Ministry of Environment of Denmark
Environmental Protection Agency

Nitrous Oxide Emissions from Ornum Waste Water Treatment Plant

Kalundborg Utility

MUDP Report

September 2022

Publisher: The Danish Environmental Protection Agency

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1. Summary

In this project, Kalundborg Forsyning (referred to in the remainder of the report as Kalfor) aims to evaluate the nitrous oxide (N_2O) emissions in the Ornum wastewater treatment plant (referred to as OR in the remainder of the report). The objective of the study is summarized as follows: (i) to collect long-term N_2O measurements and to quantify the extent of N_2O emissions, (ii) to perform a process analysis of potential factors contributing to the emissions with the help of deep learning models developed at DTU (iii) Based on the analysis, to identify whether there is a need to perform process modifications or install additional / modify their control systems to keep the N_2O emissions within the legal emission threshold.

The project has been ongoing in the period ranging between 01-01-2020 and 01-12-2021. During this period various sensor data have been collected, N_2O emissions are quantified, modeled, and analyzed. The major activities reported in this report are:

- Plant description
- Methods
- Results
- Conclusion and perspectives

The main conclusions of this project can be summarized in one point: The N_2O emission factor of the Ornum plant is found to be **0.06%** on average. This emission factor is quite low compared with the threshold/average emission factors reported in IPCC 2019 report **(1.6%)** or the Danish environmental agency **(0.84%)** for a wastewater treatment plant (Miljøstyrelsen, 2020). This finding is robust against a huge uncertainty (two sigma deviation of the mean) in the estimation of the mass transfer coefficient for N_2O. A deep neural network is trained to explain the N_2O concentration in liquid with a training R^2 of **0.81**. The sensitivity analysis using the model indicated that dissolved oxygen (DO) is the most significant process parameter (alone it explained 40% of the variation in the liquid N_2O concentration). All other measured inputs (temperature, NH_4, NO_3, and influent) were important but mainly through their interaction effects.
Overall given that N_2O emission is low and not significant, it is recommended that there is no need for changing/modifying current process control and operation strategy at this moment in time.

2. Resumé

Gennem dette projekt ønskede Kalundborg Forsyning (herfra forkortet som Kalfor) at evaluere deres lattergas (N_2O) udledning ved Ornum rensningsanlæg (herfra forkortet som OR). Hovedformålet i dette studie er følgende: (i) at samle N_2O relaterede målinger gennem en længere periode for at bestemme graden af N_2O udledningen, (ii) udføre en analyse af potentielle faktorer der bidrager til N_2O udledningen ved brug af kunstig intelligens baseret modeller som dybe neurale netværk udviklet på DTU (iii). Ud fra denne analyse identificeres, om der er et behov for at udføre proces ændringer, ved at installere eller modificere nuværende kontrol systemer, for at opretholde N_2O udledningen på et passende niveau.

Projektet har kørt i perioden mellem 01-01-2020 til 01-12-2021. I løbet af denne periode, er der samlet forskellige sensor data til at bestemme, modellere og analysere N_2O udledningen. I rapporten forekommer følgende afsnit:

- Beskrivelse af rensningsanlægget
- Metoder
- Resultater
- Konklusioner and perspektiver

Hoved konklusionen I denne rapport er at N_2O emmisionsfaktor fra OR anlægget er gennemsnitligt **0.06%**. Denne udledningsfaktor er meget lavere end grænsen defineret i rapporten af IPCC i 2019 (1.6%) og den danske miljøstyrelse (**0.84%**) for et rensningsanlæg (Miljøstyrelsen, 2020). Disse resultater kan betragtes som robuste i forhold til eventuelle usikkerheder og er stadig gældende selv ved 2 gange standardafvigelse af den bestemte masse overførelses koefficient af N_2O ($k_L a_{N_2O}$). Modellen, baseret på dybe neurale netværk, producerer en god prædiktion af N_2O koncentrationerne i væskefasen med en R^2 værdi på **0.81**. Denne model er derefter brugt til at udføre en følsomhedsanalyse som viste at oxygen koncentrationen er den vigtigste procesparameter. Følsomhedsanalysen viser, at oxygen koncentrationen har ca. 40% indflydelse på N_2O variationen i væskefasen. Øvrige proces parametre såsom temperaturen, ammonium koncentrationen (NH_4) og indløbs flow er ydermere indirekte influerende på emmisionsfaktor.

Hovedsageligt, så er N_2O udeledningen meget lave og derfor anbefaler vi ikke nogle ændringer eller modifikationer af den nuværende operation eller kontrol systemer.

