Ministry of Environment and Gender Equality
Environmental Protection Agency

TwiN$_2$Ops Digital Twin for monitoring, prediction, and reduction of N_2O emissions from Operating wastewater treatment plantS MUDP-project

MUDP Report

March 2025

Publisher: The Danish Environmental Protection Agency

Editors:
Trine Dalkvist, DHI A/S
Fabio Polesel, DHI A/S
Carles Pellicer I Nacher, Novafos
Frida Viktor, DHI A/S
Henrik Refstrup Sørensen, DHI A/S
Peter Andreasen, DHI A/S
Mette Guldborg Hansen, FORS A/S
Tine Boye Andersen, FORS A/S
Lars Lund Schjødt, FORS A/S

ISBN: 978-87-7038-729-3

Miljøteknologisk Udviklings- og Demonstrationsprogram

Projektet, som er beskrevet i denne rapport, er støttet af Miljøteknologisk Udviklings- og Demonstrationsprogram (MUDP) under Miljøministeriet, der støtter udvikling, test og demonstration af miljøteknologi.

MUDP investerer i udvikling af fremtidens miljøteknologi til gavn for klima og miljø i Danmark og globalt, samtidig med at dansk vækst og beskæftigelse styrkes. Programmet understøtter dels den bredere miljødagsorden, herunder rent vand, ren luft og sikker kemi, men understøtter også regeringens målsætninger inden for klima, biodiversitet og cirkulær økonomi.

Det er MUDP's bestyrelse, som beslutter, hvilke projekter der skal modtage tilskud. Bestyrelsen betjenes af MUDP-sekretariatet i Miljøstyrelsen.

MUDP-sekretariatet i Miljøstyrelsen
Tolderlundsvej 5, 5000 Odense| Tlf. +45 72 54 40 00

Mail: ecoinnovation@mst.dk
MUDP's hjemmeside

Denne slutrapport er godkendt af MUDP, men det er alene rapportens forfatter/projektlederen, som er ansvarlige for indholdet. Rapporten må citeres med kildeangivelse.

Contents

1. Konklusion og sammenfatning

Lattergas (N_2O) er en kraftig drivhusgas med en global opvarmningseffekt ca. 273 gange større end kuldioxid (CO_2) over en 100-årig periode (IPCC AR6). I Danmark udgør N_2O-udledninger fra spildevandsrensningsanlæg 57 % af de direkte drivhusgasudledninger fra vandsektoren, svarende til omkring 67.000 tons CO_2-ækvivalenter årligt (Regeringens klimapartnerskaber, 2020). For at nå nationale og internationale klimamål er reduktion af N_2O-emissioner fra spildevandsrensning essentiel. Den danske regering har med "Klimaplanen for en Grøn Affaldssektor og Cirkulær Økonomi" sat ambitiøse mål om betydelige reduktioner i N_2O-emissioner inden 2025, hvilket kræver nye teknologiske løsninger.

Digitale tvillinger af renseanlæg, kan blive et afgørende værktøj til evaluering og optimering af driften på renseanlæggene. Denne teknologi integrerer realtidsdata fra sensorer, procesmodeller og driftsdata, hvilket gør det muligt at simulere og optimere anlæggets ydeevne. Mens der findes digitale tvillinger inden for flere sektorer, er de sjældent anvendt inden for spildevandsrensning eller fokuseret på N_2O-emissioner. En Digital Tvilling, der inkluderer et N_2O-modul kan understøtte evalueringen af optimerede tiltag for emissionsreduktion samtidig med at anlæggets øvrige mål, som udløbskvalitet og driftsomkostninger balanceres.

Dette projekt har til formål at:

- Udvikle og validere en procesmodel for N_2O-emissioner gennem test i både pilot- og fuldskala miljøer.
- Integrere N_2O-modulet i en Digital Tvilling, for at opnå realtids overvågning samt mulighed for at kontrollere emissionerne.
- Reducere N_2O-emissioner fra spildevandsrensning og derved støtte nationale og internationale klimamål.
- Øge renseanlæggenes operationelle effektivitet og bæredygtighed.

Aktiveret slam-modeller (ASM) har gennem de seneste 40 år dannet grundlag for mekanistisk modellering af biokemiske processer i renseanlæg og er løbende udviklet til at beskrive processer som nitrifikation-denitrifikation og fosforfjernelse. Med det øgede fokus på N_2O-emissioner fra renseanlæg er der gjort flere forsøg på at inkludere N_2O-relaterede processer i ASM. Til dette projekt blev modellerne ASM-NDHA og ASM2d-N_2O valgt til indledende test i et standard renseanlægsopsætning. Resultaterne viste, at ASM-NDHA leverede mere realistiske vækstprofiler for nitrificerende bakterier og blev derfor valgt til videre anvendelse i pilot- og fuldskalaanalyser af N_2O-dynamikker.

Til kalibrering af N_2O modellen blev der anvendt en trinvis tilgang til at justere de biokinetiske parametre, som beskriver N_2O-produktion og -reduktion i spildevandsrensningsprocessen. Formålet med denne proces var at opnå en model, der præcist kan efterligne N_2O-dynamikken og niveauerne på pilotanlæg. Modellen blev kalibreret i tre hovedtrin, hvor parametrene for de biologiske processer blev justeret baseret på eksperimentelle data.

1. **Kalibrering af N_2O-reduktionsparametre for heterotrofe bakterier**
   I første trin blev modellens reduktionsparametrene for N_2O hos heterotrofe bakterier kalibreret. Dette skete ved brug af eksperimentelle data, hvor N_2O-spikes blev kombi-

neret med varierende doseringer af kulstof under anoxiske forhold. Kalibreringen fokuserede på at justere procesparameteren KF_NOS til 100 mg-N/L, hvilket gav en god tilpasning af N_2O-reduktionsdynamikken i modellen.

2. **Kalibrering af NO_3^- og NO_2^- reduktionsparametre for heterotrofe bakterier**
   Andet trin involverede kalibrering af parametre for reduktion af nitrat (NO_3^-) og nitrit (NO_2^-) hos heterotrofe bakterier. Eksperimenter med NO_3-spikes og varierende kulstofdoser under anoxiske forhold blev brugt som grundlag, og de tidligere justerede N_2O-reduktionsparametre blev fastholdt. Kalibreringen fokuserede på parametrene KF_NOR, KNO_iNIR, KNO_iNOR og KNO_iNOS, som gav en rimelig modeltilpasning, men med mulighed for forbedring ved yderligere kalibrering med NO_2-spikes.
3. **Kalibrering af parametre for N_2O-produktion af AOB**
   I tredje trin blev parametrene for ammonium-oxiderende bakteriers (AOB's) N_2O-produktion kalibreret. Eksperimenter med ammonium (NH_4^+) -pulser under overskud af ilt blev anvendt, og parametrene fra de tidligere trin blev bevaret. De kalibrerede parametre inkluderede KNH_AOB, KO_NOB og $KHNO_2$_NOB, men en lav detaljeringsgrad af spildevandets organiske indhold reducerede kalibreringens præcision for N_2O-dynamikken i denne del af testene.

Resultaterne fra kalibreringen, medfører at modellen giver en passende tilpasning til eksperimentelle data for flere nøgleparametre, men yderligere eksperimenter og finjustering af data ville kunne øge nøjagtigheden.

Efter implementering og kalibrering af N_2O-processerne blev N_2O modellen implementeret i fuld skala for Bjergmarken renseanlæg i Roskilde (125.000 PE), drevet af FORS A/S. Renseanlæggets konfiguration blev modelleret i WEST-softwaren og omfattede energibalancer, dynamisk CO_2-aftryksberegning og en indløbsgenerator til forudsigelser af flow og koncentrationer baseret på nedbørsdata og oplandets karakteristika. Modellen inkluderede også Hubgrade® beluftnings- og fasestyringslogik for en præcis beskrivelse af anlægget. For at evaluere modellens evne til at simulere Bjergmarken Renseanlæg blev data fra perioden januar-april 2024 brugt. Sensordata for indløbsflow, temperatur, RAS flow samt fasekode blev brugt som input til modellen. Simuleringsdata viste god overensstemmelse med målte værdier for TSS (total suspended solids), NH_4-N(ammonium), NO_3-N og N_2O-N i procestankene, også under intense regnvejrsperioder.

Den verificerede model af Bjergmarken renseanlæg blev anvendt til at udvikle en online digital tvilling via TwinPlant-teknologien med N_2O-modellering. Den digitale tvilling skaber en virtuel kopi af anlægget og kombinerer:

1. **Real-time dataindsamling** fra mere end 100 sensorer med kvalitetskontrol og databehandling.
2. **Simulering og forudsigelse** gennem en WEST-model, der giver realtidsindblik og 48-timers prognoser.
3. **Brugerinterface og dashboards** til visualisering af data og evaluering af alternative driftsstrategier.
4. **Scenarie konfiguration og evaluering** hvor styringsparameter og input tidsserier kan justeres og effekten på opsatte nøgletal så som energibalancer, CO_2-aftryk, udløbskoncentrationer kan evalueres.

I projektets afsluttende fase blev den kalibrerede fuldskalamodel for Bjergmarken renseanlæg anvendt til en række scenarieanalyser med fokus på optimering af driften og reduktion af drivhusgasemissioner med fokus på N_2O. Indledende analyser for 2024 viste, at anlægget har en N_2O-emissionsfaktor på 1,3%, hvilket er ca. 50% højere end det nationale gennemsnit og svarer til en CO_2-udledning på 5,5 tons pr. dag.

Analyserne omfattede en række faktorer, der påvirker N_2O-emissioner, herunder ugentlig belastningsvariation, hvor de højeste N_2O-koncentrationer og ammoniumbelastninger observeres i morgentimerne fra tirsdag til fredag. Derudover viste de indledende analyser også at øgede NH_4-oxideringsrater fremmer øgede N_2O-koncentrationer. De høje koncentrationer af NH_4-N kan fremme hydroxylamine oxidering via AOB under nitrifikationen, der kan resultere i ukomplet oxidering under stressede forhold og dermed øge dannelsen af N_2O. Desuden bidrog høje DO-koncentrationer til stigende N_2O-niveauer, idet disse tilstande fremmer ufuldstændig oxidation af ammonium og dermed øger N_2O-produktionen. Ligeledes blev det observeret at lave TSS-koncentrationer og høje NO_3-niveauer kan øge N_2O koncentrationen, da begrænset biomassetilgængelighed og højt NO_3 kan skabe ubalance i denitrifikationsprocesserne og føre til netto N_2O-produktion.

Blandt scenarierne var optimeringstiltag som implementering af bufferkapacitet ved indløbet, justering af DO setpunkterne via beluftningsstyringen i Hubgrade, indførsel af kontinuerlige returslamflowrater (RAS) for tørvejr og regnvejr, tilføjelse af kulstofdosering i de anaerobe faser, samt ændring af beluftningsstrategien til en mere simpel fase og beluftningsstyring. Resultaterne viser at der kan opnås driftsbesparelser på op imod 25% og reduceringer i CO_{2eq} på op imod 30% mens udledningskvaliteten af både kvælstof, organisk materiale samt fosfor samtidig kan forbedres. En mere dybdegående evaluering af anlægget med kombinationer af scenarierne formodes at kunne vise endnu større forbedringer.

Scenarieanalyserne viser, at de undersøgte strategier kan gøre driften af Bjergmarken renseanlæg både mere effektiv og bæredygtig. Modellerne giver et samlet overblik over, hvordan forskellige tiltag påvirker nøgleparametre som klimapåvirkning, N_2O-emissioner, udløbskvalitet og driftsomkostninger under skiftende driftsforhold. Den integrerede model fremhæver synergier og nødvendige afvejninger mellem effektivitet, emissioner og udledningskvalitet. Dette overblik er værdifuldt for en optimal beslutningsproces og kan være med til at understøtte en mere bæredygtig og effektiv drift af anlægget og modvirke at ændringer foretaget medfører uønskede effekter.

2. Conclusion and summary

Nitrous oxide (N_2O) is a potent greenhouse gas, with a global warming potential approximately 273 times that of carbon dioxide (CO_2) over a 100-year period (IPCC AR6). In Denmark, N_2O emissions from wastewater treatment plants constitute 57% of the water sector's direct greenhouse gas emissions, amounting to around 67,000 tons of CO_2-equivalents annually (Regeringens klimapartnerskaber, 2020). Reducing N_2O emissions from wastewater treatment is crucial to meet national and international climate targets. The Danish government has set ambitious goals to significantly reduce N_2O emissions by 2025 through the "Climate Plan for a Green Waste Sector and Circular Economy," which will require new technological solutions.

Digital twins of treatment plants could become essential tools for evaluating and optimizing plant operations. This technology integrates real-time data from sensors, process models, and operational data, enabling the simulation and optimization of plant performance. While digital twins are used in various sectors, they are rarely applied in wastewater treatment or focused on N_2O emissions. A digital twin incorporating an N_2O module can support the evaluation of optimized strategies for emission reduction while balancing other plant goals, such as effluent quality and operational costs.

This project aims to:

- Develop and validate a process model for N_2O emissions through testing in both pilot and full-scale environments.
- Integrate the N_2O module into a digital twin to achieve real-time monitoring and control of emissions.
- Reduce N_2O emissions from wastewater treatment, supporting national and international climate goals.
- Improve the operational efficiency and sustainability of treatment plants.

Activated Sludge Models (ASM) have provided the foundation for mechanistic modeling of biochemical processes in treatment plants for over 40 years, evolving to describe processes like nitrification-denitrification and phosphorus removal. With the increased focus on N_2O emissions from treatment plants, there have been multiple efforts to include N_2O-related processes in ASMs. For this project, ASM-NDHA and ASM2d-N_2O were initially evaluated in a standard treatment plant setup. Results indicated that ASM-NDHA provided more realistic growth profiles for nitrifying bacteria and was selected for further pilot and full-scale analyses of N_2O dynamics.

A stepwise approach was used to calibrate the N_2O model by adjusting biokinetic parameters that describe N_2O production and reduction in the wastewater treatment process. This process aimed to achieve a model that accurately replicates N_2O dynamics and levels at the pilot plant. The model calibration was conducted in three main steps, with adjustments to biological process parameters based on experimental data:

1. **Calibration of N_2O Reduction Parameters for Heterotrophic Bacteria**
   In the first step, the model's reduction parameters for N_2O in heterotrophic bacteria were calibrated using experimental data where N_2O spikes were combined with varying carbon dosages under anoxic conditions. The focus was on adjusting the process parameter KF_NOS to 100 mg-N/L, which provided a good fit for N_2O reduction dynamics in the model.
2. **Calibration of NO_3^- and nitrite NO_2^- Reduction Parameters for Heterotrophic Bacteria**
   The second step involved calibrating parameters for the reduction of nitrate (NO_3^-)

and nitrite (NO_2^-) in heterotrophic bacteria. Experiments with NO_3^- spikes and varying carbon dosages under anoxic conditions served as a basis, with the previously adjusted N_2O reduction parameters retained. The calibration focused on parameters KF_NOR, KNO_iNIR, KNO_iNOR, and KNO_iNOS, achieving reasonable model accuracy but leaving room for improvement with further calibration using NO_2 spikes.

3. **Calibration of N_2O Production Parameters for AOB**
   In the third step, parameters for N_2O production by ammonia-oxidizing bacteria (AOB) were calibrated. Experiments with ammonium (NH_4^+) pulses in the presence of excess oxygen were used, while retaining parameters from the earlier steps. Calibrated parameters included KNH_AOB, KO_NOB, and $KHNO_2$_NOB. However, a low level of detail in the organic content of the wastewater reduced the calibration precision for N_2O dynamics in this part of the tests.

