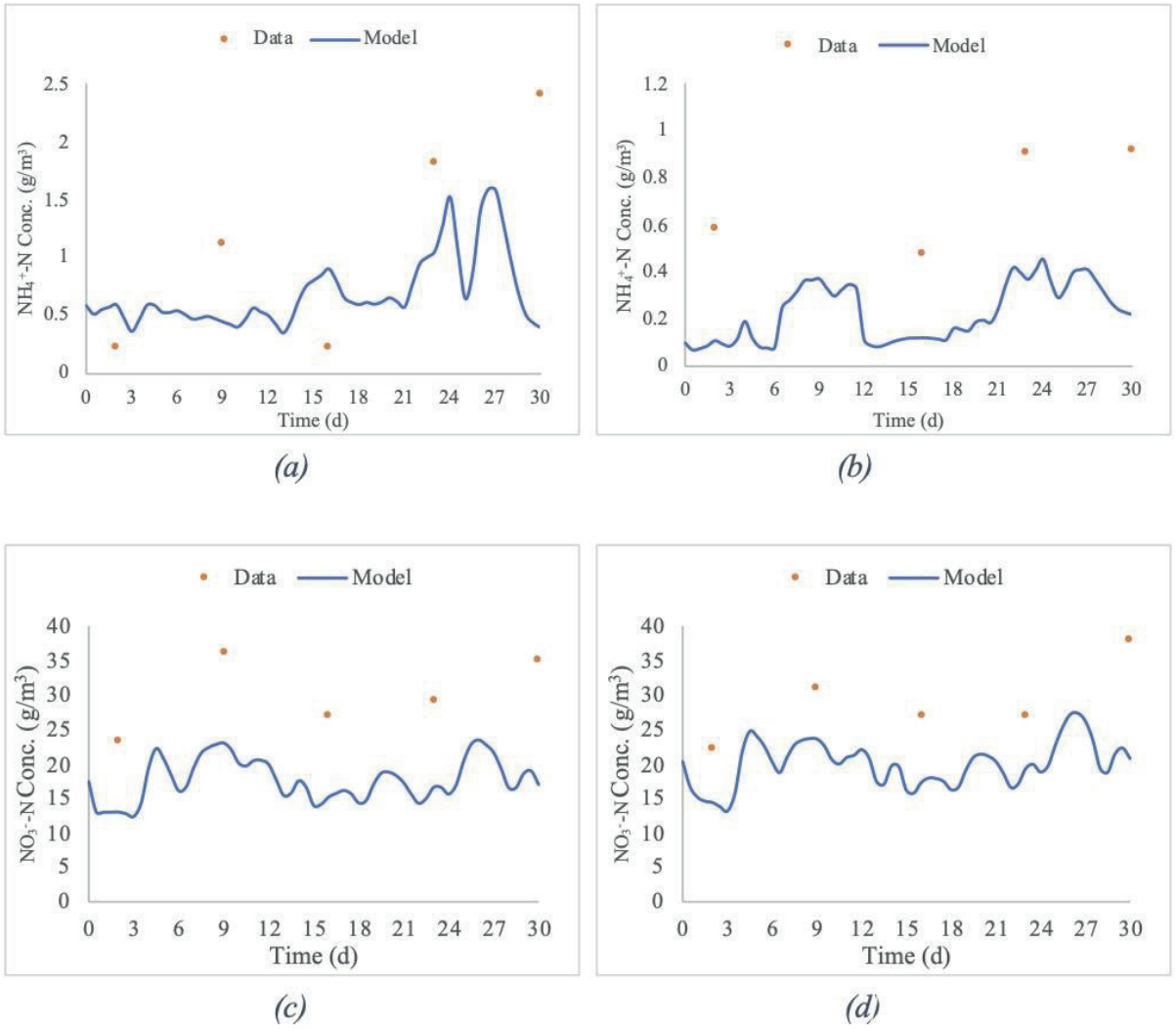
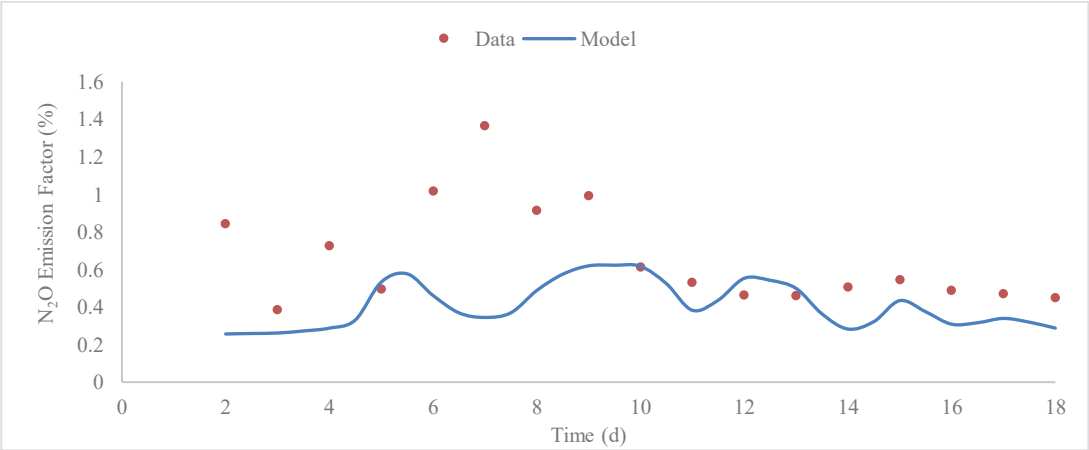


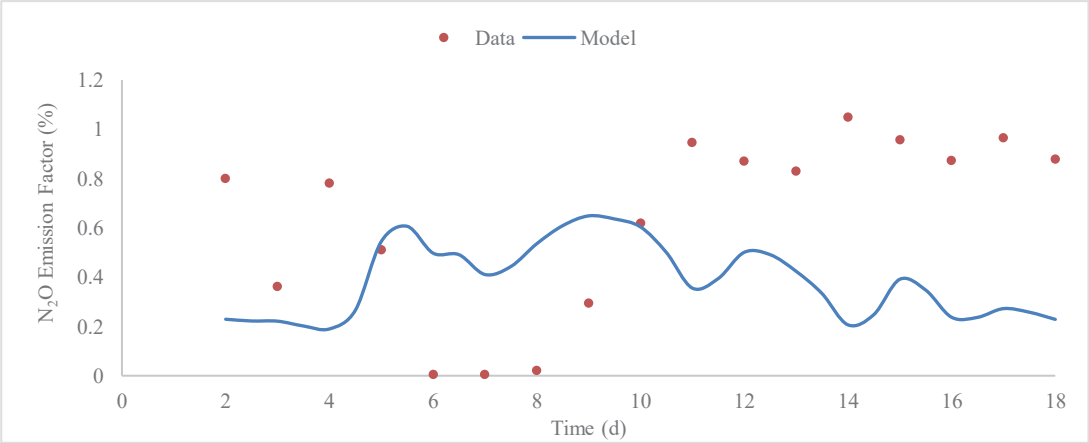
Figure 5.2.3. Calibrated results for nitrogen species in the outflow wastewater from post-sedimentation basins from both lines. Simulated results of ammonium concentration in line 1 (a) and line 2 (b), nitrate concentration calibrated for line 1 (c) and line 2 (d). Blue lines are the model calibration results and red dots are lab measurement data.