3. Plant Description

3.1 General introduction to the plant

Ornum WWTP is a medium-size WWTP (referred to as OR in the report) is located in Gørlev in the municipality of Kalundborg in the northwestern part of Zealand Denmark with a capacity of app. 16.000 PE (person equivalent). An aerial picture of the plant can be seen in Figure 1.

FIGURE 1. Aerial picture or Ornum (OR) WWTP

3.2 Plant description and sensor location

Ornum is a typical activated sludge plant that performs biological COD and nitrogen removal with chemical phosphorus removal. The process flow diagram of the plant is shown in Figure 2, which also shows the sensor locations.

The influent wastewater passes through a grit removal system, which then flows into two parallel carrousel-type aeration tanks. For the remainder of the report, the aeration tanks are abbreviated as LT01 and LT02. The activated sludge is separated into two settling tanks (EKT1 and EKT2), part of it recycled to aeration tanks to maintain desired biomass concentration. Part of the excess sludge is mineralized in nearby reed beds, while the remaining sludge is dewatered and disposed of via trucks. The treated effluent wastewater is discharged to the Great Belt through a 1.6 km pipeline.

Aeration is provided via surface aerators, which are controlled by an intermittent aeration control strategy. Aeration is activated when ammonium reaches a given setpoint determined by the operator. As DO concentration increases in the wastewater, the number of rotors to supply oxygen is regulated to maintain DO levels in between a certain min and max value. If ammonium is depleted to the minimum setpoint, the aeration system is switched off.

Thanks to the higher internal recirculation rates typical to carrousel-type tanks, the tanks are considered well mixed. Therefore the N_2O wastewater sensor (Unisense) is located next to the online sensors namely DO, NO_3, and NH_4 sensors in the two parallel tanks to obtain a representative measurement of the concentrations. This decision is also motivated to potentially consider the use of N_2O sensor in a control strategy. In this way, interpretation and analysis of the sensors can be performed consistently at this representative sampling point (middle of the carrousel reactors). In addition pH sensor (influent) and turbidity sensor (effluent) is also present and considered in data analysis.