Calibration results indicated that the model achieved an appropriate fit for experimental data on several key parameters, though additional experiments and fine-tuning would increase accuracy.

Following the calibration of N_2O processes, the N_2O model was implemented at full scale for the Bjergmarken treatment plant in Roskilde (125,000 PE), operated by FORS A/S. The plant's configuration was modeled in WEST software, incorporating energy balances, dynamic CO_2 footprint calculations, and an inflow generator for flow and concentration forecasts based on rainfall data and catchment characteristics. The model also included Hubgrade® aeration and phase control logic to accurately describe plant operations. To assess the model's ability to simulate Bjergmarken, data from January to April 2024 were used, with sensor data on influent flow, temperature, RAS flow, and phase codes as model inputs. Simulation data showed good agreement with measured values for TSS, NH_4-N, NO_3-N, and N_2O-N in process tanks, even during heavy rainfall.

The verified model of the Bjergmarken WWTP was used to develop an online digital twin through TwinPlant technology with N_2O modeling. The digital twin creates a virtual copy of the plant, combining:

1. Real-time data collection from over one hundred sensors with quality control and data processing.
2. Simulation and prediction via a WEST model, providing real-time insights and 48-hour forecasts.
3. User interface and dashboards for data visualization and evaluation of alternative operational strategies.
4. Scenario configuration and evaluation, allowing for adjustment of control parameters and input time series to assess impacts on KPIs such as energy balances, CO_2 footprint, effluent concentrations, and operational costs.

In the final project phase, the calibrated full-scale model of Bjergmarken was applied to a series of scenario analyses focused on optimizing operations and reducing greenhouse gas emissions, with an emphasis on N_2O. Initial analyses from 2024 showed that the plant has an N_2O emission factor of 1.3%, which is about 50% higher than the national average, equating to a CO_2 emission of 5.5 tons per day.

The analyses explored a range of factors affecting N_2O emissions, including weekly load variations, with the highest N_2O concentrations and ammonium loads observed in the early morning hours from Tuesday to Friday. The initial analyses also indicated that higher NH_4 oxidation rates lead to increased N_2O concentrations. High NH_4^+ concentrations can enhance hydroxylamine oxidation via AOB during nitrification, which can result in incomplete oxidation under stressed conditions, thereby increasing N_2O formation. Additionally, high DO concentrations contributed to rising N_2O levels, as these conditions favor incomplete ammonium oxidation, thus boosting N_2O production. Furthermore, low TSS concentrations and high NO_3^- levels were found to elevate N_2O concentrations, as limited biomass availability and high NO_3^- levels can create imbalances in denitrification processes, leading to net N_2O production.

Optimization measures explored included implementing buffer capacity at the inlet, adjusting DO setpoints via aeration control in Hubgrade, introducing continuous return sludge flow rates (RAS) for dry and wet weather, adding carbon dosing in anaerobic phases, and shifting to a simpler phase and aeration control strategy. Results showed that operational savings of up to 25% and CO_2 eq reductions of up to 30% could be achieved while also improving effluent quality. A more in-depth evaluation of the plant with combinations of these scenarios is expected to show even greater improvements.

The scenario analyses demonstrate that the strategies explored can make the operation of the Bjergmarken plant both more efficient and sustainable. The models provide an overview of how various measures impact key parameters like climate footprint, N_2O emissions, effluent quality, and operational costs under changing conditions. This integrated model approach highlights synergies and necessary trade-offs between efficiency, emissions, and effluent quality, providing valuable insights for an optimal decision-making process and supporting more sustainable and efficient plant operation.

3. Introduction

Nitrous oxide (N_2O) is a potent greenhouse gas with a global warming potential approximately 273 times that of carbon dioxide (CO_2) over a 100-year period (IPCC AR6). Emissions of N_2O from wastewater treatment plants represent a significant portion of the total greenhouse gas emissions from the water sector. Specifically, in Denmark, N_2O emissions account for 57% of the direct greenhouse gas emissions from wastewater treatment, equating to around 67,000 tons of CO_2-equivalents per year (Regeringens klimapartnerskaber, 2020). Reducing N_2O emissions from wastewater treatment plants is crucial for meeting national and international climate targets. The Danish government has set ambitious goals to reduce greenhouse gas emissions as part of the "Climate Plan for a Green Waste Sector and Circular Economy," targeting a significant reduction in N_2O emissions by 2025. Achieving these targets requires innovative technological solutions that can be implemented on a large scale. Digital Twin technologies could represent attractive solutions to meet these regulatory demands efficiently.

Digital Twins are a promising technology that supports the optimal operation of wastewater treatment plants. A Digital Twin is a virtual representation of a physical system that uses real-time data to simulate, predict, and optimize performance. In the context of wastewater treatment, a Digital Twin can integrate various data sources, including process models, sensor data, and operational data, to provide a holistic view of plant operations. The market for digital solutions in the water sector is expected to grow steadily over the next decade, driven by regulatory pressure. The commercial potential is significant, with global market estimates for Digital Twin technologies in the water industry expected to reach nearly DKK 21 billion by 2026 (Klima-, Energi- og Forsyningsministeriet, 2020).
Currently, Digital Twins are used in various applications worldwide, but they do not typically include the quantification and management of N_2O emissions. By developing an N_2O module for the Digital Twin, users can not only reduce the costs associated with online measurements but also continuously evaluate and automatically identify optimized control measures for emission reduction. This system could allow users to monitor whether the implemented measures compromise other operational goals of the plant, such as effluent quality or other operational costs.

The expected outcomes of this project include:

- Development of a consensus process model for N_2O emissions, validated through pilot and full-scale testing.
- Integration of the N_2O module into the Digital Twin, enabling real-time monitoring and control of emissions.
- Reduction of N_2O emissions from wastewater treatment plants, contributing to national and international climate goals.
- Enhanced operational efficiency and sustainability of wastewater treatment plants.

This project will deliver a new digital technology for monitoring, predicting, and reducing N_2O emissions, developed and tested in pilot and full-scale operational environments. The integration of modelling and control approaches into a new Digital Twin technology represents a substantial technological advancement. The long-term application of this technology has the potential to achieve significant reductions in N_2O emissions, supporting national and international efforts to combat climate change and promote sustainable development goals.

4. Review of N_2O models and emission pathways

Hundreds of scientific studies have contributed to the significant development of the modelling practice on N_2O emissions during wastewater treatment operations. Such models focus on the description of the microbial pathways that have been identified as key contributors to N_2O emissions (TABLE 1):

- Nitrifier denitrification. Ammonia-oxidizing bacteria (AOB) convert ammonia (NH_3) to nitrite (NO_2^-) under aerobic conditions. When oxygen availability is low, AOBs are known to be able to use NO_2^- as terminal electron acceptor to sustain their metabolic function and limit NO_2^- accumulation, which is known to be inhibitory. N_2O is the final product of this pathway, with Nitric oxide (NO) as an intermediate. This process is catalysed by nitrite and nitric oxide reductases (NiR, NoR). Low dissolved oxygen (DO) and high nitrite accumulation levels are known to promote N_2O production through this pathway. This pathway is significant in wastewater treatment plants (WWTPs).
- Incomplete hydroxylamine oxidation by AOB under nitrifier nitrification. Oxidation of NH_3 to NO_2^- with DO as terminal electron acceptor is catalysed by Ammonia Monooxygenase (AMO) and Hydroxylamine Oxidoreductase (HAO) in a 2-step process with hydroxylamine (NH_2OH) as an intermediate. However, this oxidation is incomplete under environmentally stress conditions, leading to the production of nitric oxide (NO) and subsequently N_2O, as described in the nitrifier denitrification pathway Low DO and high ammonia oxidation rates are known to favour this pathway.
- Heterotrophic denitrification. Heterotrophic bacteria sustain the microbial aerobic oxidation of a wide range of organic carbon contaminants into CO_2. Under DO limitation, this bacterial group can utilize nitrate or nitrite as electron acceptor to sustain their metabolism. This process plays a crucial role in nitrogen removal processes in most WWTPs. The main product of this microbial reaction is nitrogen gas (N_2), with NO, and N_2O as intermediates. Situations of environmental stress such as low C (electron donor) availability or suboptimal pH and temperature conditions, can influence the electron affinities of the different enzymes catalysing the process and lead to net N_2O emissions.
- Abiotic production. High NO_2^- or NH_2OH concentrations in combination with presence of trace metals such as Fe or Mn or low pH (<5) are known to catalyse chemical reactions that lead to the production of N_2O.

TABLE 1. N_2O pathways.

Pathway	Microorganisms Involved	Key Steps	Conditions Favouring N_2O Production
Nitrifier Denitrification	Ammonia-oxidizing bacteria (AOB)	$NH_3 \rightarrow NH_2OH \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O$	Low DO, high nitrite, NH_2OH accumulation
Incomplete Hydroxylamine Oxidation	Ammonia-oxidizing bacteria (AOB)	$NH_3 \rightarrow NH_2OH \rightarrow NO \rightarrow N_2O$	High NH_3 oxidation rates, low DO, NH_2OH accumulation
Heterotrophic Denitrification	Heterotrophic Bacteria (HB)	$NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2$	Adequate carbon, low DO, optimal pH and temperature, high nitrate/nitrite
Abiotic Pathways	None	$NH_2OH + HNO_2 / O_2 \rightarrow N_2O$; $HNO_2 + Fe^{2+} \rightarrow N_2O$	High nitrite/NH_2OH, presence of trace metals, acidic pH

5. Model selection and initial evaluation

In the past four decades, Activated Sludge Models (ASM) have represented the conventional framework for mechanistic modelling of biochemical processes in biological wastewater treatment systems. These models have progressively evolved to describe dynamics of nitrogen removal (nitrification-denitrification), chemical and enhanced biological phosphorus removal, substrate storage and utilization.

Due to the emerging relevance of N_2O generation in wastewater treatment plants, several attempts have been made to incorporate the relevant processes in the ASM framework. Prominent examples of mechanistic models describing N_2O generation and utilization mechanisms include:

- ASMN (Hiatt and Grady, 2008)
- ASMG1 (Guo and Vanrolleghem, 2014)
- ASM-NDHA (Doming Felez and Smets, 2020)
- ASM2d-N2O (Solis et al., 2022), including the description of autotrophic N_2O generation made by Pocquet et al. (2016).

Considering the detailed description of the underlying mechanisms, as well as the comprehensive model development, calibration and validation using laboratory-scale and full-scale data, the models ASM-NDHA and ASM2d-N2O were selected for initial testing using a conventional wastewater treatment configuration (the benchmark simulation model no. 1, BSM1: Alex et al., 2008). The configuration, including a typical influent, five activated sludge reactors in series (two non-aerated and three aerated) and a secondary settler, was implemented in the software WEST (DHI A/S, Denmark) along with the two process models. An extension of the ASM-NDHA including phosphorus removal processes (Chrysochoidis et al., 2023) was considered. The comparison of the two models (FIGURE 1) revealed that AOB and NOB growth was realistic as resulting from ASM-NDHA simulations, while limited NOB growth could be achieved using ASM2d-N2O. This finding, while not ruling out the capabilities of the ASM2d-N2O model, revealed the potential need for a more thorough calibration effort to adjust the default parameter set. Therefore, the ASM-NDHA model was selected for further use in the project to describe N_2O dynamics pilot-scale and full-scale WWTPs.

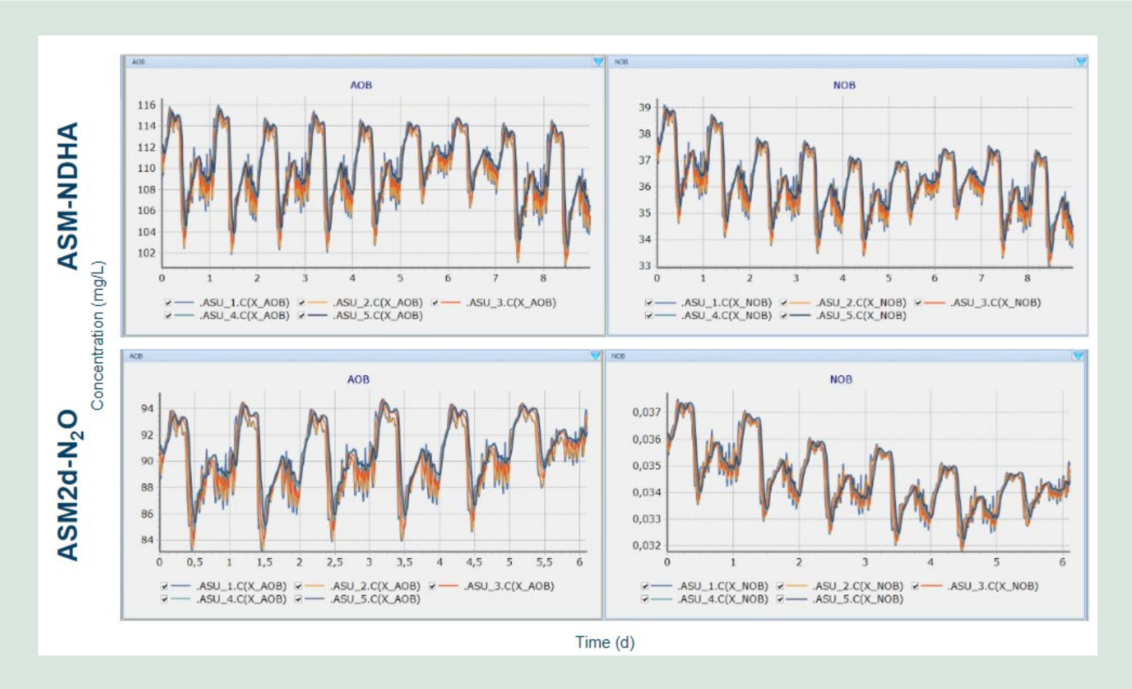

FIGURE 1. Comparison of simulation results (AOB and NOB concentrations) using ASM-NDHA and ASM2D-N2O process models in the BSM1 configuration.

6. Access to N_2O and process data from the pilot plant at Marselisborg AAV

Aarhus Vand kindly provided data for model calibration from a series of tests carried out in their Activated Sludge pilot plant at the Marselisborg WWTP, Denmark. This test facility is fed with primary treated wastewater from the WWTP with intermittent additions of reject from the dewatering process of their digested sludge. Dencerin (DAKA A/S, Denmark) was dosed at varying rates as organic carbon supplement to sustain or boost denitrification.

The plant is equipped with a Hydrolysis tank followed by 2 process tanks and a small secondary clarifier with sludge recirculation and sludge wasting capabilities (FIGURE 2). The bioprocesses taking place are monitored with TSS, NH_4-N NO_3-N, N_2O, DO, Temperature, flow, pH, and conductivity sensors at key locations. The online data collected, with a resolution of 1 min, provided enough level of detail to undertake the calibration of the selected process model.

A series of batch experiments were conducted by Aarhus Vand with the aim to investigate if an increased load or nitrification rate impacts nitrous oxide formation in the aerobic stage, and to explore the relationship between carbon dosing, denitrification rate, and nitrous oxide in the anoxic stage. Only one tank was used for the tests using bacterial biomass from the plant's process tanks. The only liquid addition during the tests was Dencerin. The amounts dosed did not impact the liquid volume at the tank significantly. A detailed description and interpretation of the results can be found in (Rebsdorf et. al. 2024). Here we will focus on the changes to the model structure and parameter calibration to make the model fit the experimental observations by Aarhus Vand.