Dynamic calibration was conducted for N_2O emissions from the biological secondary treatment process for both lines for 18 days and the simulated results are compared with the measured data. Figure 5.2.4 a and b visualizes the comparison of simulated results of the total emission factor of N_2O from all eight zones in the activated sludge unit stage in line 1 and 2. The model predicted well in line 1 after 10 days of simulation and the predictions are within the measured data except for the peak values. The simulations couldn't capture the peak N_2O emissions during the calibration in line 1 from day 6 to 9, which is because the DO set point is low for line 1 during that period as you can see in DO values from Figure 8. (I) in the Appendix, and also that the incoming flowrate is also low for these days (see figure 8 in appendix). Regarding the results for line 2 (see figure 5.2.4 (b)), predictions are lower than the measured data for the last half of the simulated days. In the beginning days, the simulations are within the measured values but after 10 days of simulation N_2O production decreased much lower than the measured data. The reason for these low results might relate to influent concentrations. When analyzing the TN, COD, and NH_4^+-N from the influent, it is observed that total nitrogen and ammonium

concentrations are lower for those days and have high COD than the first 10 days of the simulation period. As the COD/N ratio is higher than the other days, N_2O production got reduced during these days.



(a)



(b)

Figure 5.2.4. Calibrated results of the total N_2O emissions from line 1(a) and line 2 (b). The total indicated the addition of emissions from all the zones where floating hoods are arranged at the Klagshamn treatment plant.

Figure 5.2.5 shows the N_2O emissions results for each zone where the floating hoods have been installed in the treatment process. Figure 5.2.5 (a) is the second zone calibrated results along with measured data. When analyzing the results, all the zones showed a similar trend in capturing the emissions except for the last zone. Zone 2 in both lines underestimated the emissions and in zone 4 and zone 6, the model is able to capture the trend in line 1 but line 2 is underestimated and doesn't match the measurements. In the last zone, the predictions are different in the emission pattern than the other zones where line 1 is overestimated and emissions are low in line 2 during the last 5 days. It is difficult to understand the reason for differences in different zones as it depends on many factors like process configuration, the activity of the microorganisms, and availability of the aerobic and anoxic conditions within each zone and pathway dominations with oxygen availability, etc. If the measured emissions

are associated with a particular pathway and in the model, they might not have captured well from that pathway due to the available conditions and microorganism behaviour in the model.

Figure 5.2.5. Calibration results of the N_2O emissions calibrated for each zone of both lines where floating hoods are arranged in the treatment plant and are compared with the measured data. (a) Zone 2, (b) Zone 4, (c) Zone 6, (d) Zone 8b. Simulated data is represented with lines and dotted values are measured data for N_2O emissions and blue colour is related to line 1 and the grey colour shows the values for line 2.

5.2.3 N_2O production pathways:

It is observed that the emissions are produced from two pathways i.e., the AOB nitrifier denitrification pathway and the heterotrophic denitrification pathway. As described in section 5.2.1, the N_2O production got increased when heterotrophic kinetic parameters have adjusted. This explains that the heterotrophs played a role in producing the N_2O emissions. Nitrite concentrations were observed to be very low (around 0.05 g/m^3) which indicated that the nitrite is actively converted into nitrate by autotrophic bacteria and thus emissions are also observed from nitrifier denitrification. As per the literature, with high DO set values (> 2.5 mg/l), hydroxylamine pathways are considered to be the dominant pathway for N_2O emissions, and

heterotrophic denitrification is considered a less contributed pathway. But in this case, the heterotrophic denitrification pathway showed a significant role in N_2O emissions with high DO values. This can be justified that even though pathway contributions depend on DO set points, it also depends on various other factors, and considering the process configuration, operating conditions, and incoming wastewater, emissions cannot solely depend on DO set points and that the ASM2dISS model used in this study doesn't include hydroxylamine pathway. It is also confirmed in recent studies by Domingo-F Elez et al. (2017) where the heterotrophic denitrification pathway showed predominant contributions to N_2O emissions under aerobic conditions ranging from 0.2-6.5 mg O_2/l at low COD/N ratios which is also the same case with low COD/N ratio which is discussed in section 4.2.2.

5.3 Validation

The model has been validated for the periods of 2022-11-01 to 2022-11-30. The validated results are presented in Figures 5.3, 5.3.1, 5.3.2 and 5.3.3, which showed similar results to those obtained from calibration. Compared with the calibrated results, validation simulations resulted in a better fit with the measured values.

Figure 5.3. Validated results of the solids in the treatment process. (a) solids content in the outflow from the pre-sedimentation basin in lines 1 (Blue line) and 2 (Grey line), (b) combined solids in the underflow sludge from pre-sedimentation basin, (c) MLSS in activated sludge unit reactors in zone 8b for line1, (d) MLSS in activated sludge unit reactors in line 2, (e) Solids

content in the underflow sludge from post-sedimentation for line 1, (f) Solids content in the underflow sludge from post-sedimentation in line 2. Blue lines represent the calibrated model results and red dots are measured data.