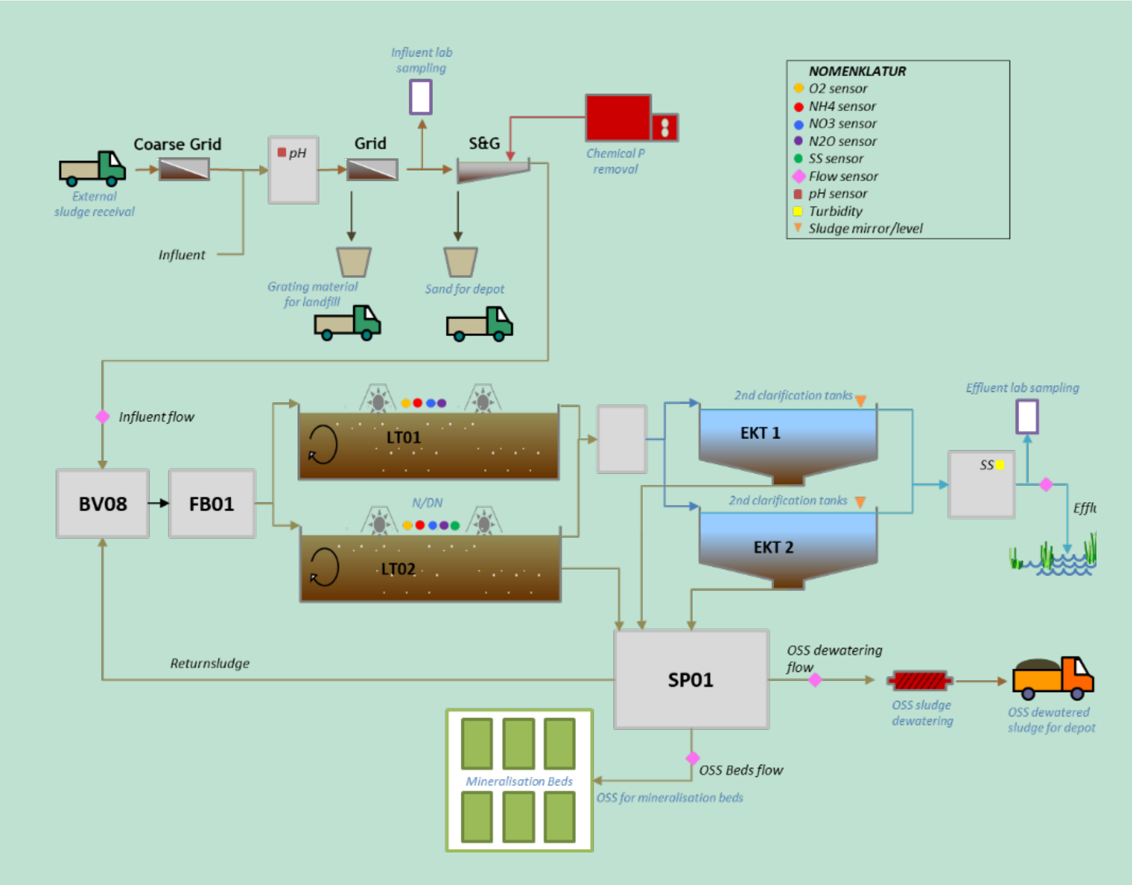

FIGURE 2. Process flow diagram of Ornum WWTP and location of the sensors

4. Methods

4.1 Data Treatment and Pre-processing

The data collected during the project period can be classified into high-frequency data (usually provided every minute or couple of minutes using the online sensors) and low-frequency data provided at a maximum of once a day from offline laboratory measurements. The overall data used in the deep learning modeling and analysis are reported in Table 1. Some data concern the whole sludge system some are distinct for each of the two aeration tanks LT1 and LT2.

TABLE 1: Overview of measurement data from OR

High-frequency data (online sensors)	Low-frequency data (offline measurements)
• Influent flow rate (Q in [m3/h])	• Total Flow (Q^{tot} in [m^3/h])
	• Chemical Oxygen Demand (COD in [mg/l])
Individual tank data	• Ammonia concentration (NH_4 in [mg/l])
	• Nitrate concentration (NO_3 in [mg/l])
• Dissolved Oxygen (DO in [mg/l])	• Total N concentration (TN in [mg/l])
• Ammonia concentration (NH_4 in [mg/l])	
• Nitrate concentration (NO_3 in [mg/l])	
• Liquid Nitrous Oxide concentration (N_2O in [mg/l])	
• Temperature (T in [ºC])	

The data were collected in the period ranging between 03-03-2021 and 30-09-2021 with varying frequency and timestamps. The workflow of the data processing can be seen in Figure 3.

FIGURE 2: Data preprocessing steps

The first step consists of performing a sanity check on the collected data. This is done by examining the values of the measured data and making sure it is consistent with the physical meaning, e.g. concentrations cannot be negative, etc. Corrective actions are taken such as identifying any negative concentrations that might be a result of bad calibration or measurement drift. Time alignment consists of establishing a common timestamp for all collected data, which is important for any proper analysis in particular modeling of the data. This is done by for example first rounding up all timestamps to the closest minute and then finding the common timestamps between all the measurements. This will result in creating timestamps for which a measurement value does not exist (also known in programming terms as *"NaNs"*). These are corrected using linear interpolation. The method was chosen since the time between two measurements is not large and would therefore be a suitable approximation. As a last remark in data quality check, a potential issue with the daylight saving time (DST) changes which shifts (up or down) timestamps is corrected. In total **152,307** data points were collected. The overall statistics of the measured data can be seen in Table 2 (Units are indicated in Table 1). Important to note is that the influent flow is measured in terms of total influent flow and it is assumed that LT1 and LT2 receive half the amount each and thus have similar statistics, which is the design/control strategy for influent flow distribution.

TABLE 2: Statistics on the collected data from OR

	Min	mean	median	Max	Std.dev
Q (LT1)	0.00	66.79	80.95	333.35	55.93
Q (LT2)	0.00	66.79	80.95	333.35	55.93
DO (LT1)	0.00	0.11	0.00	9.06	0.44
DO(LT2)	0.00	0.13	0.00	9.10	0.43
NH_4(LT1)	0.00	1.50	1.53	4.47	0.55
NH_4(LT2)	0.00	1.53	1.56	4.90	0.53
NO_3(LT1)	0.00	0.97	0.10	25.89	2.28
NO_3(LT2)	0.00	1.21	0.32	28.21	2.54
N_2O(LT1)	0.00	0.01	0.00	1.64	0.01
N_2O(LT2)	0.00	0.01	0.00	1.30	0.01
K(LT1)	0.00	34.30	33.50	87.79	7.63
K(LT2)	0.00	31.42	31.85	105.00	7.05
T(LT1)	6.80	14.73	16.40	21.90	4.31
T(LT2)	6.60	14.62	16.30	21.60	4.31

4.2 Modeling the Liquid N_2O concentration

Building mathematical models capable of describing the dynamics of N_2O production in activated sludge systems is a challenging task because the complete mechanism for such process is still not fully understood and activated sludge models (ASM), in addition to not providing the full mechanism, contains various parameters that must be determined through calibration experiments (Sin and Al, 2021). Data-driven models have proven to be a useful tool to describe complex systems such as the dynamics of N_2O production in WWTP (Hwangbo *et al.*, 2020).