The biokinetic parameters for the different processes in the model were calibrated using a stepwise approach:

1. N_2O reduction parameters for Heterotrophic Bacteria were calibrated using data from experiments with N_2O pulses and varying carbon dosing under anoxic conditions.
2. NO_3^- and NO_2^- reduction parameters for Heterotrophic Bacteria were calibrated using data from experiments with NO_3-N pulses and varying carbon dosing under anoxic conditions. The parameters identified in step 1 above were locked.
3. Parameters associated with N_2O production by AOB were calibrated using data from experiments with NH_4-N pulses under excess DO. The parameters identified in steps 1 and 2 above were locked.

A simple model was built in WEST with a single process tank (FIGURE 2). Carbon dosing was simulated as an influent stream to the tank, with the C and N content of Dencerin. Bubbling of N_2O was simulated with a typical mass transfer function (N_2O transfer rate = kLa * ($S_{N_2O\_gas}$/H – $S_{N_2O\_process\ tank}$)) with a fitted kLa while N_2O was sparged in the tank and a kLa of 0 when the bubbling was turned off. Initial biomass concentrations were estimated from previous pilot operational data and typical stoichiometric relationships (Henze et al., 2008).

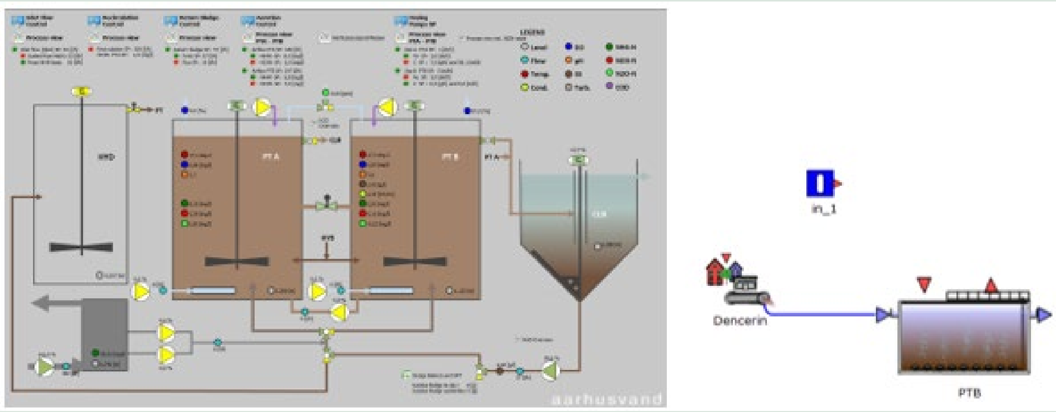

FIGURE 2. WEST process model for the batch tests performed in the Marselisborg pilot plant.

6.1 Calibration step 1: Removal of N_2O pulses with varying C dosing during denitrification

Evaluation of the data suggests that N_2O denitrification is catalysed by a higher C dosing rate (FIGURE 3). The correlation between C dosing rate and specific N_2O reduction rate was improved by normalizing the data at 20° C and a pH of 7,9 by using the equations suggested in the chosen model. Consequently, those corrections were incorporated into the model. pH and temperature were given as known inputs.

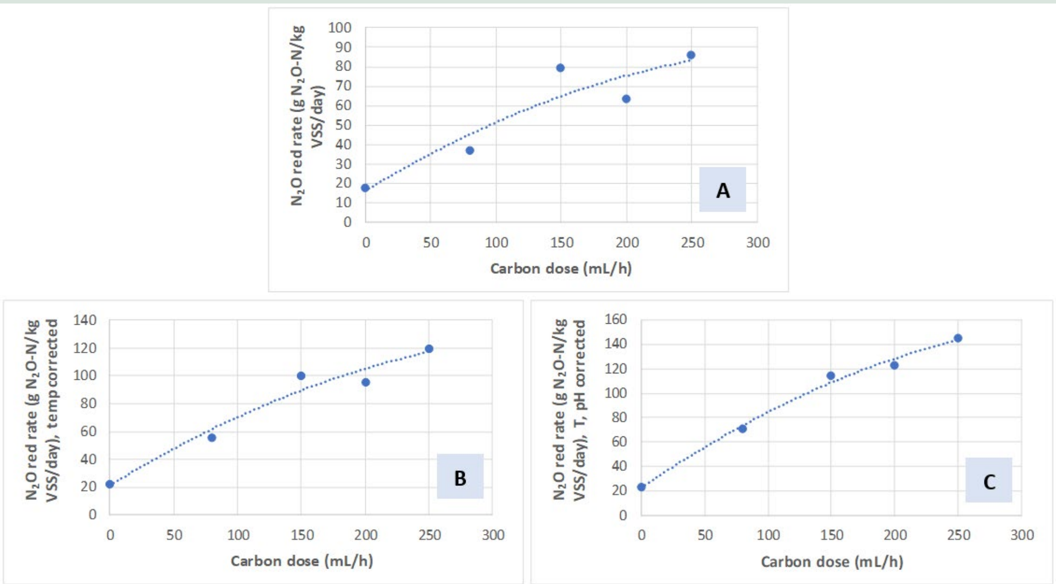

FIGURE 3. A) Correlation of N_2O reduction rate with C dose as collected in the batch tests. B) Normalised at a temperature of 20 °C. C) Normalised at a temperature of 20 °C and pH 7,9.

Manual calibration of the process parameter K_{F_NOS} (100 mg-N/L) yielded a good fit of the N_2O reduction dynamics for all experiments (FIGURE 4). The rest of the parameter were left as shown in the original dataset of the calibrated NADH model (Domingo-Felez and Smets, 2020). The very high value for the fitted parameter could be explained by insufficient data on the organic C fraction of the wastewater.

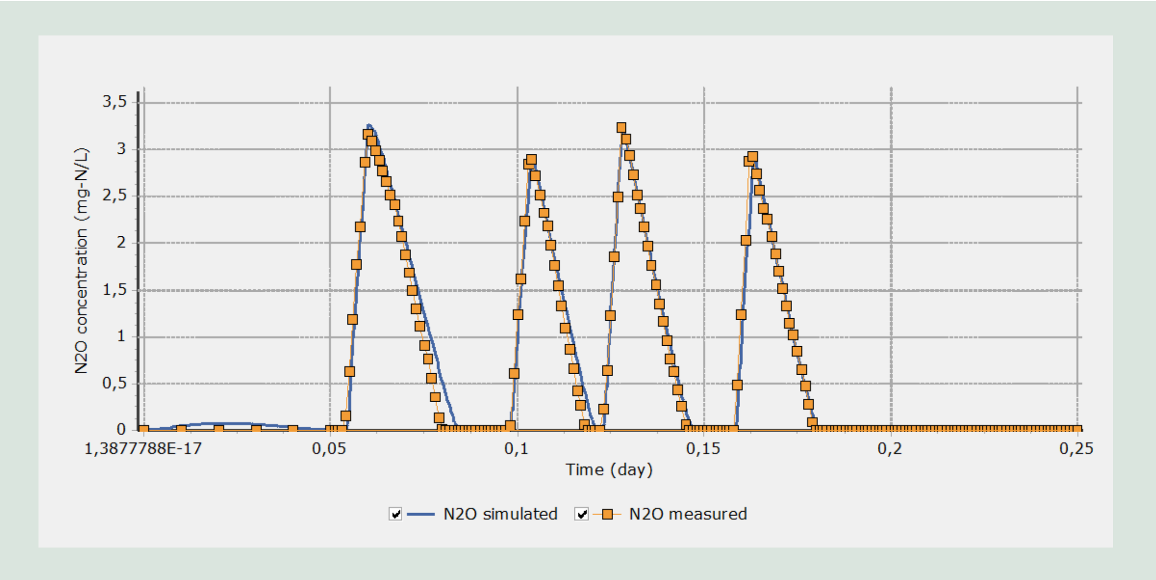

FIGURE 4. Model fit for the N_2O sparging and reduction with a C dose of 250 ml/h.

6.2 Calibration step 2: Nitrous oxide production during denitrification of NO_3-N pulses with varying C dosing

As expected, NO_3^- reduction is catalysed by a higher dosing rate of organic C (FIGURE 5). Normalization of the data at 20°C improved the correlation slightly. Normalization of the data collected in the different tests at a pH of 7,9 did not show any improvement in the fit. Therefore, it was discarded to include a correction factor for pH in the process equations for NO_3^- reduction. The temperature corrections were implemented as suggested in (Domingo-Félez and Smets, 2020).

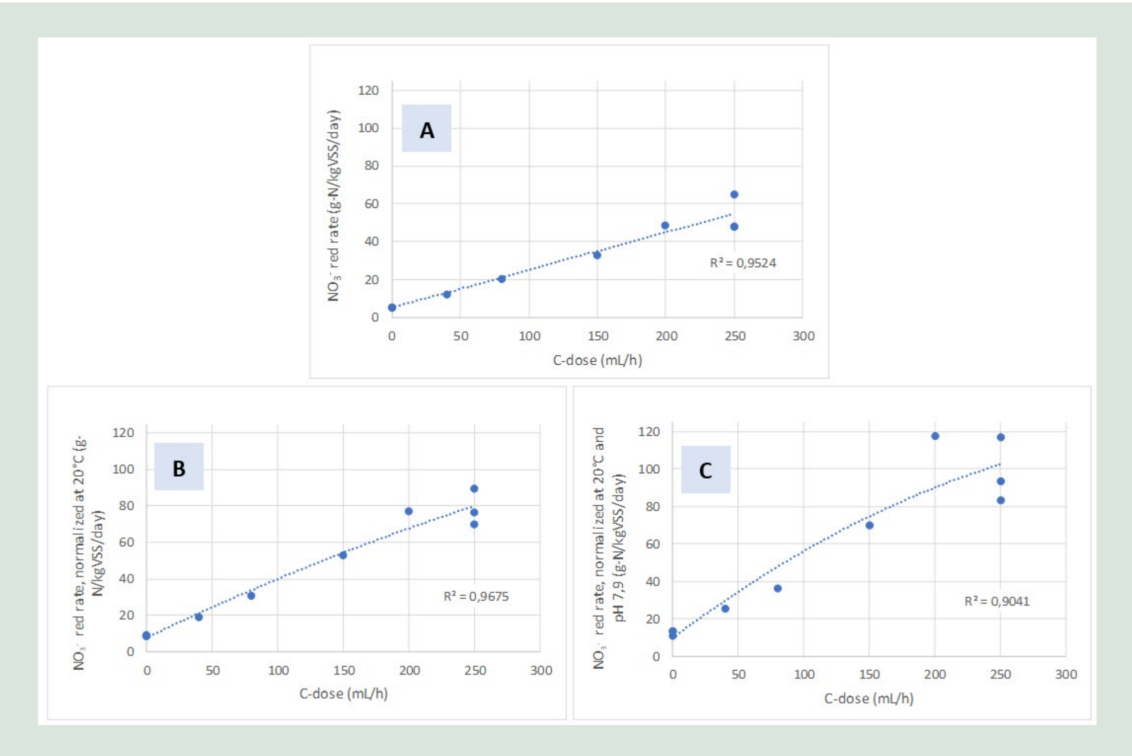

FIGURE 5. A) Correlation of NO_3^- reduction rate with C dose as collected in the batch tests. B) Normalised at a temperature of 20 °C. C) Normalised at a temperature of 20 °C and pH 7,9.

The NO_3^- reduction rates observed are low in comparison to standard design values for traditional Activated Sludge systems (Ye et al., 2020) but are within the range observed in systems with simultaneous N/DN (FIGURE 6). Data does not show a strong correlation between the NO_3^- reduction rate and N_2O production rates. However, the highest dosing rates of C seem to be associated to high N_2O emissions. Therefore, there could be a critical C-dose rate at which nitrate reduction rates are enhanced, while keeping a balanced electron supply to the N_2O reduction step in the denitrification process. This could be justified by a lower competition ability for the N_2O reductase enzyme to divert the electrons available from the C source into the N_2O reduction pathway (Pan et al. 2013).

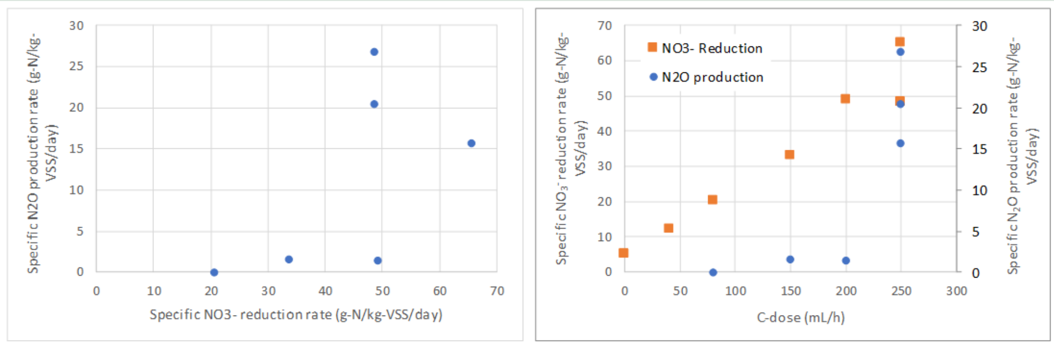

FIGURE 6. Correlation of NO_3^- reduction rate with N_2O production rate.

A reasonable model fit to the available experimental data could be achieved by manually calibrating the following parameter set on top of the parameters calibrated in Step 1: K_{F_NOR} (100 mg-N/L), K_{NO_iNIR} (0,2 mg-N/L), K_{NO_iNOR} (0,1 mg-N/L), and K_{NO_iNOS} (0,01 mg-N/L) (FIGURE 7). Higher accuracy could probably be obtained by including the calibration experiments with NO_2-N spikes. As for the previous case, the high half saturation constant for fermentables in the NO reduction step, could be related to insufficient characterization of the organic C fraction in the wastewater.