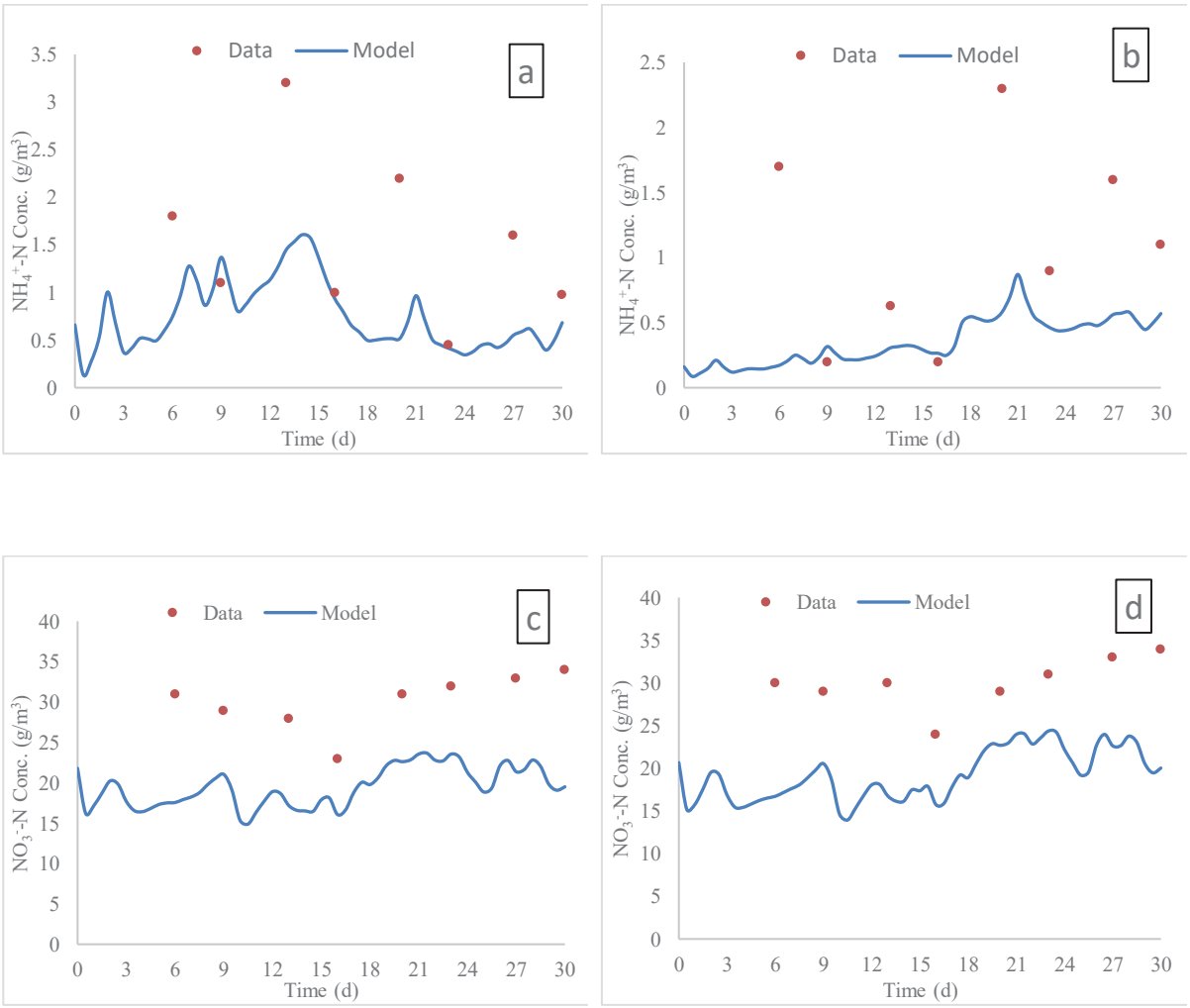
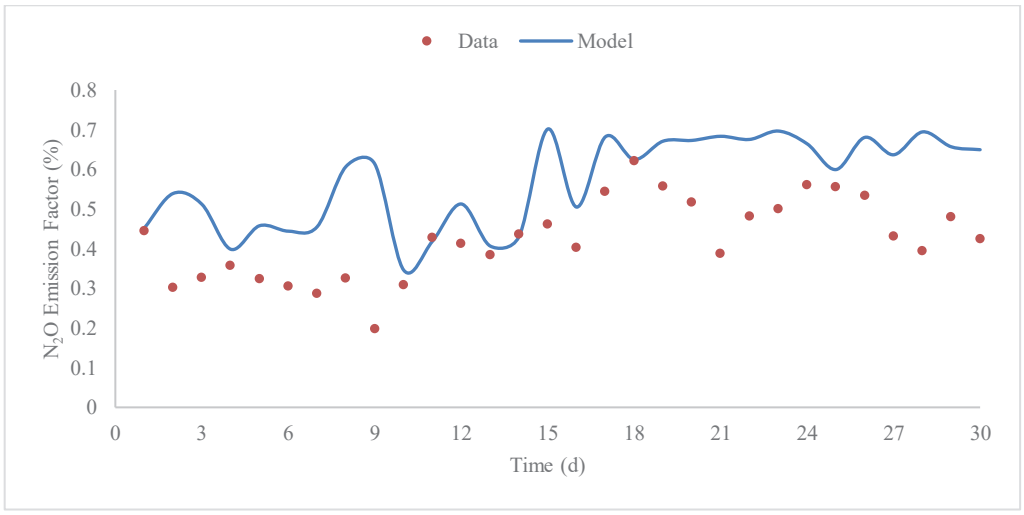
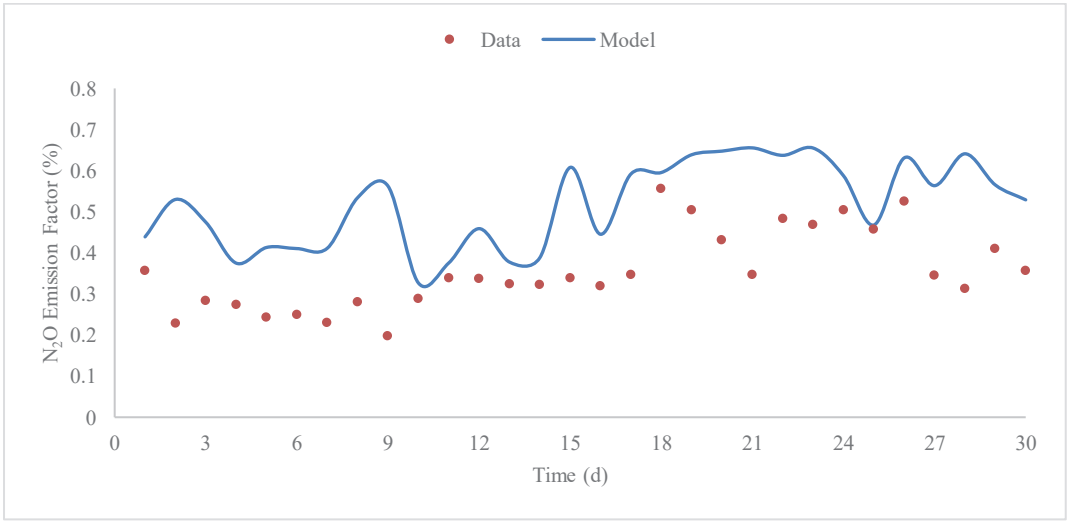


Figure 5.3.1. Validated results for nitrogen species in the outflow wastewater from post-sedimentation basins from both lines. Simulated results of ammonium concentration in line 1 (a) and line 2 (b), nitrate concentration calibrated for line 1 (c) and line 2 (d). Blue lines are the model calibration results and red dots are lab measurement data.