In this work, we use a DTU software tool for performing global system analysis namely *deepGSA.* The tool is capable of building deep artificial neural network (DNN) models by providing the dependent variable also known as target variable (y: N_2O concentration) and the input process variables (x: Q, NO_3, NH_4, DO, K, T). The tool performs the training and selection of hyperparameters for the deep neural network models. A schematic of such a model can be seen in Figure 4 taken from (Hwangbo *et al.*, 2020).

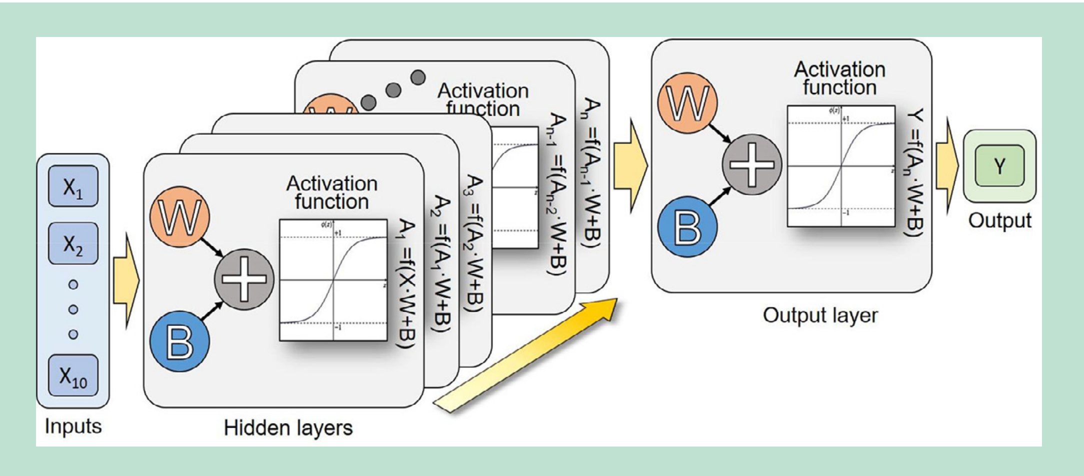

FIGURE 3. Deep-Learning structure (adapted from (Hwangbo et al., 2020))

Constructing a DNN is associated with a high degree of freedom expressed through the hyperparameters that must be selected to construct such models. These hyperparameters are the depth of the model (number of hidden layers), the width of the layers (number of neurons in each layer), the activations function, and the training algorithm (how the backpropagation is approximated). *deepGSA* allows the user to define a pool for each of these hyperparameters to construct a grid-search and systematically evaluate the various combination of these. In this work, a systematic workflow is used to tune this pool of hyperparameters as shown in Table 3.

TABLE 3: Hyperparameter pool for the DNN model

Hyperparameter	Pool
Number of layers	[2, 3, 4, 5]
Number of neurons	[4, 8, 16, 32, 64, 128]
Activation functions	[linear, tanh, rectified linear (ReLU)]
Training algorithms	[Levenberg-Marquardt, Bayesian backpropagation]

A common practice when developing data-driven models is to scale the inputs and to smooth them in case they are sensor data. In this work, min-max scaling is used according to our earlier study (Hwangbo *et al.*, 2021). Median smoothing with a moving window of 12-time steps is used according to the previously developed work by (Hwangbo *et al.*, 2020). The model providing the lowest root-mean-square error (RMSE) for the validation data is selected.

4.3 Calculating the N_2O emissions

OR uses surface aerators in their activated sludge system. The N_2O emissions were calculated according to the methods provided and recommended by (Unisense, 2019). The N_2O emission rate in the aerated zone is calculated through Eq.(2).

$$\mathrm{NTR}_{\mathrm{aerated}}\left[\frac{\mathrm{g}_{\mathrm{N_2O}}}{\mathrm{h}}\right]=\mathrm{k_L a}_{\mathrm{N_2O}_{\text{T-process}}}\cdot \mathrm{C}_{\mathrm{N_2O}}^{\mathrm{process}}\cdot \mathrm{V}_{\text{aerated tank}} \tag{2}$$

For non-aerated periods, the emission rate is calculated through Eq (3) where $k_L a_{N_2O_{T-process}}^{non-aerated}$ is usually set between 2 - 4 d^{-1}.