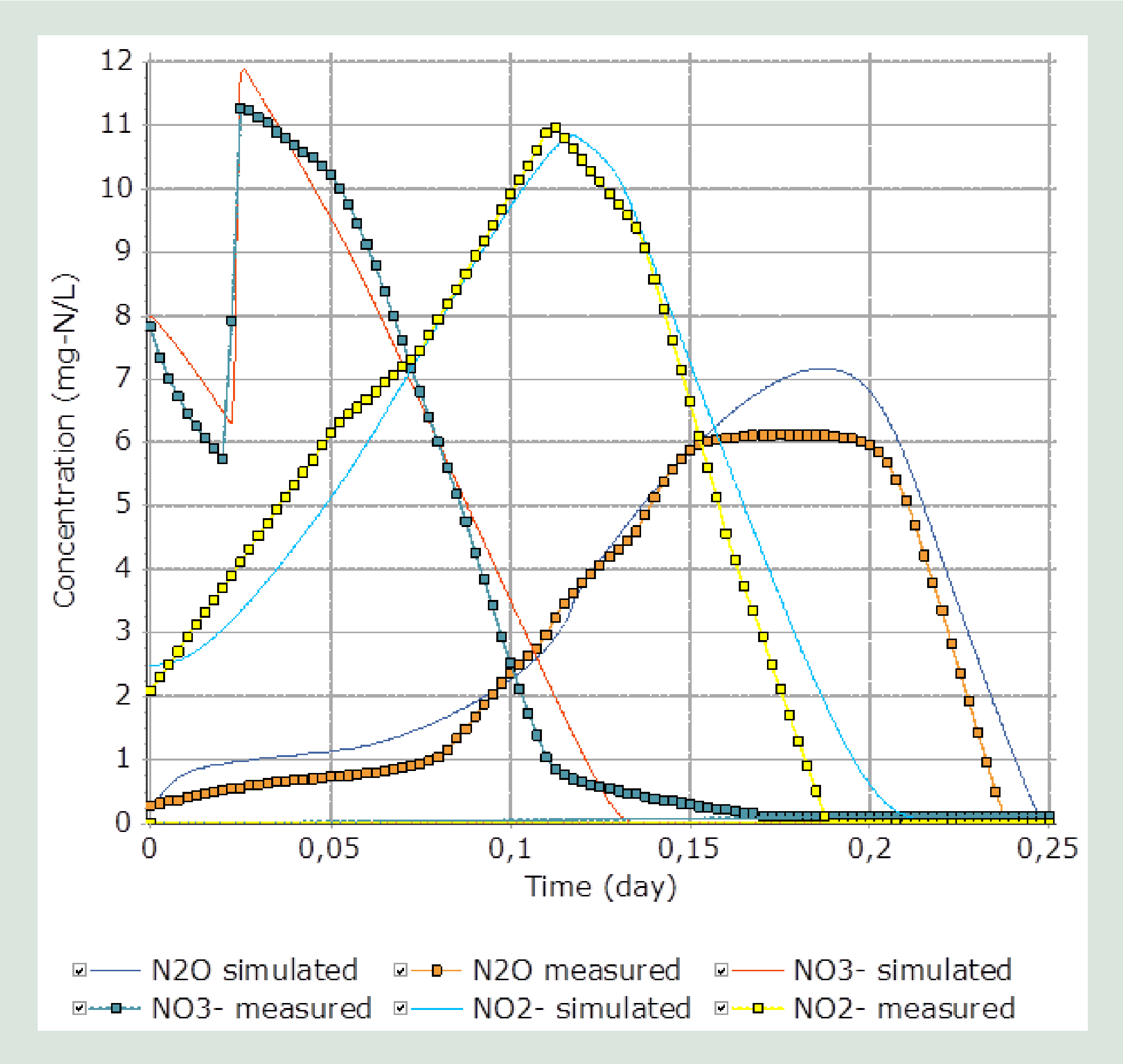

FIGURE 7. Model fit for experiments with NO_3-N spiking and external carbon dosing.

6.3 Calibration step 3: N_2O production during nitrification of an NH_4-N pulse

NH_4-N and NO_3-N in aerobic experiments at full blower capacity were fitted by the model by modifying the parameters KNH_AOB (0,02 mg-N/L), KO_NOB (0,15 mg/L), and KHNO2_NOB (0,001 mg-N/L). The parameters determined in Step 1 and 2 of this calibration exercise were left untouched. Inflow and RAS into the pilot were restarted around time 0,22 days. The wastewater fed into the process tank did not have a high level of characterization. As a result, the calibration of the N_2O dynamics for this test showed reduced accuracy (FIGURE 8).

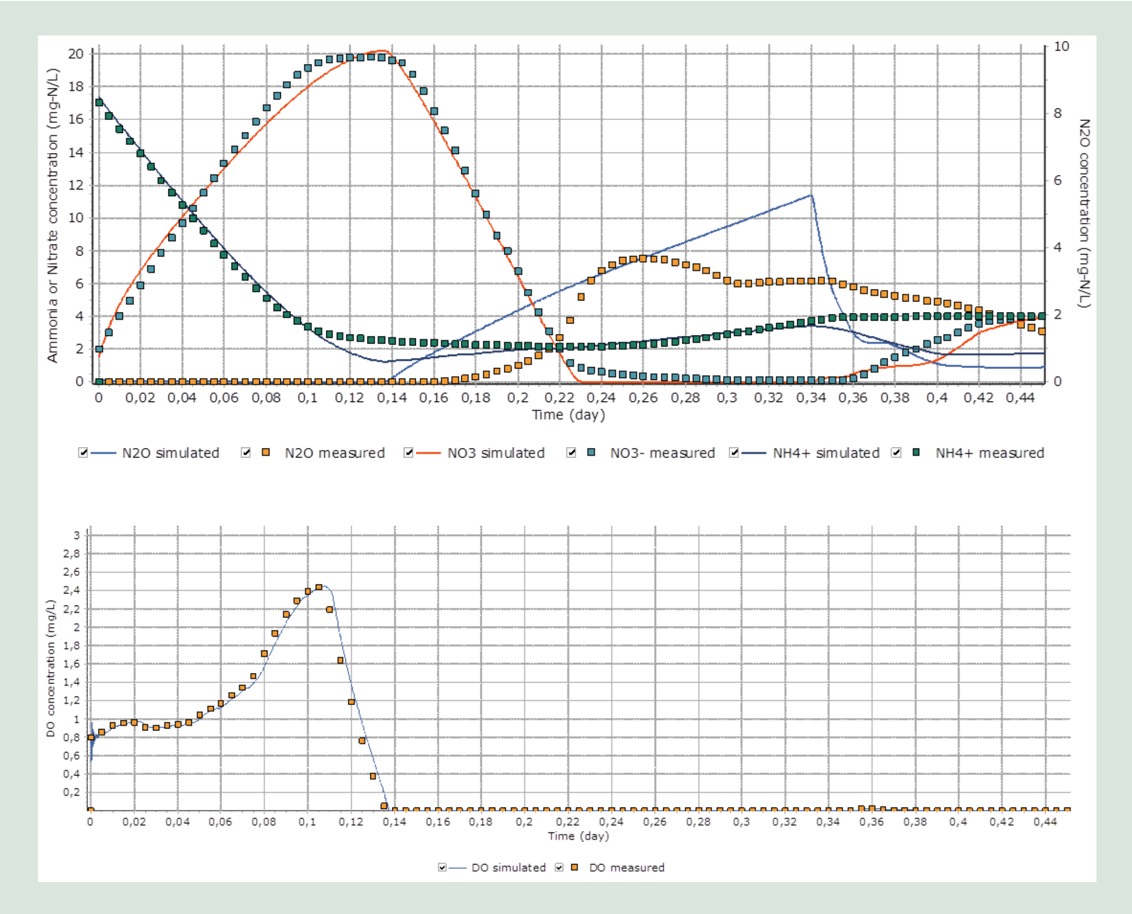

FIGURE 8. Correlation of NO_3^- reduction rate with N_2O production rate.

7. Full scale implementation of N_2O module at Bjergmarken WWTP

Following the evaluation of N_2O generation and utilization processes under controlled conditions in a pilot-scale system, the resulting mechanistic model was applied to describe N_2O dynamics in a full-scale WWTP. The WWTP considered for this task was Bjergmarken WWTP (125,000 PE), operated by FORS A/S and located in Roskilde (Denmark). The WWTP (FIGURE 9) configuration includes (i) biological treatment using the BiodeniPho® process, with a pre-anaerobic tank and 6 alternating aerated/non-aerated tanks (four with bottom aeration – L01, L02, L03 and L04 – and two with surface aeration – L11 and L12); (ii) 10 secondary settlers (nine longitudinal and one circular); (iii) dosing (PAX and PIX) for chemical phosphorus removal; (iv) sludge treatment including pre- and post-dewatering and mesophilic anaerobic digestion.

The configuration of the WWTP was implemented in the software WEST, and included (i) the description of energy (power and heat) balances including consumption (aeration, pumping, mixing), production from biogas, solar photovoltaic and heat pump installed at the WWTP effluent; (ii) the dynamic calculation of the CO_2 footprint of the WWTP based on direct emissions (e.g., N_2O-N) and indirect emissions (e.g., power and chemical use).

Being of high importance for an accurate description of N_2O dynamics in biological process tanks, the model also incorporates a detailed description of the control logics at the WWTP, specifically for aeration. The implemented logic reproduces the Hubgrade® aeration control, i.e.: (i) the alternation of up to 36 states for each process tank line, resulting from the combination of aeration/non-aeration/settling phases and inflow/outflow directions between process tanks in each line; (ii) the calculation of the dissolved oxygen (DO) set-point as a function of the measured NH_4-N concentration in the process tank.

FIGURE 9. Aerial view of Bjergmarken WWTP (Roskilde, Denmark).

Due to low frequency (monthly or bi-monthly) of water quality laboratory data (e.g., COD, TN, TP) available for the influent, the WWTP model was complemented by an influent generator model, which allows predicting influent flows and concentrations at high resolution based on catchment characteristics (population, area) and precipitation data. An example of the predictions provided by the influent generator is provided in FIGURE 10.

For the modelling of N_2O dynamics in Bjergmarken WWTP, the period January-April 2024 was selected due to the availability of measured data from online sensors. Data used for the model evaluation included, among others, NH_4-N concentration in the influent to the pre-anaerobic tanks, MLSS concentrations in process tanks (L02 and L03), NH_4-N and NO_3-N concentrations in process tanks (L01, L02, L03, L04, L11, L12) and liquid phase N_2O-N concentrations in process tanks (L02, L03, LT11, LT12).

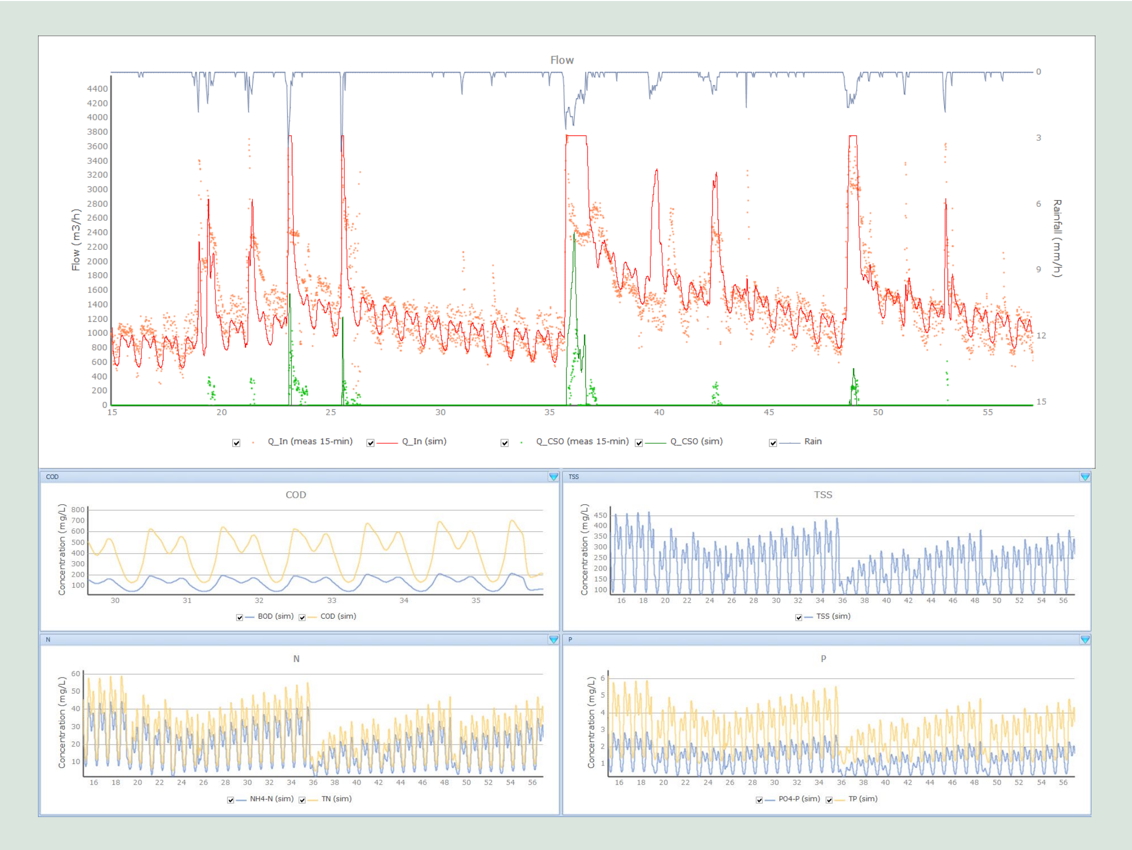

FIGURE 10. Influent generator simulation results for Bjergmarken WWTP: Influent flow (including comparison of measurements (markers) and simulaitons (line) and concentrations of COD, TSS, TN, NH_4-N, TP and PO4-P.

Modelling results for Bjergmarken WWTP are presented in FIGURE 11-FIGURE 14. The results show details of model predictions and measured data for process tanks L02 in February 2024, showing generally a good match both in terms of values and dynamics for MLSS, NH_4-N, NO_3-N and N_2O-N concentrations.

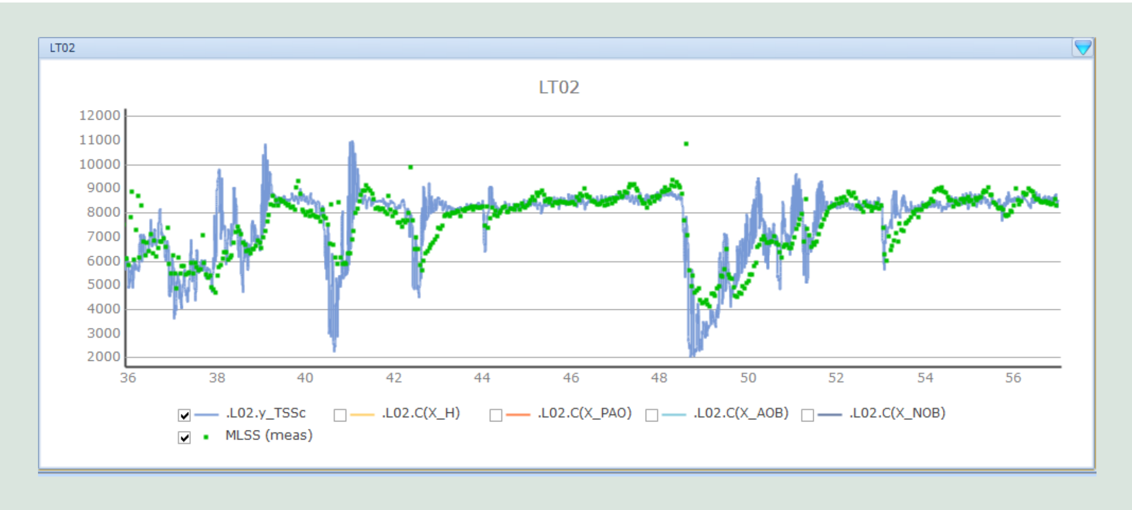

FIGURE 11. Simulation results (line) and measurements (markers) for MLSS concentrations in process tank LT02.

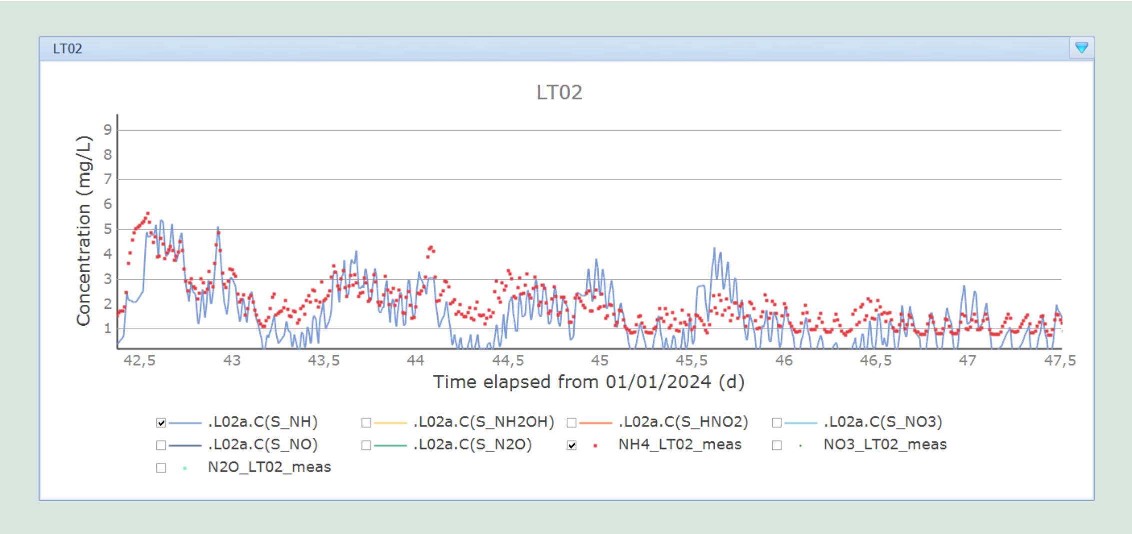

FIGURE 12. Simulation results (line) and measurements (markers) for NH_4-N concentrations in process tank LT02.