(a)



(b)

Figure 5.3.2. Validated results of the total N_2O emissions from line 1(a) and line 2 (b). The total indicated the addition of emissions from all the zones where floating hoods are arranged at the Klagshamn treatment plant.

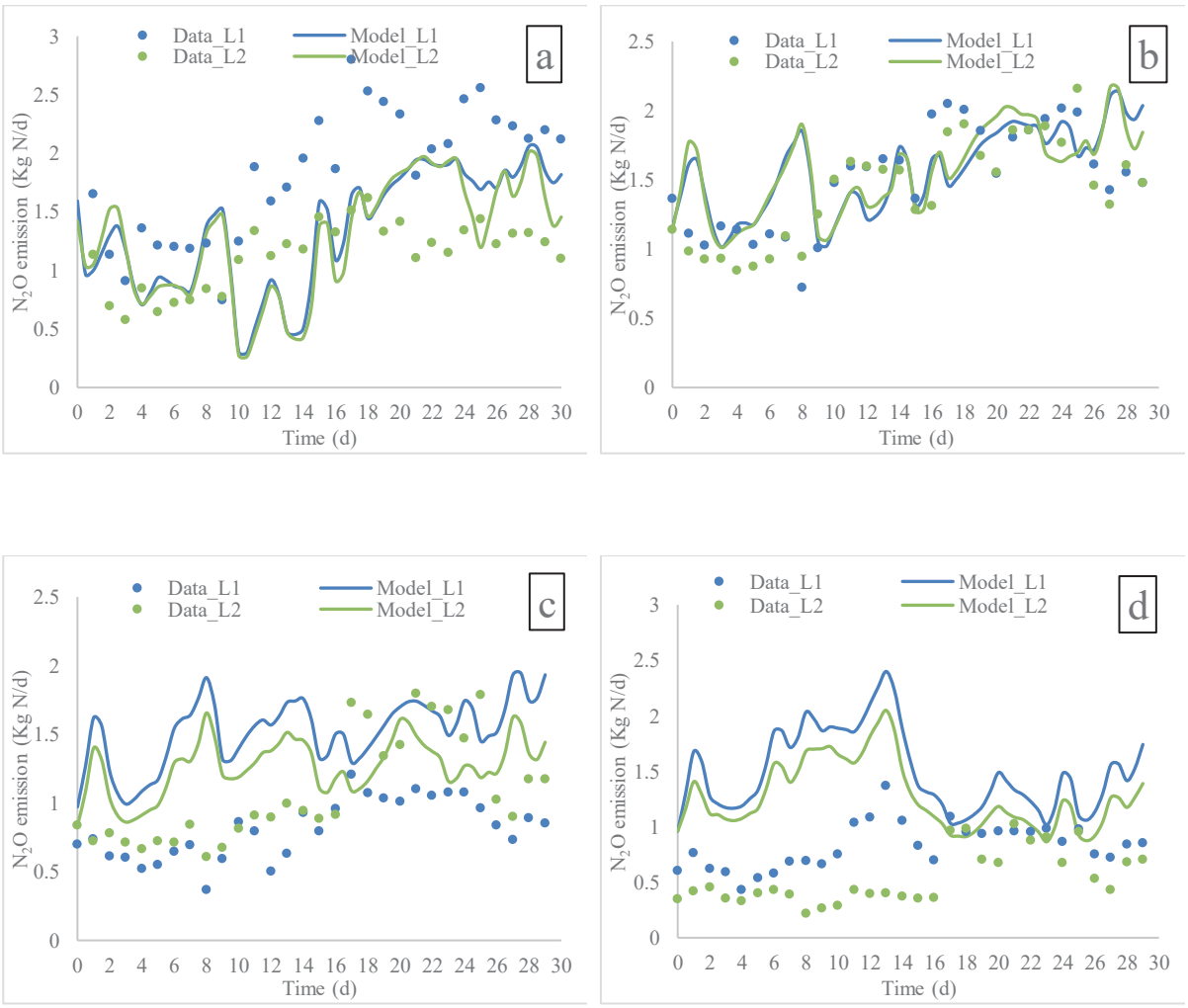


Figure 5.3.3. Validation results of the N_2O emissions calibrated for each zone of both lines where floating hoods are arranged in the treatment plant and are compared with the measured data. (a) Zone 2, (b) Zone 4, (c) Zone 6, (d) Zone 8b. Simulated data is represented with lines and dotted values are measured data for N_2O emissions and blue colour is related to line 1 and the grey colour shows the values for line 2.

5.4 Mitigation strategies

It has been observed from the calibration and validation results that two approaches are reasonable to propose as mitigation strategies to reduce N_2O emissions. Two approaches are:

- SRT variations
- Implementing internal recirculation

The process configuration of the second approach can be seen in Figure 4.5 with introducing internal recirculation to the secondary treatment process along with an anoxic zone. The reason for proposing these two strategies is based on the simulation results which showed heterotrophic denitrification as a dominant pathway and therefore the incomplete denitrification can be resolved using the proposed strategy. Also that the discussion with treatment plant organizers expressed their willingness to do modifications to the process. Simulation results for both approaches are presented and discussed in sections 5.4.1 and 5.4.2.