$$\mathrm{NTR}_{\text{non-aerated}}\left[\frac{\mathrm{g}_{\mathrm{N_2O}}}{\mathrm{h}}\right]=\mathrm{k_L a}_{\mathrm{N_2O}_{\text{T-process}}}^{\text{non-aerated}}\cdot \mathrm{C}_{\mathrm{N_2O}}^{\mathrm{process}}\cdot \mathrm{V}_{\text{non-aerated tank}} \tag{3}$$

Determining the $\mathrm{k_L a}_{\mathrm{O_2}}$ can be a challenging problem as it is associated with high local variation and will vary based on the process configuration such as the submersion depth. Unisense provides three methods to determine this (Unisense, 2019)

1) Calculation based on power consumption (method 1)
2) Calculation based directly on $\mathrm{k_L a}_{\mathrm{O_2}}$estimation (method 2)
3) Calculation based on online $\mathrm{k_L a}_{\mathrm{O_2}}$ estimation (method 3)

In the case of OR, the power consumption is not monitored and thus method 1 is excluded. Due to the complex geometry method, 2 is not a viable option, furthermore, it has been reported to overestimate the $\mathrm{k_L a}_{\mathrm{O_2}}$ (Uri Carreño *et al.*, 2020) (Unisense, 2019). Therefore, in this project, method 3 is used to determine the $\mathrm{k_L a}_{\mathrm{O_2}}$.

The $\mathrm{k_L a}_{\mathrm{O_2}}$ is estimated by calculating the oxygen transfer rate (OTR) through the aeration data collected by the sensors if the oxygen level reaches a steady state for several minutes. The $\mathrm{k_L a}_{\mathrm{O_2}}$ is calculated using the respiration rate ($\mathrm{q}_{\mathrm{O_2}}\,\mathrm{x}\,\mathrm{X}_{\mathrm{biomass}}$) corresponding to the linear slope of the oxygen decrease during the phase immediately after stoppage of the surface aerators and the steady oxygen reading ($\bar{C}_{O_2}^{process}$) according to Eq (4).

$$\mathrm{k_L a}_{\mathrm{O_2}\,\text{T-process}}=\frac{\mathrm{q}_{\mathrm{O_2}}\,\mathrm{x}\,\mathrm{X}_{\mathrm{biomass}}}{\mathrm{CO}_2^{\text{Sat, T-process}}-\bar{\mathrm{C}}_{\mathrm{O_2}}^{\mathrm{process}}} \tag{4}$$

Figure 5 provides a visual explanation of the various parameters involved in the calculation and is provided from (Unisense, 2019).

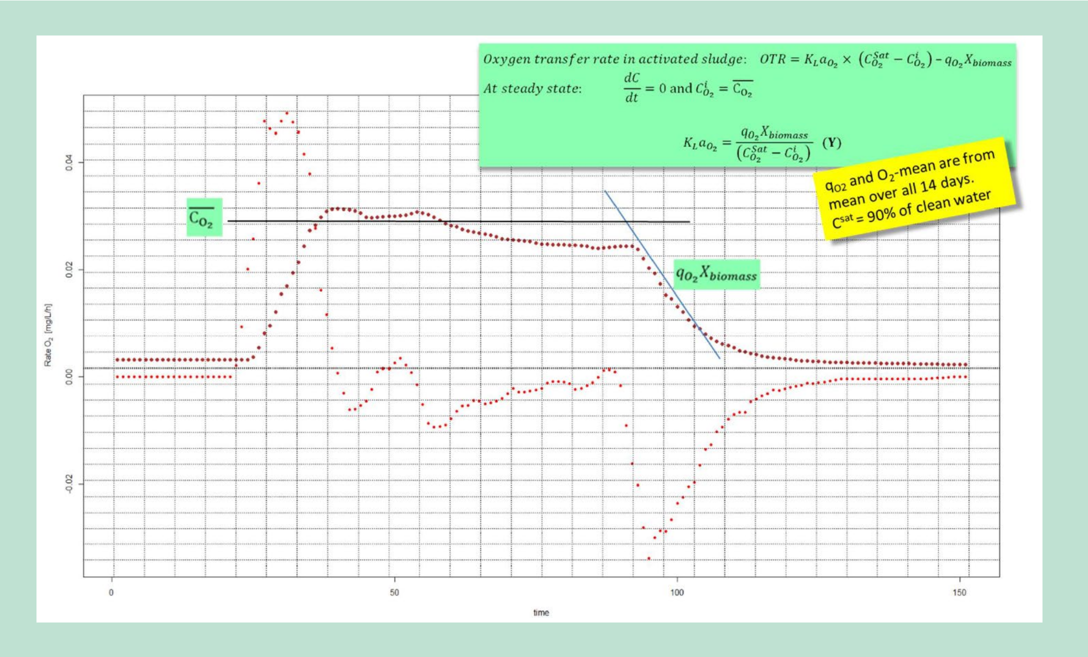

FIGURE 4. Oxygen trends during the steady-state and shut down of aerator (From (Unisense, 2019)