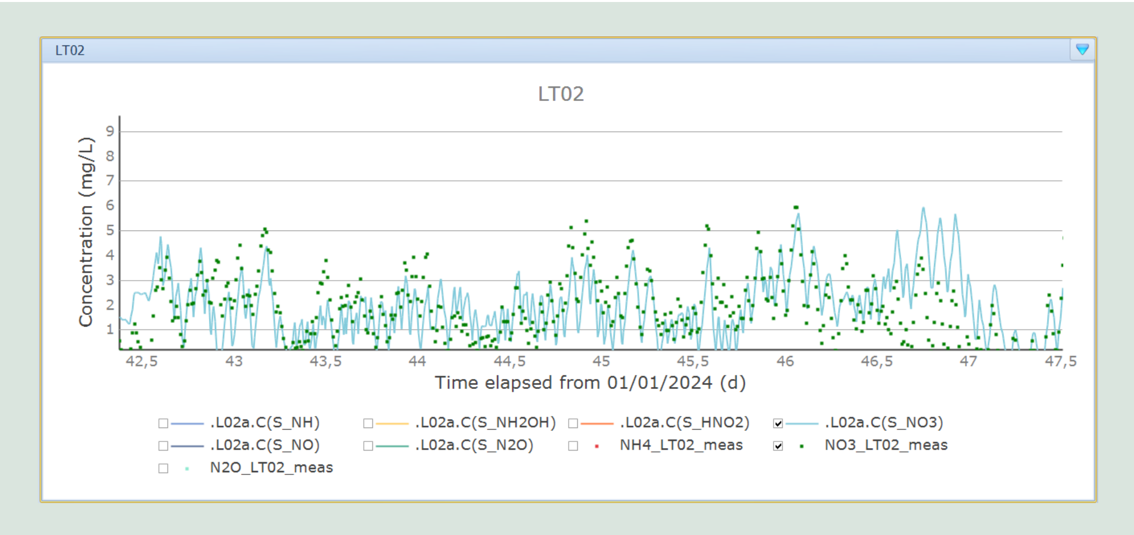

FIGURE 13. Simulation results (line) and measurements (markers) for NO_3-N concentrations in process tank LT02.

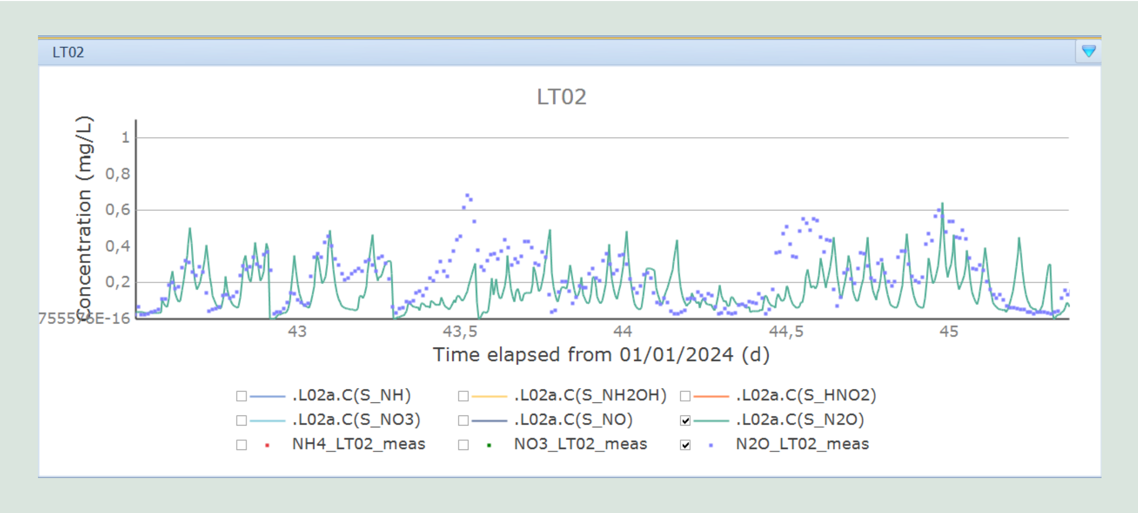

FIGURE 14. Simulation results (line) and measurements (markers) for N_2O-N concentrations in process tank LT02.

Fluctuations in liquid-phase N_2O-N concentrations were observed during the period of interest, and specific focus was given to ensure that the modelling approach used could capture these fluctuations. An example of this is presented in FIGURE 15, showing a considerable increase in N_2O-N concentrations as a result of a fast decrease in the MLSS concentration in process tank L03, possibly due to biomass washout (and thus reduced biological capacity) during a wet-weather event. The model accurately captured this event, which likely contributed to a major, yet temporary, increase in the N_2O emissions from the WWTP.

FIGURE 15. Example of increased N_2O-N concentrations as a result of biomass washout in process tank LT03.

8. Implementation of a digital twin of Bjergmarken WWTP

The verified model of Bjergmarken WWTP, as presented in the previous chapter, was used as the backbone for the implementation of an online digital twin of the WWTP. The digital twin implementation, based on the TwinPlant technology with integration of N_2O modelling, aimed at providing a virtual replica of the WWTP and combines the following elements:

1) Acquisition of real-time data from more than 100 sensors and meters installed at Bjergmarken WWTP, occurring with an hourly schedule and a 1-minute resolution. Real-time data are quality checked and pre-processed (e.g., in case of gaps or unrealistic values) as well as post-processed, allowing for the identification of possible sensor anomalies.
2) A WEST model of the WWTP (see chapter 5), providing live simulations of the plant behaviour based on the acquired online data as well as forecasting in the following 48 hours through influent predictions and weather forecast data.
3) A web-based user interface for the visualization and advanced dashboarding of post-processed measured and simulated data, as well as the evaluation of alternative operational scenarios.

The information provided by the digital twin is exemplified in FIGURE 16-FIGURE 19. FIGURE 16 presents the visualization of measured and simulated nitrogen species concentrations in process tank L02, comparing online data with modelling results and allowing to keep track of the reliability of the underlying process model. This further allows to identify potential pitfalls in the model (requiring adjustment and/or recalibration) and/or in the data (e.g., requiring sensor maintenance). The visualization of historical and real-time data is complemented by a forecast, where simulation results are presented for the 48 hours following the time of forecast (ToF).

FIGURE 17 shows an example for MLSS concentration in L02, where the prediction defines the expected MLSS concentration based on the current operation of the plant and expected influent conditions. The digital twin also provides predictions for typical indicators in locations not monitored using online sensors, thereby effectively providing “soft sensor” data, as shown for effluent COD and BOD (FIGURE 18).

A dedicated dashboard is also provided for key performance indicators (KPIs) (FIGURE 19), summarizing the status of the plant with respect to holistic parameters and therefore allowing to benchmark the performance against, e.g., country-wide data. In relation to the carbon footprint, the digital twin also provides a detailed and high-resolution prediction of the contribution to CO_2 emissions from different sources, including N_2O.

Furthermore, the digital twin provides scenario generation capabilities, where the user can configure scenarios, run simulations and compare results to baseline simulations (FIGURE 20). Bjergmarken TwinPlant is configured with Learning and Predictive Plant allowing the user to run scenario simulations on historical and predictive data.

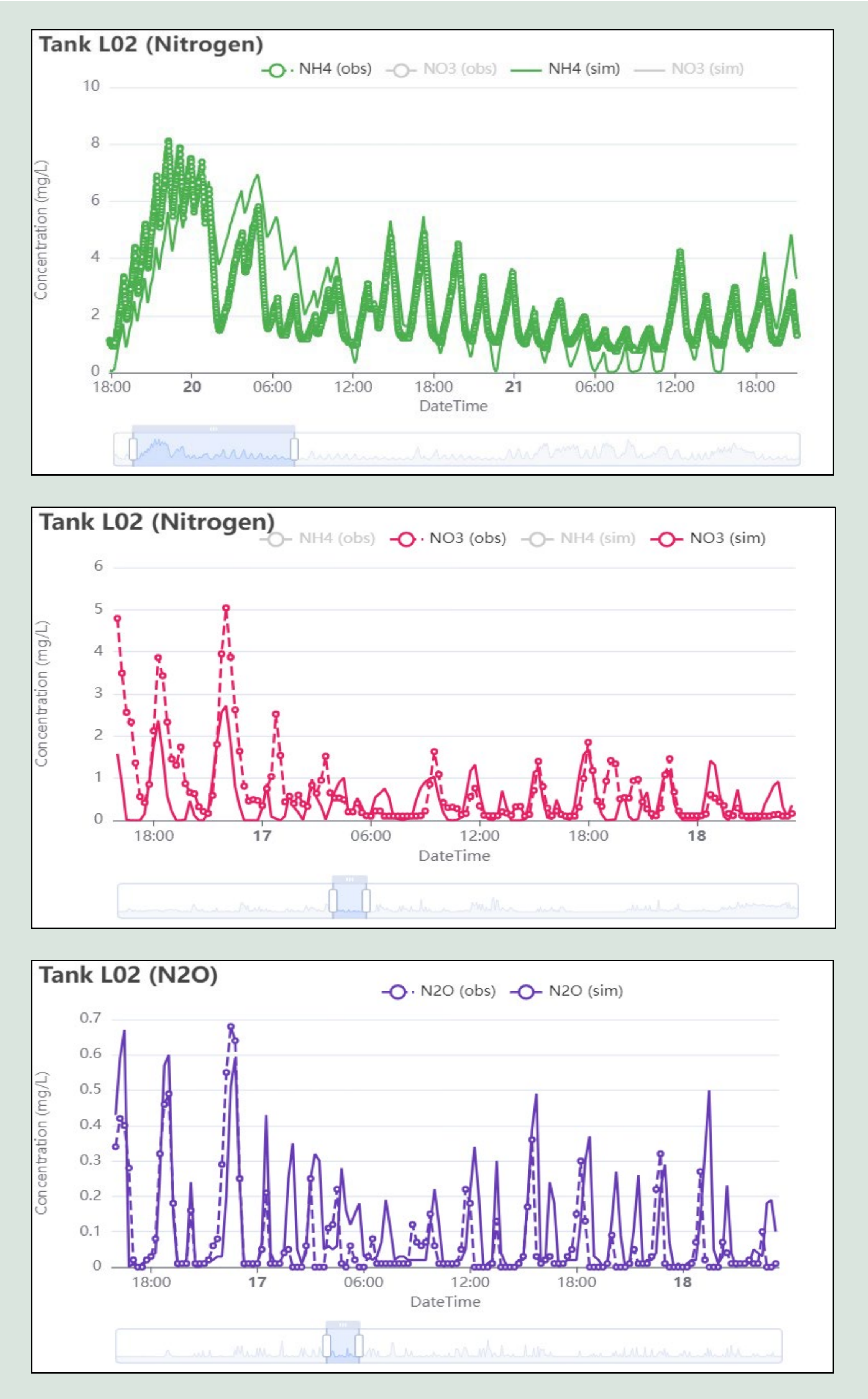
Tank L02 (Nitrogen)
NH4 (obs)
NO3 (obs)
NH4 (sim)
NO3 (sim)
Concentration (mg/L)
DateTime
Tank L02 (Nitrogen)
NH4 (obs)
NO3 (obs)
NH4 (sim)
NO3 (sim)
Concentration (mg/L)
DateTime
Tank L02 (N2O)
N2O (obs)
N2O (sim)
Concentration (mg/L)
DateTime

FIGURE 16. Visualization of NH_4-N, NO_3-N and N_2O-N concentrations in process tank LT02 (hindcast data only. Simulations (line), measurements (dotted line with markers).

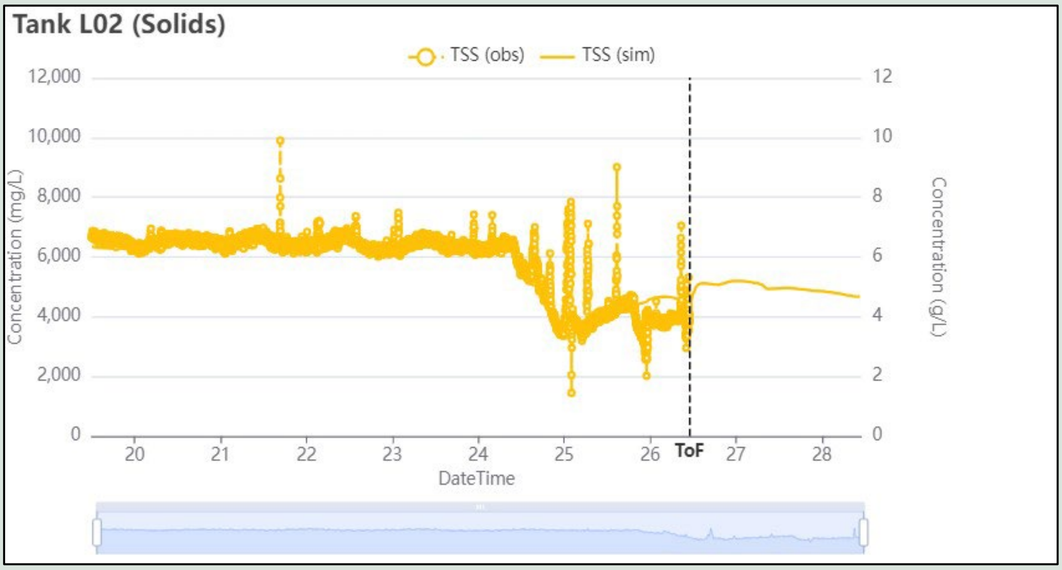

FIGURE 17. Visualization of MLSS concentrations in process tank LT02. Hindcast is left of ToF (dotted vertical black line), and forecast is right of ToF. Simulations (line), measurements (dotted line with markers).