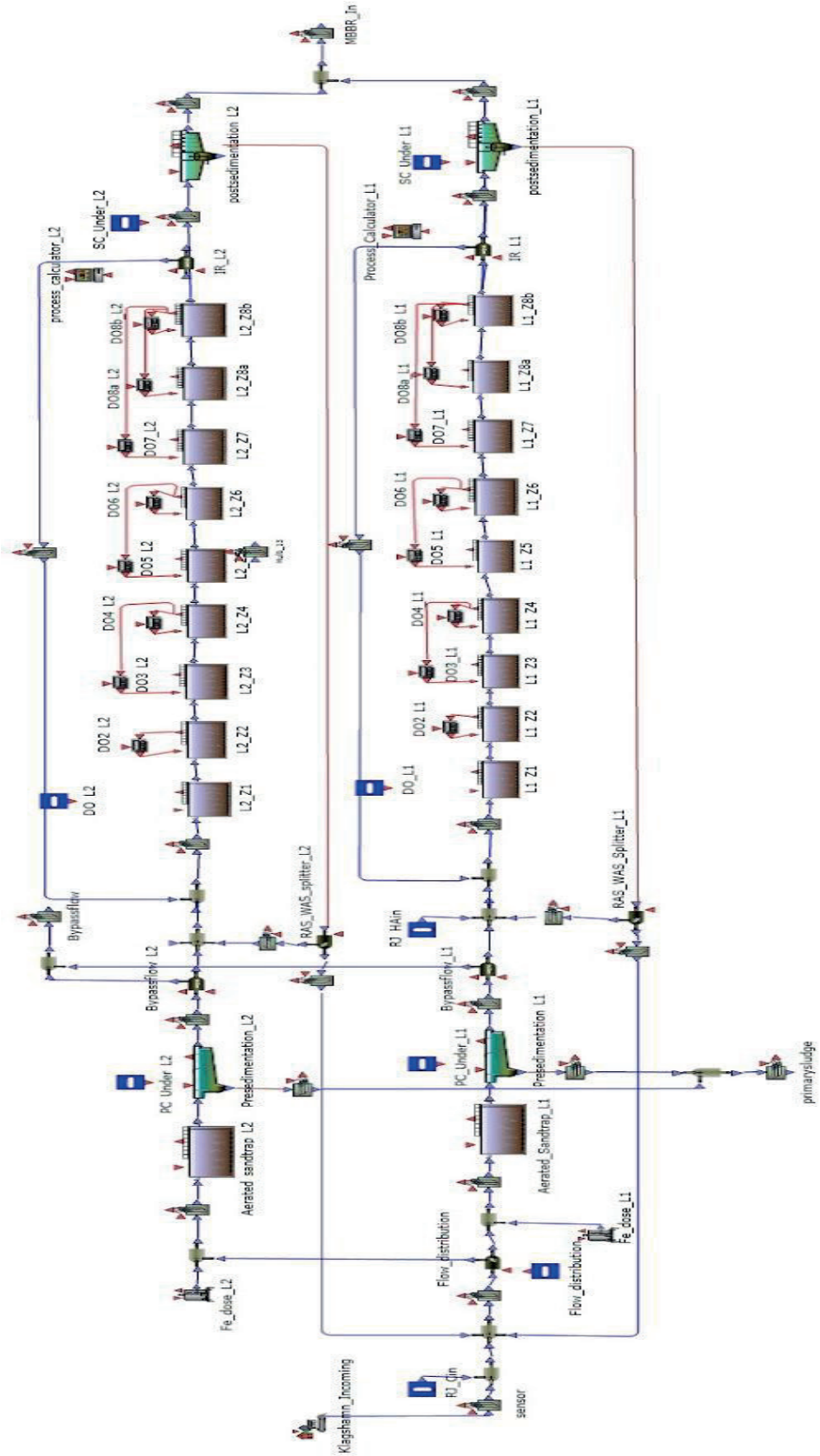
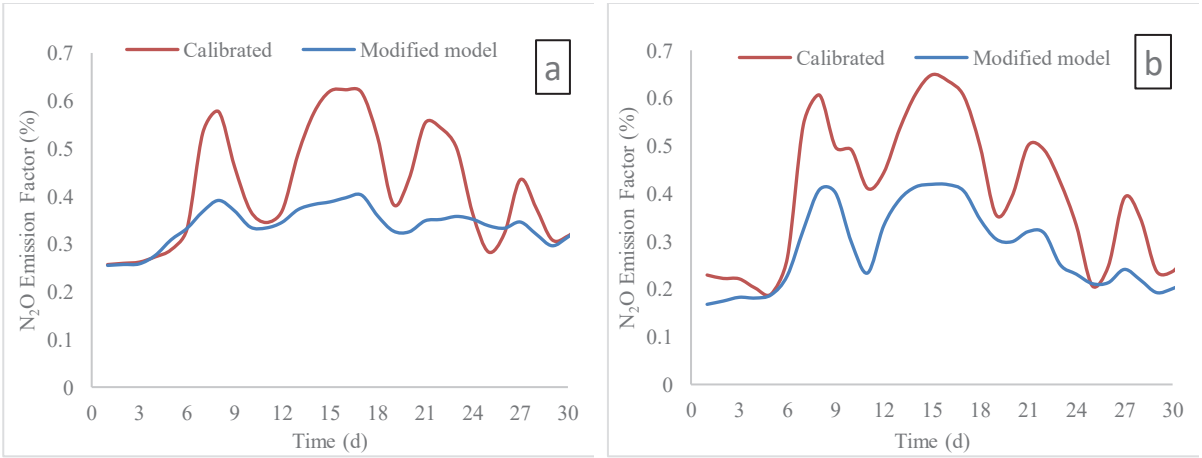


Figure 4.5. Model construction layout of the Klagshamn treatment plant process in the WEST for the primary and secondary treatment processes for mitigation strategies with internal recirculation and anoxic zone.

5.4.1 SRT variations

Without any changes in the process configuration, this approach is to adjust the SRT in both lines showing a reduction in the overall N_2O emissions in both lines (see Figure 5.4.1). Results showed an average reduction of 17% of emissions from the treatment process. In this approach, underflow from the post-sedimentation is adjusted which in turn changes WAS flow rates as it contains both RAS and WAS flows. 25% of the underflow from sedimentation is reduced which indicates that WAS is also reduced by 25%. The reduction of WAS gave less sludge to pass to the inlet of the plant and allowed the sludge to have a higher retention time in the activated sludge reactors. As it is shown in Figure 5.4.1, SRT is increased from 8 to 13 days in line 1 and 11 to 15 days in line 2 with this approach. In this approach, biomass activity increases for the consumption of produced N_2O to convert it into Nitrogen, and thus N_2O emissions got decreased. When analyzing the treatment efficiency of this approach, it is identified that nitrification is happening with reasonable concentrations of ammonium and nitrate and the results are somewhat similar to what is obtained from calibration results. Even though the overall emissions are reduced with this approach in both the lines when looking at each zone where floating hoods are arranged, emissions are reduced only in zone 2 and 4 in both the lines, and the emissions from other zones are slightly reduced. This could be because reducing the WAS has affected the initial zones and the final zones might be having the same conditions. This is because the reduction in WAS allowed less RAS flow to enter the activated sludge reactors and where the conditions might have changed only until the flow passed through the initial zones. This is an efficient approach as a mitigation strategy as it involves no additional modifications to change the treatment process configurations. In the treatment plant, this approach also allowed for reducing the energy consumption in the process operation as the pumping flow is reduced.