An empirical correlation is then used to calculate the N2O mass transfer coefficient $k_L a_{N_2O}$ according to Eq (5) where D_{N_2O} and D_{O_2} are diffusion coefficients with the same temperature dependence, hence the ratio is constant.

$k_L a_{N_2O\ \text{T-process}} = k_L a_{O_2\ \text{T-process}} \cdot \sqrt{\frac{D_{N_2O}}{D_{O_2}}} = k_L a_{O_2\ \text{T-process}} \cdot \sqrt{\frac{1.77 \cdot 10^{-9}\ m^2\ s^{-1}}{2.12 \cdot 10^{-9}\ m^2\ s^{-1}}}$	(5)

Eq (2) and Eq (3) can then be used to calculate the emission rates.

The calculation is carried out for each time step and is then converted to emissions daily. Thus the emission factor can be calculated as shown in Eq (6).

$N_2O \text{ emission factor } [\%] = \frac{N_2O_{emitted}}{N_2O_{influent}} \cdot 100$	(6)

In this work, the volume of the aerated and non-aerated tanks is set to the total volume of the tank. The $k_L a^{non-aerated}_{N_2O_{T-process}}$ is set to 2 d^{-1}.

5. Results

5.1 N_2O emissions calculation and analysis

Figure 6 shows an example of the oxygen profile observed during one intermittent aerated and the non-aerated period from the Ornum plant. As mentioned above, the actuators namely the surface aerators are used in on-off operation mode as part of the aeration control strategy. The plateau of the oxygen profile is used to estimate average oxygen concentration, and the slope of the right tail of the oxygen profile is used to determine the oxygen consumption rate of activated sludge, which is used in Eq (4) to estimate the volumetric mass transfer coefficient of the system.

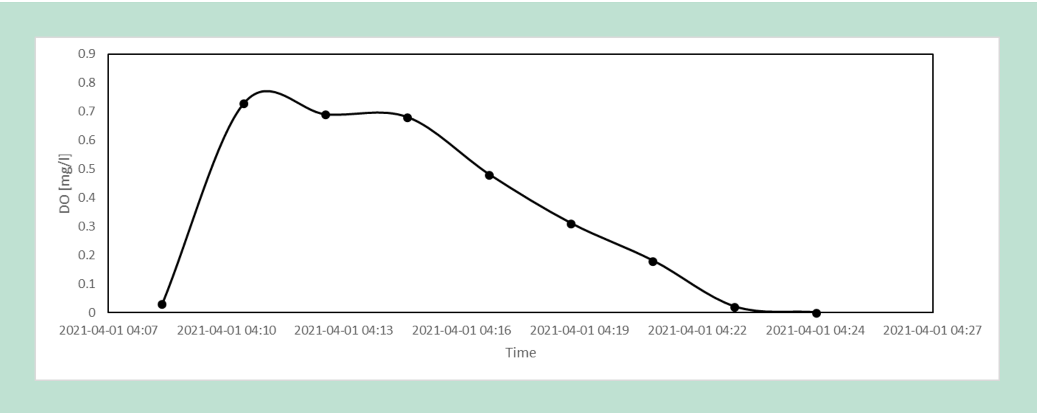

FIGURE 5. Oxygen (DO) profile for LT1 at a specific time step

These calculations are performed for surface aerators in both LT1 and LT2 tanks separately on a series of time locations, which are reported in Table 4 and Table 5 respectively. These calculations are used to infer mean and standard deviation for $\mathrm{k_La_{N_2O}}$ estimations.