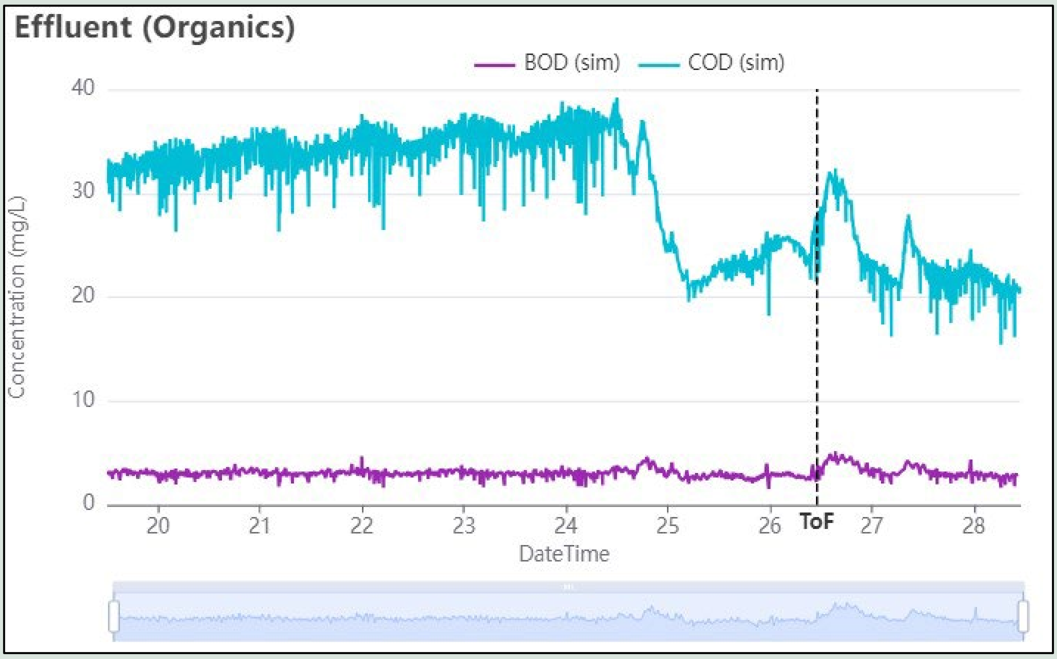

FIGURE 18. Visualisation of COD and BOD concentrations in the effluent. Hindcast is left of ToF (dotted vertical black line), and forecast is right of ToF. Simulations (line).

FIGURE 19. KPI dashboard and relative contribution of different sources (N_2O, power, non-biogenic $_B$COD removal and biogas leaks) to the carbon footprint of the WWTP.

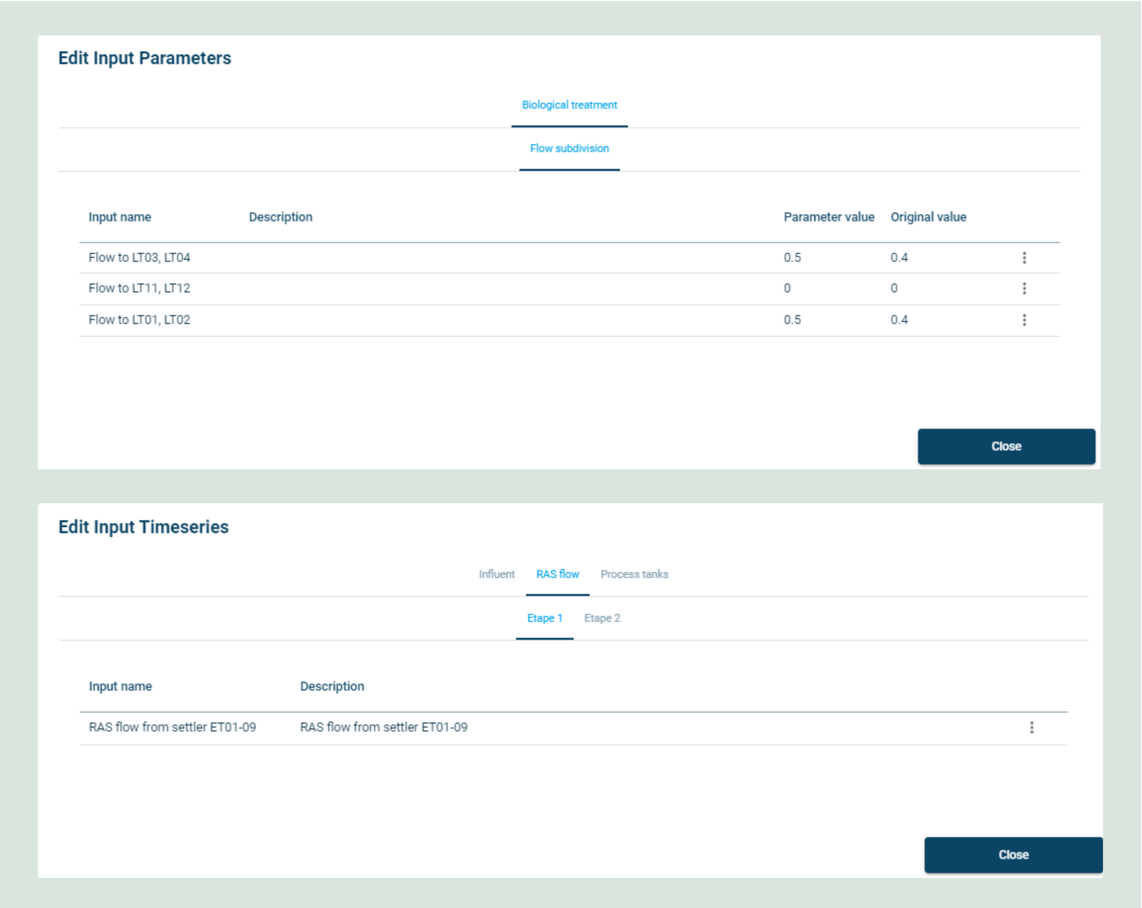

FIGURE 20. Scenario configuration in TwinPlant, which allows for changing input parameters and timeseries. The illustration presents some of the available options. Additional options can be made available through the configuration management system (CMS) to TwinPlant.

9. Evaluation of N_2O reducing scenarios in TwinPlant

9.1 Initial evaluation of data

Evaluation of the data collected at the Bjergmarken WWTP between January and May 2024 show that the plant has an N_2O emission factor of 1,3%, ca. 50% higher than the national standard (Vangsgaard and Madsen, 2020). The CO_2 emissions associated are as high as 5,5 tons per day, similar to the emissions of a commercial plane flying from London to Sidney (sustainabletravel.org). When looking at the aggregated operational data during the mentioned period, there seems to be a series of typical factors triggering peaks of N_2O concentrations in the liquid phase. Here we will focus our analysis on aerated tank 2, where the N content is highest and there is higher risk for N_2O emissions (FIGURE 21).

a) High precipitation events. High treatment flows associated with wet weather events seem to result in sudden drops in biomass concentration in the system (represented by the TSS). Such behaviour could be caused by severe dilution or washout events. The plant is configured to use a process tank as biomass settling tank under extreme flow conditions. This situation, together with low recirculated sludge rates in the range of 20-30% can result in lower biomass availability to deal with eventual first flush ammonia peaks. Some examples of this trend are seen on February 5th, February 19th, and April 3rd.
b) High NH_4-N peaks at the influent of the process tank, such as the event seen in the first half of March.
c) Low MLSS concentrations in the process tank, such as the event seen in the first half of January.

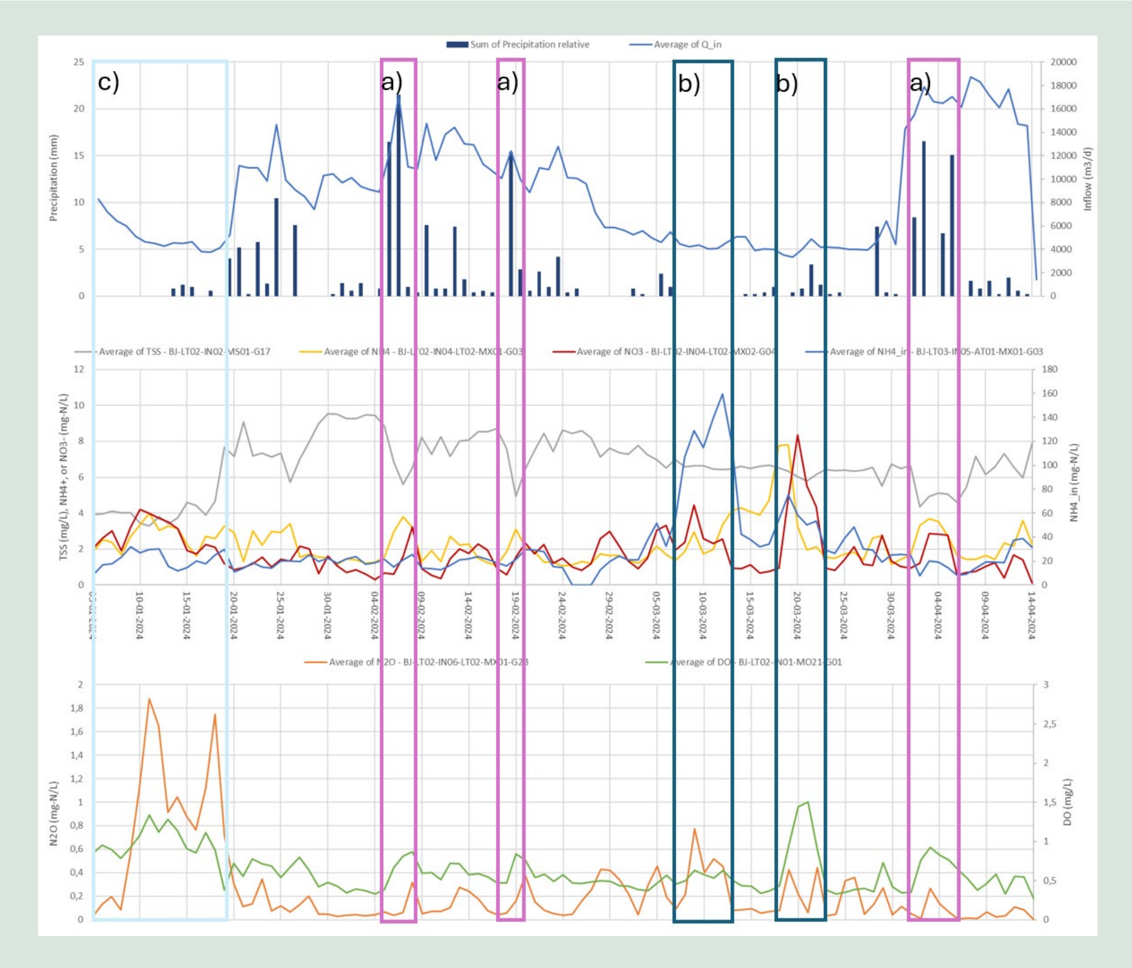

FIGURE 21. Visual assessment of factors contributing to elevated N_2O concentrations. The top graph shows the daily average inflow (blue line) and precipitation (bars). The middle graph presents the average daily TSS concentrations in LT02 (grey line), NH_4-N concentrations in LT02 (yellow line), NO_3-N concentrations in LT02 (orange line), and NH_4-N concentrations in the pre-anaerobic tank (blue line). The bottom graph illustrates the average daily N_2O concentrations in LT02 (orange line) and DO concentrations in LT02 (blue line). The vertical squares display periods with a) high precipitation, b) high nitrogen loads and c) low TSS concentrations.

Based on the initial findings a more thorough analysis of the data was conducted.

9.2 Data analysis and scenario evaluation

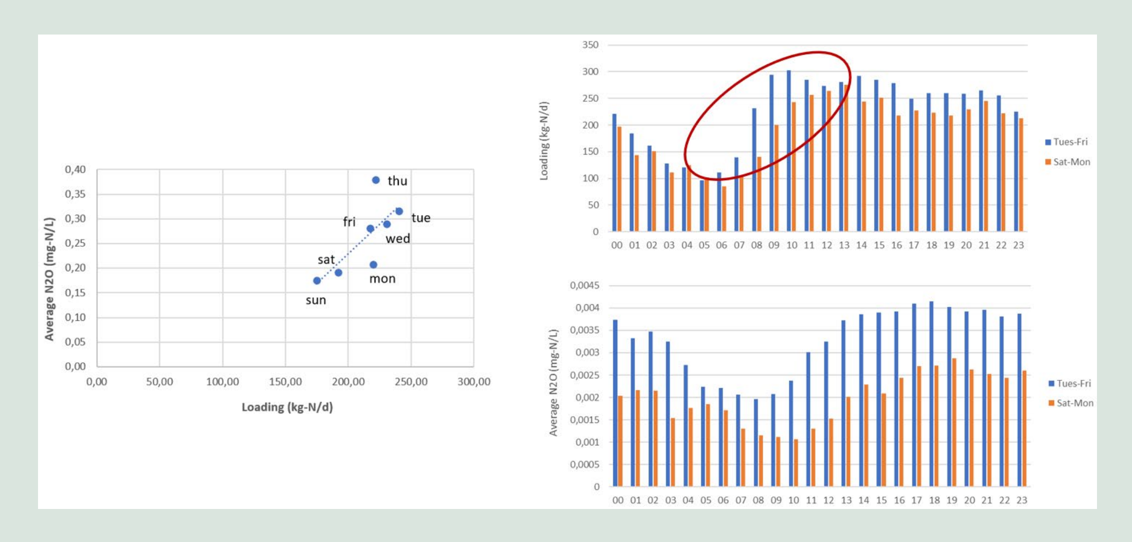

FIGURE 22. Evaluation of the impact of nitrogen loadings on the average N_2O concentrations, considering the time of the day and the influence of the weekday.

The influence of weekdays on average N_2O concentrations and loads was evaluated by categorizing the data by day of the week and calculating the average N_2O concentrations and nitrogen loadings for each day. FIGURE 22 (left) shows the results, indicating that Tuesday through Friday have higher loadings and average N_2O concentrations compared to the other weekdays. On the right side of FIGURE 22, the data are grouped into two categories: Tuesday-Friday (blue) and Saturday-Monday (orange). The top graph displays the nitrogen load, while the bottom graph shows the average N_2O concentration throughout the hour of the day. The results clearly demonstrate a significant increase in load during the morning hours on Tuesday-Friday compared to the rest of the day (highlighted in the red circle). Average N_2O concentrations are consistently higher on Tuesday-Friday, with the smallest difference between the two groups occurring between 4 am and 9 am.

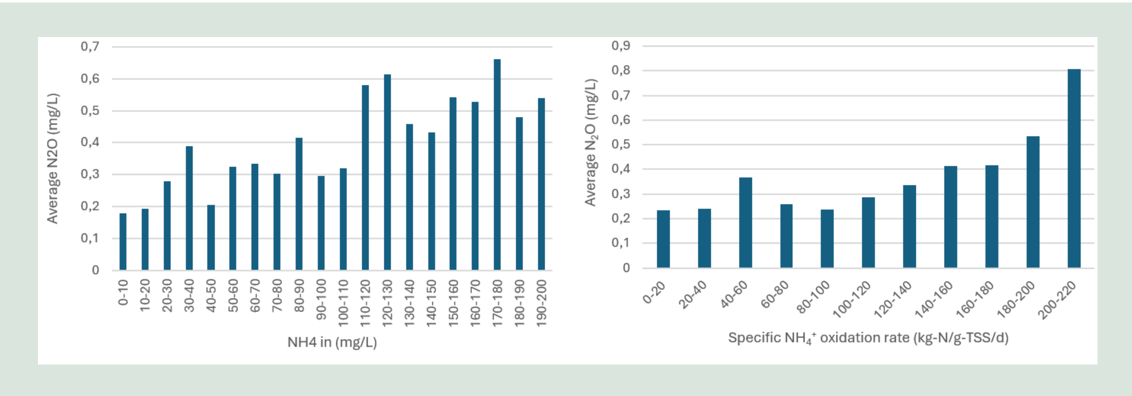

FIGURE 23. Assessment of the influence of NH_4-N concentrations and the specific NH_4-N oxidation rate in the pre-anaerobic tank on average N_2O concentrations.

The impact of the incoming NH_4-N load to the Bjergmarken treatment plant was evaluated further by categorizing the data into twenty groups based on daily average NH_4-N concentrations. The average N_2O concentration for each category is shown on the y-axis in FIGURE 23 (left side). For the calculated NH_4-N oxidation rates, the calculated data were divided into eleven categories, with the corresponding average N_2O concentrations displayed on the y-axis FIGURE 23 (right side).