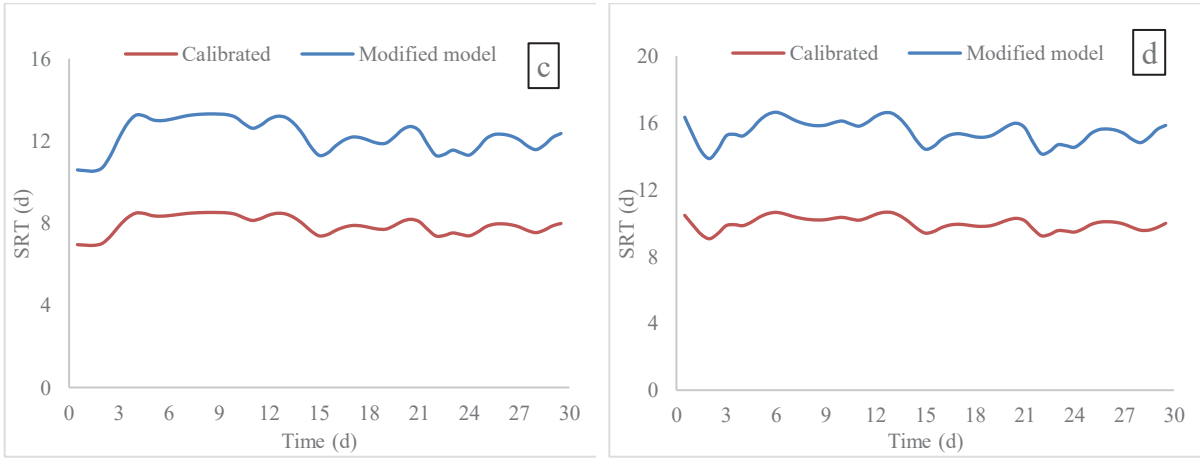


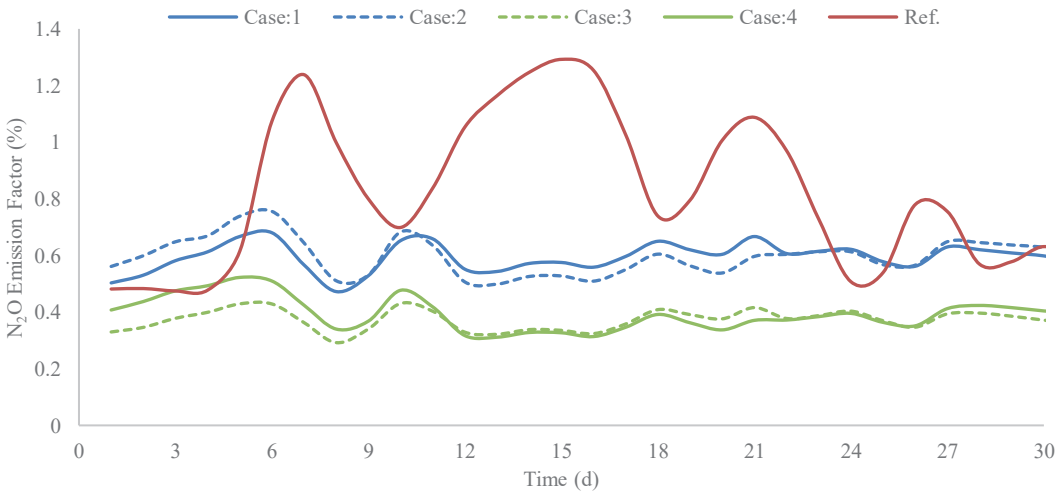
Figure 5.4.1. Simulated results of the mitigation strategy approach of SRT variations for total N_2O emissions from lines 1 (a) and 2 (b) and SRT variations in lines 1 (c) and 2 (d). The red line indicated calibrated model results and the blue line indicates simulation results from the modified model with the mitigation strategy.

5.4.2 Implementing internal recirculation

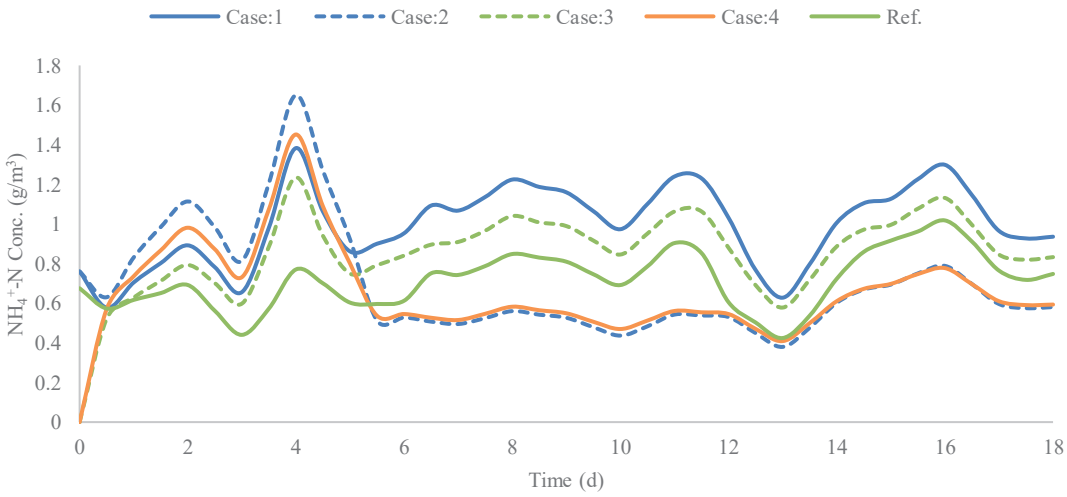
As the model predicted N_2O emissions from both autotrophic and heterotrophic pathways, the addition of internal recirculation to the treatment process can be efficient as a mitigation strategy. This can be justified that the N_2O is produced as a by-product of incomplete nitrification of the heterotrophic microorganisms and therefore, internal recirculation can be considered a better way to resolve this. The results of this strategy are estimated, and the model results are compared with the calibrated results as a reference. The approach is investigated with 4 cases:

- Case 1: Internal recirculation with 2 times the influent flow and 1 anoxic zone (ie., zone 1)
- Case 2: Internal recirculation with 2 times the influent flow and 2 anoxic zones (ie., Zone 1 and 8b)
- Case 3: Internal recirculation with 3 times the influent flow and 1 anoxic zone (ie., Zone 1)
- Case 4: Internal recirculation with 3 times the influent flow and 2 anoxic zones (ie., Zone 1 and 8b)

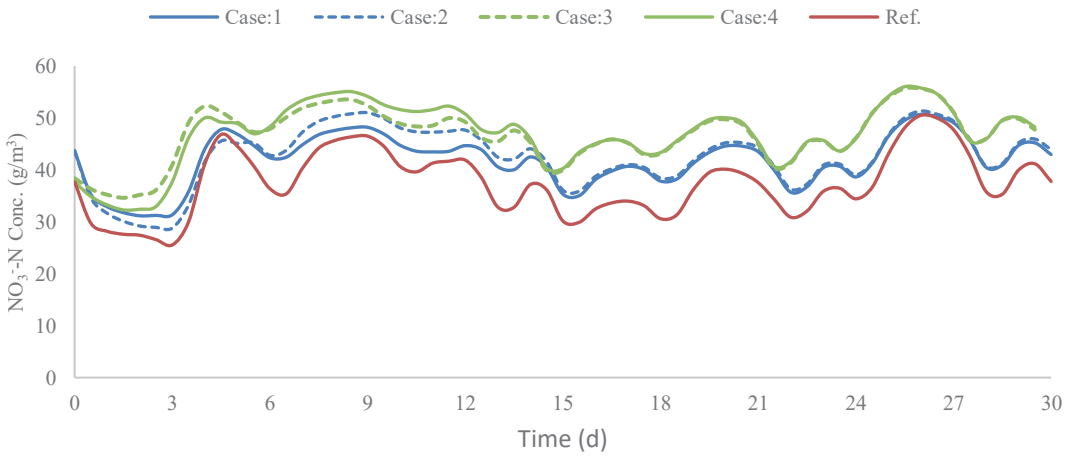
Internal recirculation is introduced, and anoxic zones are analyzed for 2 cases, one with only one zone and another with 2 zones with anoxic conditions. The simulated results for all the cases are presented in Figure 5.4.2, which showed a reduction in the emissions in all the cases than the reference calibrated emissions. Out of all the cases, 3 times the internal recirculation with 1 zone gave better outcomes for reducing the N_2O emissions compared with all the other cases, see Figure 5.4.2 (a). The reason for giving better results from this case is that increased internal recirculation impacts denitrification with the availability of nitrate as an electron acceptor. This resulted in efficient denitrification and acts as a sink for the produced N_2O.


Case:1
Case:2
Case:3
Case:4
Ref.
N2O Emission Factor (%)
Time (d)

(a)


Case:1
Case:2
Case:3
Case:4
Ref.
NH4+-N Conc. (g/m3)
Time (d)

(b)



(c)

Figure 5.4.2. Simulated results of the mitigation strategy approach of implementing internal recirculation for total N_2O emissions (a) from all the zones where floating hoods are arranged along with ammonium (b) and nitrate (c) concentrations. The red line indicates the reference line indicated the calibrated results.

Ammonium and nitrate concentrations are also investigated, and the simulated results are shown in Figure 5.4.2 (b and c). Results showed that both cases of internal recirculation with one anoxic zone showed less nitrification with high ammonium concentration and nitrification is high for the cases with two anoxic zones with almost similar ammonium concentrations for both cases. Regarding the nitrate concentrations, all the cases showed higher concentrations than the reference values this could be the reason that the addition of internal recirculation also has an impact on autotrophic microorganisms. Internal recirculation increases the population dynamics of autotrophs which enhances the nitrification process. Due to better nitrification, high nitrate can be available as electron acceptors to perform denitrification by heterotrophic denitrifiers and it is also explained in section 5.2.1 that nitrate is strongly correlated with N_2O emissions.

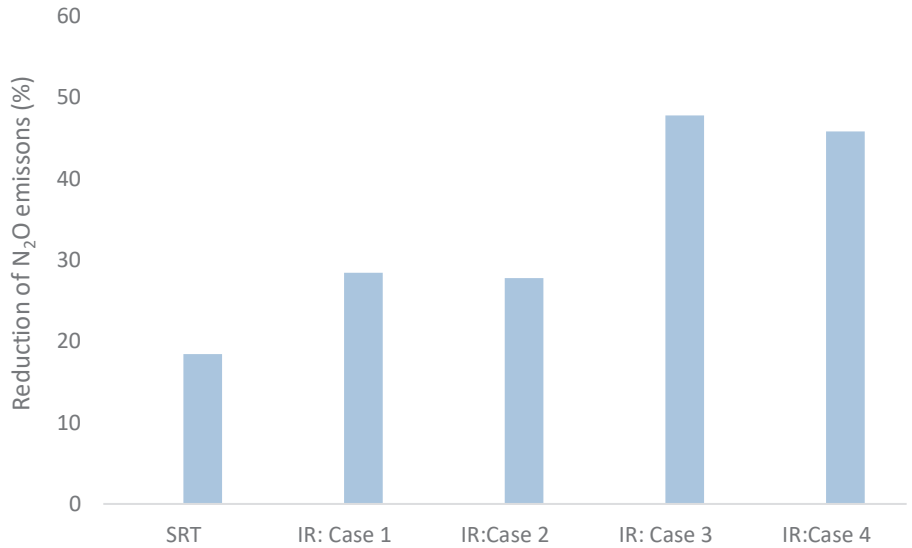


Figure 5.4.3. Comparison of all the proposed mitigation strategies for reducing total N_2O emissions.

When evaluating the percentage decrease of N_2O emissions from all the strategies, it is observed that (see Figure 5.4.3), all the strategies gave a good amount of reduction for N_2O emissions, but case 3 of internal recirculation with 1 anoxic zone provided the best results with a reduction of 46%. Variations in SRT with no requirement for process modifications and less energy demand reduced emissions by 18%. Even though this strategy comes with less energy demand, it is also crucial to take into account the increase of solids content in the activated sludge reactors and in RAS flows and additional air supply due to an increase in the SRT of the process. Internal recirculation can be implemented for mitigating N_2O emissions, but it requires modifications for process configuration and also the circulating flow demands energy for pumping the wastewater. As the Klagshamn treatment plant is willing to do modifications to the treatment plant it is efficient to implement internal recirculation with 1 anoxic zone to reduce the high N_2O emissions without compromising the effluent quality.