TABLE 4: k_La for N_2O at different time locations for LT1

$q_{O_2} x\, X_{biomass}$ [g/m^3-d]	$\bar{C}_{O_2}^{process}$ [mg/l]	$CO_2^{Sat,T-process}$ [mg/l]	$k_La_{O_2}$ [1/d]	$k_La_{O_2}$ [1/h]	$\mathrm{k_La_{N_2O}}$ [1/h]
-116.6	0.70	9.9	12.68	0.53	0.48
-378.1	1.12	9.9	43.04	1.79	1.64
-295.2	0.92	9.9	32.85	1.37	1.25
-147.6	0.50	9.9	15.71	0.65	0.60
-144.0	0.61	9.9	15.51	0.65	0.59
-363.6	1.08	9.9	41.22	1.72	1.57
-276.5	1.39	9.9	32.48	1.35	1.24

TABLE 5: k_La for N_2O at different time locations for LT2

$q_{O_2} x\, X_{biomass}$ [g/m^3-d]	$\bar{C}_{O_2}^{process}$ [mg/l]	$CO_2^{Sat,T-process}$ [mg/l]	$k_La_{O_2}$ [1/d]	$k_La_{O_2}$ [1/h]	$\mathrm{k_La_{N_2O}}$ [1/h]
-319.5	2.33	9.9	42.17	1.76	1.62
-322.6	1.83	9.9	39.97	1.67	1.52
-203.76	0.87	9.9	22.56	0.94	0.86
-259.2	0.85	9.9	28.63	1.19	1.10
-324.7	1.56	9.9	38.91	1.62	1.48

Based on the results in Table 4 and 5, the average and standard deviation for the mass transfer coefficients are summarized as:

$$\mathrm{k_L a_{N_2O}}\ \left[\frac{1}{\mathrm{h}}\right](\mathrm{LT1}){=}1.05\ \pm 0.49$$

$$\mathrm{k_L a_{N_2O}}\ \left[\frac{1}{\mathrm{h}}\right](\mathrm{LT2}){=}1.31\ \pm 0.32$$

The corresponding 95% confidence interval for these estimates (calculated as 2 standard deviations around the mean) are as follows:

$$k_L a_{N_2O}(LT1) = [0.08 \quad 2.02]$$

$$k_L a_{N_2O}(LT2) = [0.66 \quad 1.95]$$

The obtained results are comparable to the results obtained at Ejby Mølle, another WWTP that uses surface aerators ($k_L a_{N_2O}\ \left[\frac{1}{h}\right] \sim 0.5 - 1.1$) (Uri Carreño *et al.*, 2020).
Using the average values of the estimated $k_L a_{N_2O}$, the emission factors and long-term N_2O emissions are calculated and plotted in Figure 7 and Figure 8 respectively. Key emission numbers for OR are summarized in Table 6.

TABLE 6: Summary statistics for N_2O emissions for OR plant (Match-September 2021)

	kg N_2O-$N_{emitted}$ [per day]	**kg N_2O-$N_{emitted}$ [per year]**	**kg $N_2O_{emitted}$ [per year]**	**kg $CO_{2equivalent}$ [per year]**	**Emission factor [%]**
Min	0.00005	0.01	0.03	8.97	0.000
Max	0.60030	219.10	344.31	102,604.	0.337
Mean	**0.08584**	**31.30**	**49.23**	**14,671**	**0.061**
Median	0.04120	15.00	23.63	7,041	0.034
Std. dev.	0.11192	40.90	64.20	19,130	0.077

A plot of the daily emission factors is shown in Figure 8, while the average daily emissions are shown in Figure 8. We have observed several peaks (three in total) in N_2O emissions during the monitoring period. We believe these peaks correspond to sensor drift and the need for recalibration. For example concerning the peak around April 14th, 2021, these values were not observed after the calibration of the N_2O sensor on April 19th,2021. From biological perspectives, such peaks may also correspond to a transient response to shock load or disturbances. Since we did not have any additional measurements to rule these out, we have kept these peaks in the statistical analysis of the emission factors for the plant. This decision was taken as a precautionary principle