Assessing the impact of incoming NH_4-N load on average N_2O concentrations based on daily NH_4-N concentrations in the pre-anaerobic tank gives an unclear result. However, analysing the specific NH_4-N oxidation rate reveals a clear trend: as the NH_4-N oxidation rate increases, the average N_2O concentrations also rise. This aligns with the theory discussed in Section 2, which explains that hydroxylamine oxidation by ammonia-oxidizing bacteria (AOB) during nitrification can lead to incomplete oxidation under environmental stress, producing nitric oxide and, subsequently, N_2O. High ammonia oxidation rates are known to promote this pathway.

Based on these findings, which demonstrate that increased nitrogen loadings and NH_4-N oxidation rates result in higher N_2O concentrations, a scenario was devised involving the introduction of a buffer tank at the WWTP influent. Scenarios with varying buffer tank volumes and retention times were evaluated, with each scenario doubling the tank's retention time from 2 to 6 hours, resulting a volume increase from 2800 to 8300 m^3. Four scenarios were assessed in total (TABLE 2).

TABLE 2. Equalisation of influent loads**.**

Retention time [h]	**Volume of buffer tank [m^3]**
0 (baseline)	0
2	2.800
4	5.600
6	8.300

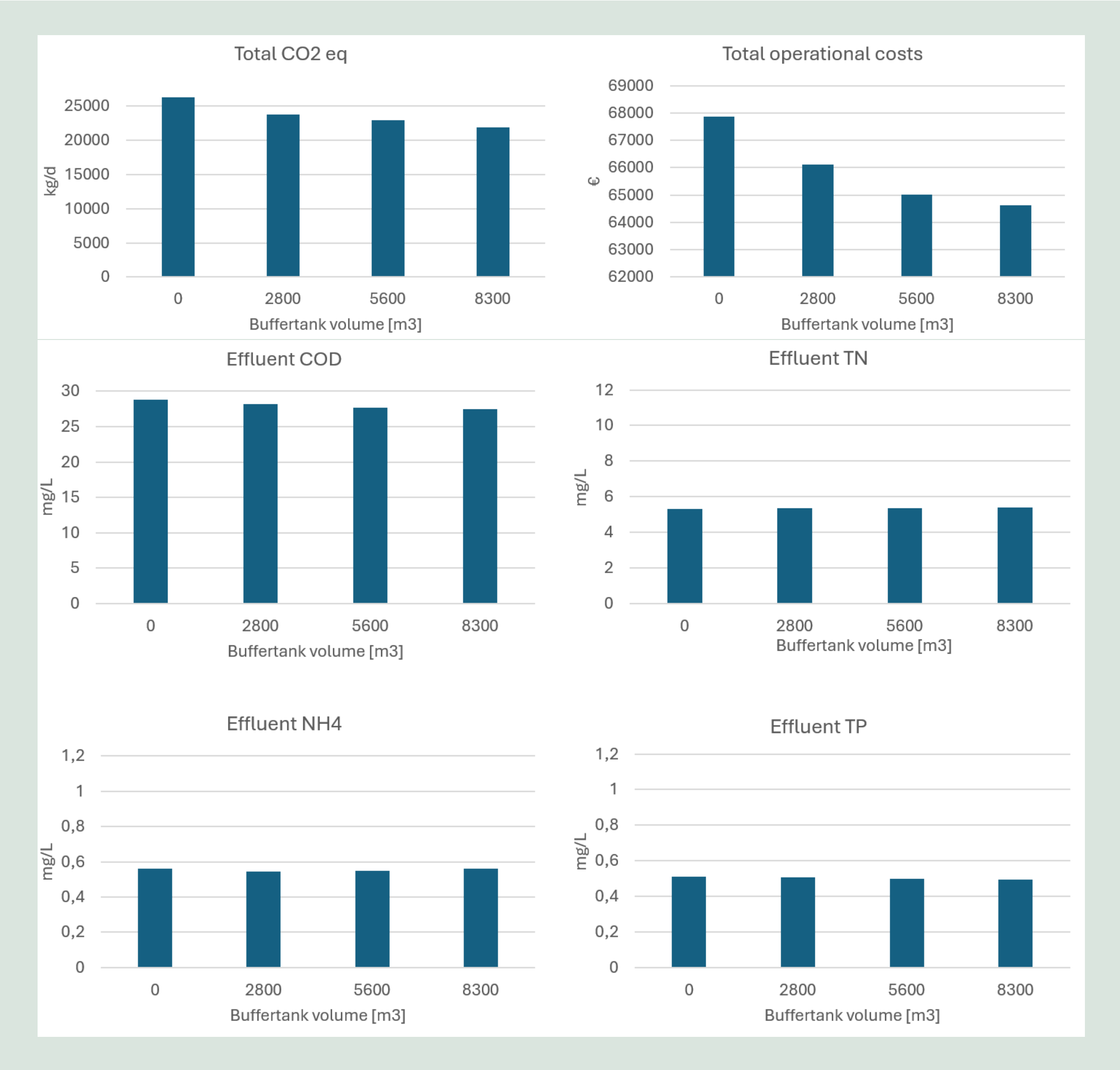

FIGURE 24. Evaluation of scenarios with a buffer tank introduced at the influent of the WWTP. The baseline scenario represents a buffer tank of volume of 0. Scenarios are constructed by doubling of the retention time in the buffer tank from 2 to 6 hours resulting in a volume of 2800-8300m^3.

Scenario evaluations clearly demonstrate that introducing a buffer tank to the influent of the WWTP lowers both the total CO2eq for the evaluated period (10-17%) but also the operational cost (3-5%) (FIGURE 24).

Assessing the impact of DO concentration in the process tank on average N_2O concentration (FIGURE 25) reveals a clear trend: as DO concentrations increase, average N_2O concentrations rise as well. This observation is consistent with existing theory. High DO concentrations promote hydroxylamine (NH_2OH) oxidation, an intermediate in ammonia oxidation by AOB. When suboptimal conditions for complete nitrification exists, such as high DO combine with environmental stresses like high ammonium loads or imbalances in the nitrifying microbial community, AOB may produce N_2O as a side product through the incomplete oxidation of hydroxylamine to nitric oxide (NO), which can be converted to N_2O.

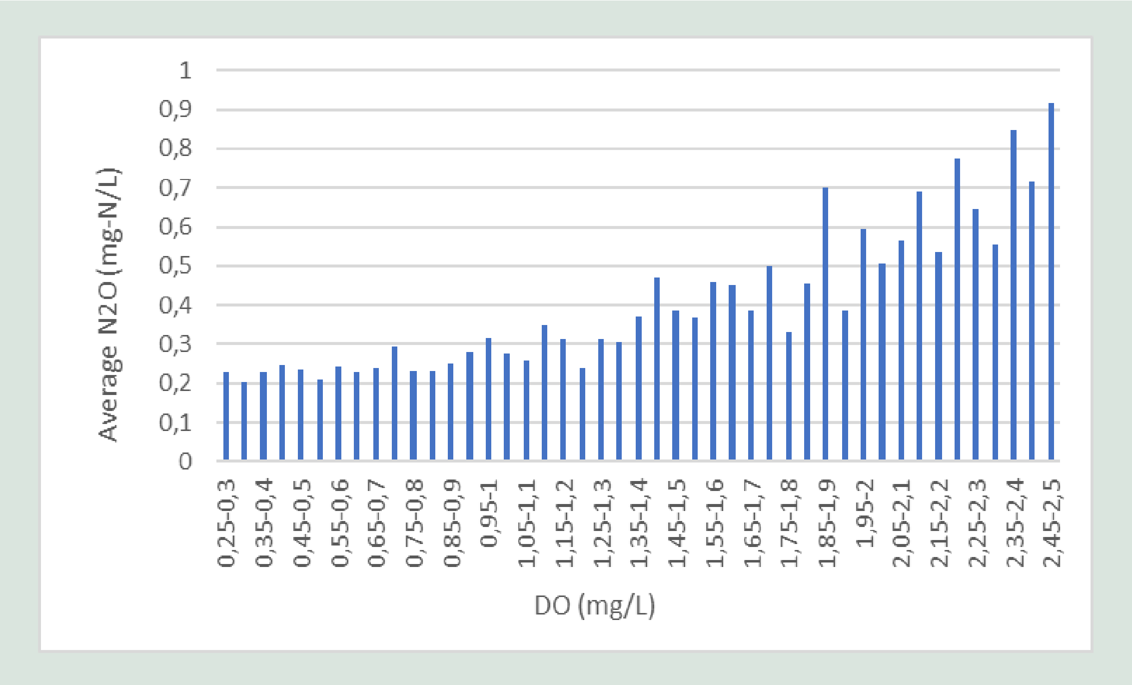

FIGURE 25. Assessment of the influence of DO concentrations in the process tanks, on average N_2O concentrations, using LT02 as the example.

Scenarios were developed to evaluate the impact of adjusting the maximum and minimum DO setpoints for the Hubgrade aeration controller. The minimum DO concentration was varied between 0.2 and 1 mg/L (baseline), while the maximum concentration was adjusted between 2 and 2.5 mg/L (baseline).

FIGURE 26 illustrates how the optimal DO setpoint can be identified. The KPIs at the right of the figure can be adjusted based on the utility's specific priorities. In this case, the results show that lowering the setpoints reduce CO_S emissions and operational costs, but negatively impacts effluent quality, particularly in terms of COD and NH_4-N concentrations.

0,5	2	4	6	CO_2 eq released (kg/d)	Cost (€/m3)	COD (mg/L)	NH4 (mg-N/L)	TN (mg-N/L)	TP (mg-P/L)
DOsp_0	DOsp_1	DOsp_2	DOsp_3						
0,2	0,2	1,0	1,0	16312,4	0,4	26,8	1,4	4,1	1,0
1,0	0,2	1,0	1,0	18323,9	0,4	26,8	1,1	4,5	1,1
0,2	1,0	1,0	1,0	17444,0	0,4	26,8	1,2	4,7	1,0
1,0	1,0	1,0	1,0	17556,2	0,5	26,7	0,7	6,3	1,1
0,2	0,2	2,5	1,0	16901,2	0,4	26,8	1,1	4,1	1,0
1,0	0,2	2,5	1,0	18862,6	0,4	26,8	0,9	4,7	1,1
0,2	1,0	2,5	1,0	17660,8	0,4	26,8	0,7	4,9	1,1
1,0	1,0	2,5	1,0	18166,6	0,5	26,7	0,5	6,5	1,2
0,2	0,2	1,0	2,5	16791,6	0,4	26,8	1,3	4,1	1,0
1,0	0,2	1,0	2,5	18386,6	0,4	26,8	1,1	4,5	1,1
0,2	1,0	1,0	2,5	16616,0	0,4	26,8	1,0	4,7	1,0
1,0	1,0	1,0	2,5	17728,0	0,5	26,7	0,7	6,3	1,1
0,2	0,2	2,5	2,5	17029,3	0,4	26,8	1,1	4,1	1,0
1,0	0,2	2,5	2,5	19566,9	0,4	26,8	0,9	4,7	1,1
0,2	1,0	2,5	2,5	18175,1	0,4	26,8	0,7	4,9	1,1
1,0	1,0	2,5	2,5	18329,2	0,5	26,7	0,5	6,5	1,2

FIGURE 26. Assessment of the impact of Hubgrade DO setpoints on average N_2O concentrations shows controller settings in light to dark blue (lowest to highest) on the left and outputs (CO_{2eq}/day, cost/day, effluent COD, NH_4-N, TN, TP) on the right. Columns are color-coded: green for lowest values, red for highest. The red rectangle marks the baseline simulation with default settings. Cost, effluent COD, and TP impacts are minimal, with only decimal-level variations.

Assessing the impact of NO_3-N concentrations in LT02 on the average N_2O concentration (FIGURE 27), clearly demonstrates that as NO_3-N concentrations increase, the average N_2O concentration rise as well. Heterotrophic bacteria can under low DO concentrations utilise nitrate or nitrite as the electron acceptor to sustain their metabolism. The main product of this pathway is nitrogen gas with NO and N_2O as intermediates. If organic carbon is limited, this pathway can result in net N_2O emissions.

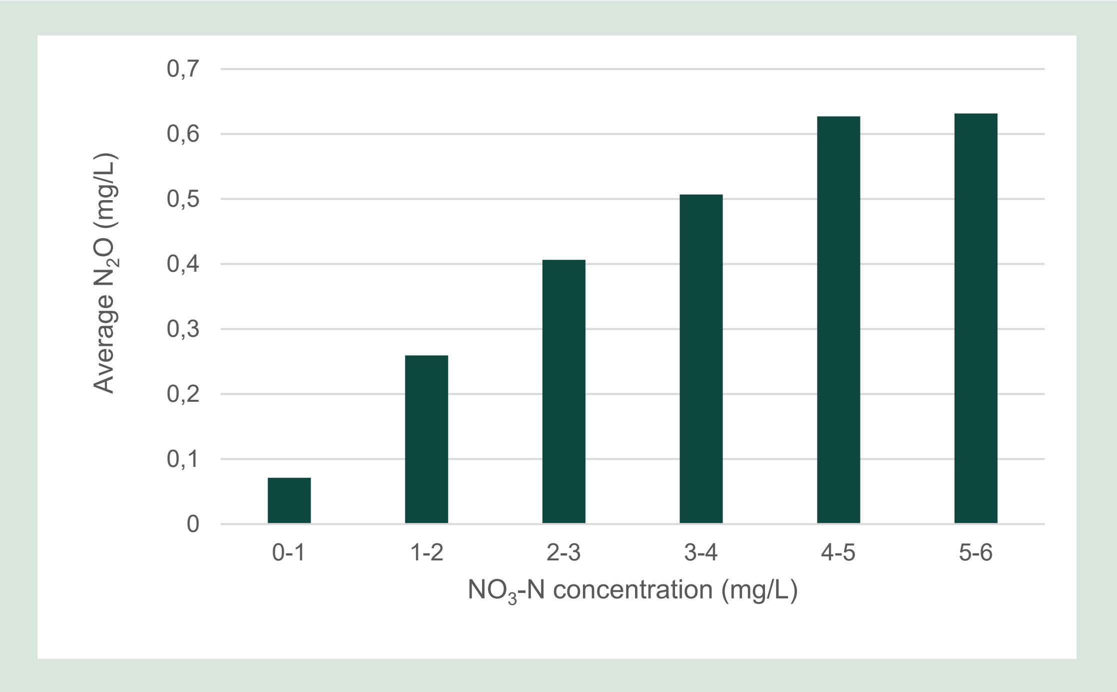

FIGURE 27. Assessment of the influence of NO_3-N concentrations in the process tanks, on average N_2O concentrations, using LT02 as the example.

To investigate if carbon dosing could reduce the average N_2O concentrations a scenario was constructed with dosing of acetate between 0,0 m^3/d and 0,714 m^3/d to each of the process lines. The dosing unit was controlled by an on/off controller and a timer also linked to the aeration controller to accommodate dosing only when aeration if off. Eleven simulations, including the baseline with no carbon dosing, was executed.

The results suggest that catalysing the heterotrophic denitrification pathway has a broadly positive effect on overall operation. FIGURE 28 demonstrates that increasing acetate dosing can reduce the cost per treated volume of wastewater by up to 25%, while also lowering CO_2 emissions (CO_{2eq}) by 30%. Additionally, carbon dosing improves effluent quality by reducing TN, NH_4-N, and TP levels, though a slight increase in COD is observed. The cost calculator in WEST accounts for expenses related to chemicals (such as acetate (670 €/ton), PIX (233 €/ton), and PAX (283€/ton)), sludge disposal, effluent taxes (based on measurements), and power consumption for equipment operation, including blowers and pumps. The additional cost of acetate is offset by reductions in both power consumption and effluent taxes.