6 Conclusion

This study demonstrated a mechanistic model-based approach for identifying mitigation strategies for N_2O emissions from a full-scale WWTP. N_2O emissions are quantified at full-scale using multiple floating hoods arranged at the treatment process. Full-scale measurements are pre-processed and analysed for model simulations. The main findings from the modelling studies with the research question are:

- Calibration and validation results showed generally good results with few uncertainties regarding nitrate concentrations.
- With the adjusted set of kinetic parameters, the model predicted lower N_2O emissions for a few simulated periods due to high COD/N ratios in the incoming water for those periods.
- Model simulations were able to capture the N_2O emissions that are contributed by both heterotrophic denitrification pathways by OHOs and nitrifier denitrification by AOB organisms.
- Uncertainty is related to the method used for processing the data, as it involves various considerations and the dynamic variations are uncertain as the simulation results are compared with lab measurements, which are available only for a few days.
- The simulated model was capable to identify and evaluate different approaches for mitigation strategies to reduce N_2O emissions. Simulations revealed that internal recirculation for the secondary treatment process with one anoxic zone showed better results with 46% emission reductions.
- It is not observed a significant difference in treatment efficiency in terms of ammonium and nitrate concentrations with all the proposed strategies and the treatment efficiencies are within the acceptable range with the modifications.

7 Future Studies:

The following points can be considered suggestions for modelling N_2O emissions in future studies.

- Calibration and validation of the airflow rate and energy consumption of the proposed approaches could be useful for accurately understanding the efficiency of the proposed strategies.
- Model simulations can be performed for capturing the accurate dynamic variations of the process using hourly measurement values of the treatment process.
- Other process models which include all the pathways of N_2O emissions can be considered to precisely evaluate the contribution of each pathway for emissions.
- Studies can be performed to develop data-driven and hybrid models to integrate the mechanistic model with the data-driven model to accurately predict N_2O emissions.

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9 Appendix

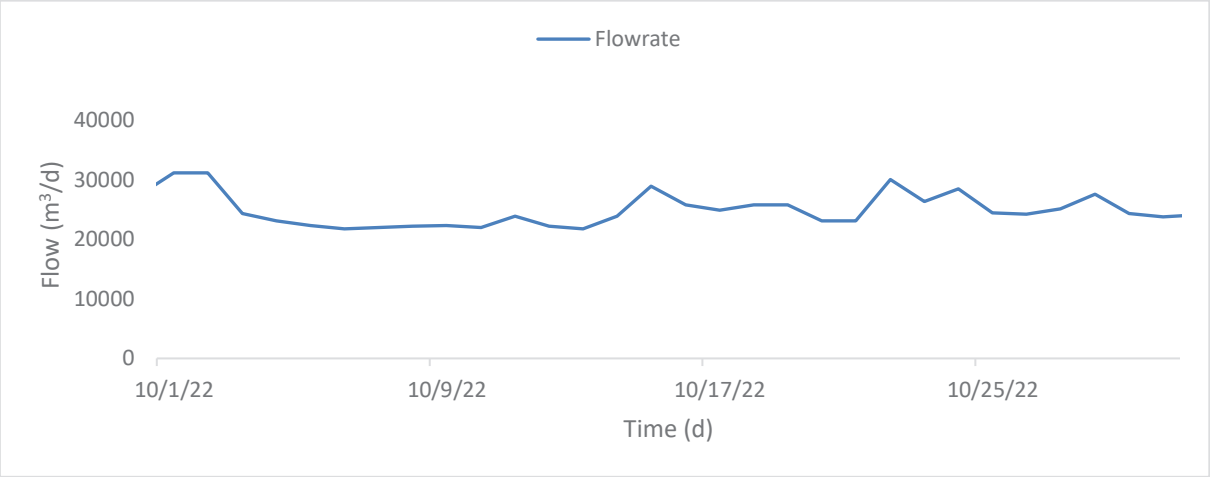

Figure 8. Incoming flow data for the periods 2022-01-01 to 2023-01-01

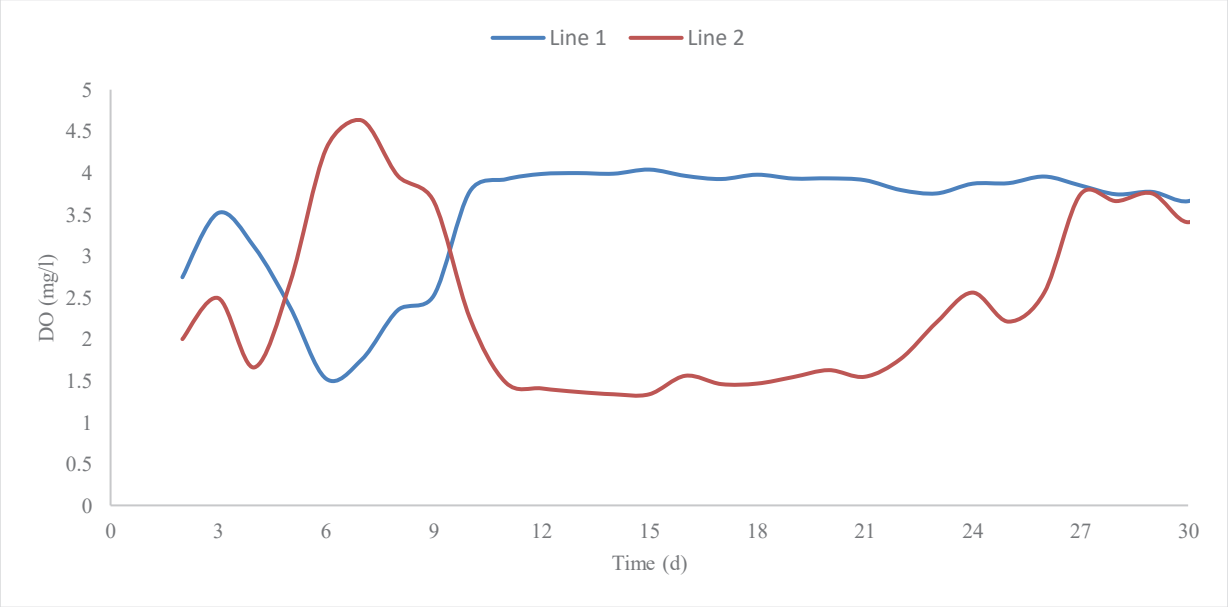

Figure 8 (I). Average DO set point values for line 1 and line 2 for the simulated periods 2022-10-01 to 2022-10-30.

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