FIGURE 28. Assessment of the impact of carbon dosing on the total CO_{2eq} per day (top graph) and the effluent concentrations of COD, TN, NH_4-N and TN. Baseline simulation has no carbon dosing and is included as the first bar in the plots. Acetate was used as the carbon source and was dosed during non-aerated phases to the process tanks.

Evaluating the impact of TSS concentrations in LT02 on average N_2O levels clearly shows that increasing the solids concentration in the process tank reduces average N_2O concentrations (FIGURE 29). Initial analysis suggests that events like heavy precipitation led to sudden drops in biomass (TSS) concentrations within the system (FIGURE 21), which could be due to significant dilution or washout of TSS. However, at Bjergmarken WWTP, the process tank functions as a settling tank during extreme flow conditions. Combined with low sludge recirculation rates of 20-30%, this can result in reduced biomass availability to manage ammonia peaks during first flush events. FIGURE 30 shows that recirculation rates fluctuate throughout the day, with periods of very low rates.

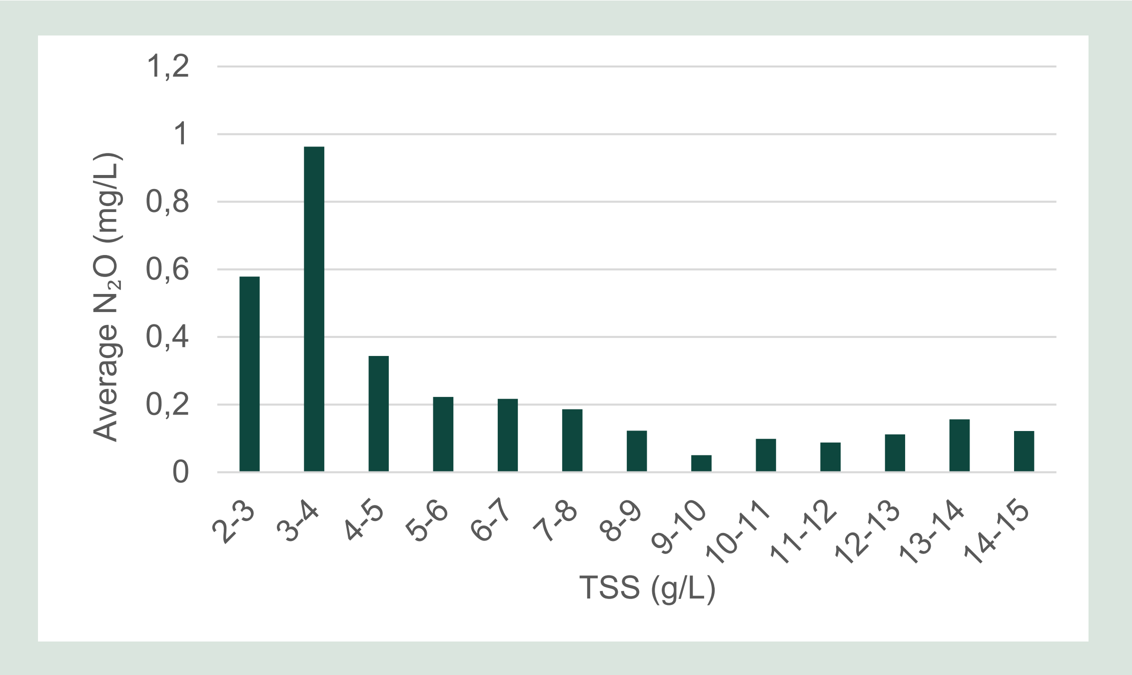

FIGURE 29. Assessment of the influence of TSS concentrations in the process tanks, on average N_2O concentrations, using LT02 as the example.

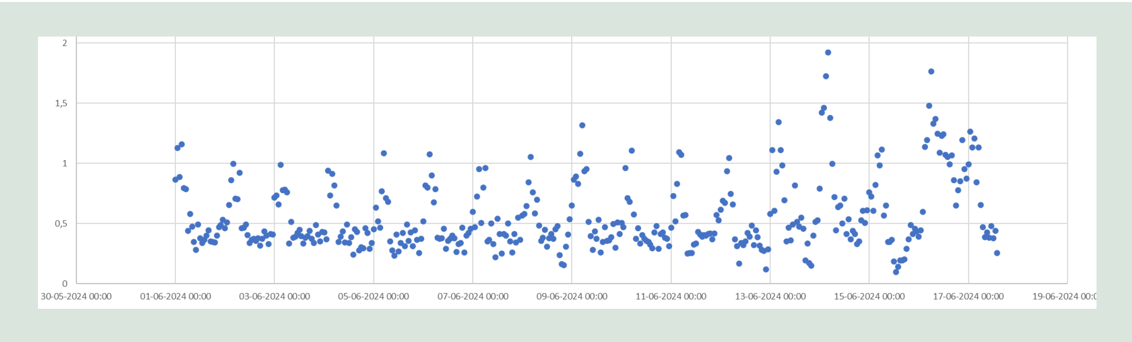

FIGURE 30. Measured recirculation rates relative to influent flow at Bjergmarken WWTP.

A scenario was developed to evaluate the impact of maintaining a more consistent recirculation rate, with distinct fixed rates for wet and dry weather conditions. Fifteen scenarios were created, where the recirculation rates during dry weather were set at 0.2, 0.4, 0.6, 0.8, and 1 relative to the influent flow. For wet weather, the recirculation rates were set at 0.8, 1, or 1.2, and all combinations of these rates were tested. FIGURE 31 presents the results from this scenario analysis. The results show that the total CO_{2eq} can be reduced by operating the RAS flow at a constant rate, while the impact on operational costs where of minor effect. Effluent concentrations of NH_4-N and TN were reduced at higher recirculation flows during dry weather. The effect during wet weather was less pronounced. However, COD and TP concentrations increased with higher RAS ratios in dry weather, suggesting that additional measures should be considered alongside RAS strategy adjustments to address the increased return of internal load.

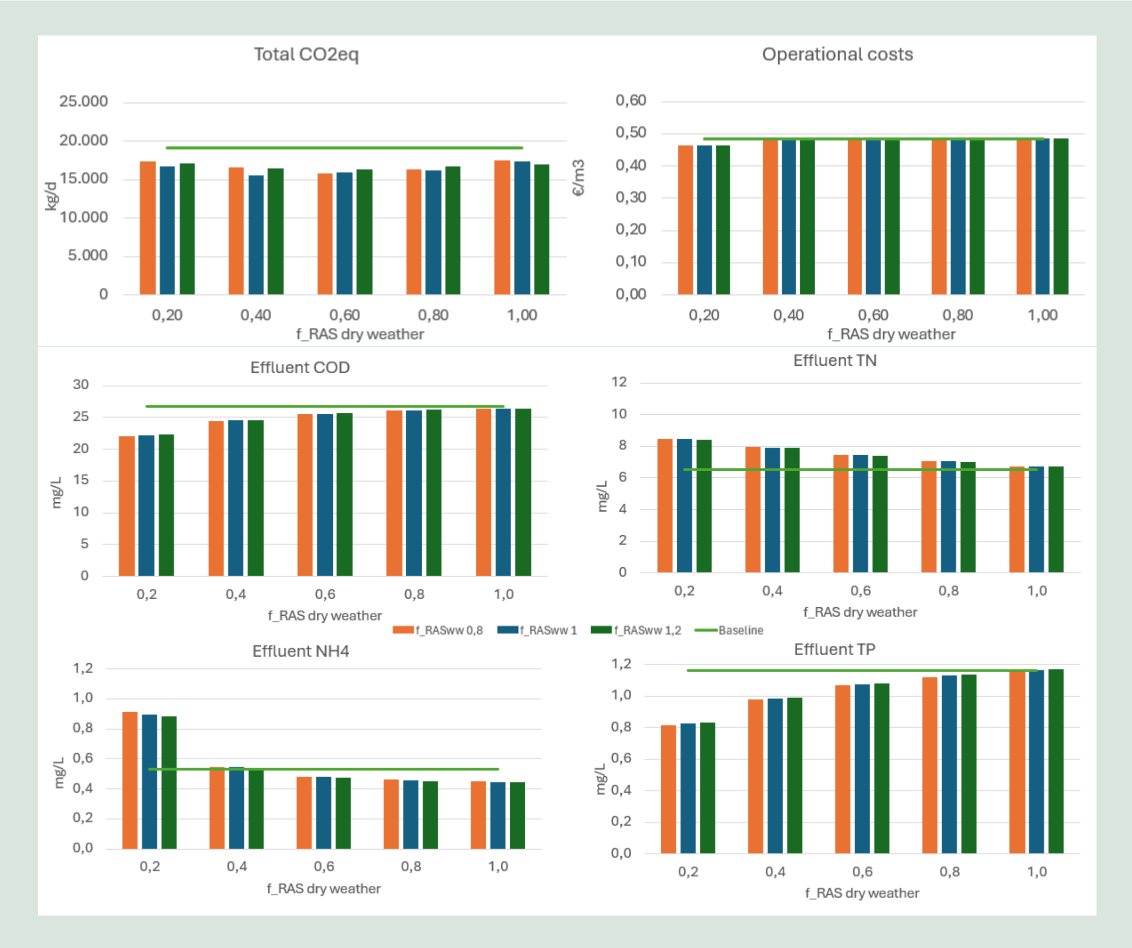

FIGURE 31. Assessment of the impact of constant RAS flow during dry weather at ratios of 0.2, 0.4, 0.8, and 1 relative to influent flow, and during wet weather at ratios of 0.8 (orange), 1 (blue), and 1.2 (dark green). The green horizontal line represents the baseline simulation.

As a final scenario evaluation, a simpler aeration controller was developed and implemented in WEST to address if a less complex operation could benefit the plant. This controller was developed to operate at constant phases. Six phase durations were assessed (0,25; 0,5; 1; 1,5; 2 and 4 hours) resulting in equal N/DN time. In addition, the aeration controller was evaluated in combination with the phases by varying DO max (1,5 or 2,5 mg/L) and min (0,5 or 1,5 mg/L) setpoints. In total 24 scenarios were simulated.

The results indicate that both the highest and lowest phase durations led to a reduction in total CO2eq per day (FIGURE 32). In terms of DO setpoints, the lowest minimum DO setpoint proved to be most effective during the shorter phase durations, while minimal differences were observed at the longest phase duration. The maximum DO setpoint had a negligible impact on the outcomes. Effluent concentrations show that while NH_4-N is effectively oxidized during aeration, nitrogen removal via denitrification is less efficient, resulting in elevated TN values at short phase durations and a minimum DO setpoint of 1.25.

FIGURE 32. Assessment of the impact of a simpler aeration controller with fixed phase durations of 0,25-4 h and a combination of DO setpoints of min 0,5; max 1,5 (dark blue), min 0,5; max 2,5 (dark green, min 1,25; max 1,5 (orange) and min 1,25; max 2,5.

10. References

Alex, J., Jeppsson, U., et al. (2008). Benchmark Simulation Model no. 1 (BSM1).

Chrysochoidis, V., Andersen, M.H., Remigi, E.U., Faragó, M., Smets, B.F., Domingo-Félez, C., Valverde-Perez, B. (2023). Critical evaluation of different mass transfer equations to model N_2O emissions from water resource recovery facilities with diffuse aeration. Environmental Technology 45, 3339-3353.

Domingo-Félez, C., Smets, B.F. (2020). Modelling N_2O dynamics of activated sludge biomass: Uncertainty analysis and pathway contribution. Chemical Engineering Journal 379, 122311.

Guo, L., Vanrolleghem, P. (2014). Calibration and validation of an activated sludge model for greenhouse gases no. 1 (ASMG1): prediction of temperature-dependent N_2O emission dynamics. Bioprocess Biosystems Engineering 37, 151–163.

Henze, M., van Loosdrecht, M. C. M., Ekama, G. A., & Brdjanovic, D. (2008). *Biological wastewater treatment: Principles, modelling and design*. IWA Publishing.

Hiatt, W.C, Grady, C.P.L. (2008). An updated process model for carbon oxidation, nitrification, and denitrification. Water Environment Research 80, 2145-56.

IPCC AR6 (2024) Green House Gas Protocol.

Klima-, Energi-, og Forsyningsministeriet. (2020) Klimaprogram 2020. Klimaprogram_2020.pdf (kefm.dk).

Pan Y., Ni B., Yuan Z., Modeling electron competition among nitrogen oxides reduction and N_2O accumulation in denitrification, Environ. Sci. Technol. 47 (2013) 11083–11091,

Pocquet, M., Wu, Z., Queinnec, I., Sperandio, M. (2016). A two pathway model for N_2O emissions by ammonium oxidizing bacteria supported by the NO/ N_2O variation. Water Research 88, 948-959.

Refdorf, M., Poulsen, L. D., Fredenslund, A., Scheutz, C., Thomsen, M., Thornberg, D., Eriksson, M., Mielczarek, A., Vangsgaard, A. K., Madsen, J. A., Askjær, N. M., Nielsen, P. N., Hansen, R., Knudsen, A. S., Almind-Jørgensen, N. (2024). ARES Aktiv Reduktion af Emissioner fra Spildevandsanlæg MUDP-projekt. Miljøstyrelsen ISBN 978-87-7038-657-9.

Regeringens klimapartnerskaber (2020). Affald og vand, cirkulær økonomi.

Solis, B., Guisasola, A., et al. (2022). Systematic calibration of N_2O emissions from a full-scale WWTP including a tracer test and a global sensitivity approach. Chemical Engineering Journal 435, 134733.

Vangsgaard, A., Madsen, J.A. (2020). MUDP Lattergaspulje. Dataopsamling på måling og reduktion af lattergasemissioner fra renseanlæg. Miljøministeriet Microsoft Word - Rapport N2O Endelig.docm.

Ye, L., Porro, J., Nopens, I. (2020). Quantification and modelling of fugitive greenhouse gas emissions from urban water systems. IWA Publishing.

TwiN2Ops

Purpose:

The project addresses the reduction of nitrous oxide (N_2O) emissions from wastewater treatment, a significant source of greenhouse gases within the water sector. The goal is to develop and validate a Digital Twin with an integrated N_2O module that combines real-time data and advanced process models. This technology aims to optimize plant operations, reduce climate impacts, and balance effluent quality with operational costs.

Results:

The developed model was evaluated and calibrated at both pilot and full-scale facilities. At the pilot scale, the model accurately replicated N_2O dynamics under controlled experimental conditions, providing insights into the processes governing emissions. At Bjergmarken Wastewater Treatment Plant, DK (125,000 PE), the model demonstrated strong agreement between simulated and observed values for key parameters such as ammonium, nitrate, TSS, and N_2O under varying operating conditions, including wet weather events. Scenario analyses identified optimization strategies that could reduce CO_2-equivalent emissions by up to 30% and operational costs by 25%, while also improving effluent quality.

Conclusion:

The implementation of the Digital Twin technology, evaluated at both pilot and full-scale facilities, shows significant potential for optimizing wastewater treatment operations and reducing climate impacts. This virtual tool allows plant operators to evaluate and assess strategies in a simulated environment before applying them in practice. The project illustrates that Digital Twin technology can enhance sustainability in the water sector, support national climate goals, and provide a robust platform for improved decision-making.

The Danish Environmental
Protection Agency
Tolderlundsvej 5
DK - 5000 Odense C

www.mst.dk