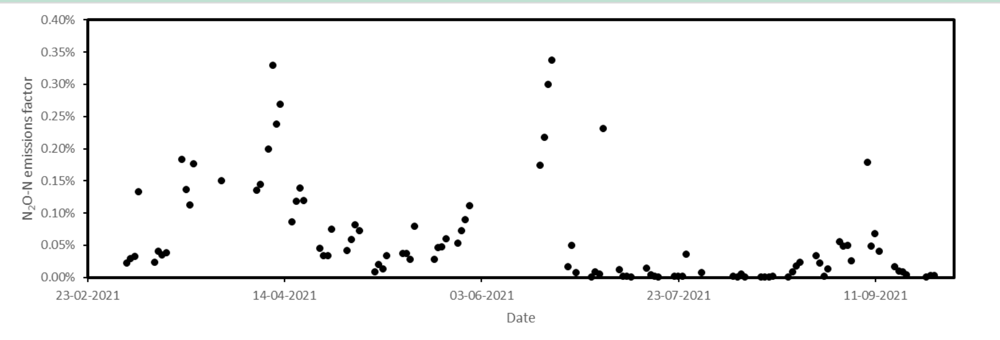

FIGURE 7. N2O emission factor for OR plant

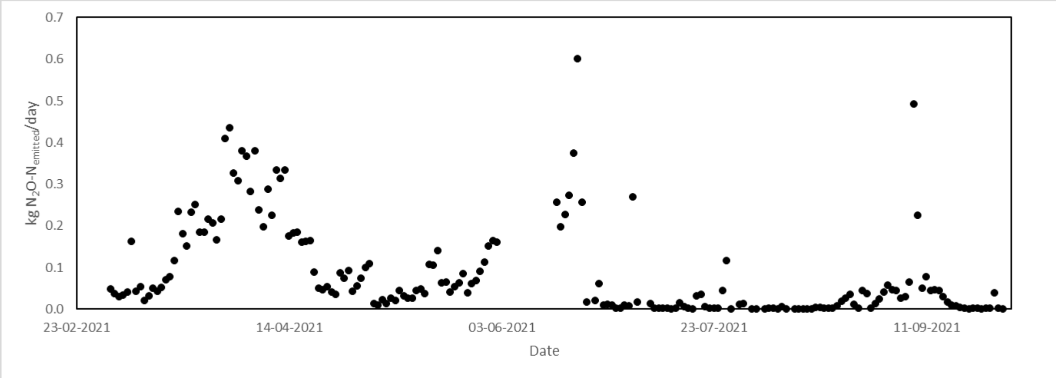

FIGURE 8. N2O emitted per day for OR plant

We have compared this emission statistics of the Ornum plant with another WWTP, Kalundborg Centrale Rensningsanlæg (denoted KCR) operated by Kalundborg utility for which the key emission numbers are reported in Table 7. This is reported here for comparative purposes. Based on the comparison, it becomes clear that the yearly N_2O emissions from Ornum (ca 15 tCO_2/yr) are much lower than the KCR plant (ca 236 tCO_2/year), which is about 15 times lower. Relative to the influent nitrogen load, that is the emission factor, Ornum's emission factor (0.06%) is about 6 times lower than that of KCR (0.38%).

TABLE 7: Key emission number for KCR (Match-April 2020) (Miljøstyrelsen, 2020)

	kg N_2O-$N_{emitted}$ [per day]	kg N_2O-$N_{emitted}$ [per year]	kg $N_2O_{emitted}$ [per year]	kg $CO_{2equivalent}$ [per year]	Emission factor [%]
Min	0.04	14.0	22.1	6.579	0.06
Max	2.63	958.6	1506.4	448,913	0.58
Mean	1.39	505.7	794.7	236,826	0.38
Median	1.32	481.4	756.4	225,415	0.38
Std. dev.	0.72	263.6	414.2	123,446	0.15

5.2 Sensitivity analysis of N_2O quantification

One of the key parameters that affect the calculation of N_2O emission from the plants is namely the mass transfer coefficient, K_La_{N2O}. To reflect this we have performed a calculation by considering the upper bound (upper 95% confidence level), K_La_{N2O} which corresponds to mean plus 2 sigmas (standard deviation). Hence we performed calculations using K_La_{N2O} 2.03 h-1 and 1.95 h-1 for LT1 and LT2 tanks. A summary statistics of the calculated emissions under these increases is shown in table Table 8. Although we have increased k_La_{N2O} by roughly 100% in these new calculations, there was only about a 33% increase in the calculated emission factors compared to the baseline (Table 6). This shows that even if considered a huge uncertainty in the estimation of the k_La_{N2O} value, the conclusion for the Ornum plant doesn't change much. In other words, the N_2O emissions are not significant for the Ornum plant.

TABLE 8: Sensitivity analysis on N_2O emissions: Emission calculations using upper 95% confidence value of k_La_{N2O}

	kg N_2O-$N_{emitted}$ [per day]	kg N_2O-$N_{emitted}$ [per year]	kg $N_2O_{emitted}$ [per year]	kg $CO_{2equivalent}$ [per year]	Emission factor [%]
Min	0.00001	0.0	0.0	3	0.000
Max	0.74100	270.5	425.0	126,655	0.484
Mean	0.11763	42.9	67.5	20,105	0.082
Median	0.05153	18.8	29.6	8,807	0.040
Std. dev.	0.16075	58.7	92.2	27,477	0.112

5.3 Predicting the Liquid N_2O concentration and global sensitivity analysis

The results from deep learning models to predict the liquid N_2O concentration is shown below as a parity plot for a portion of the data (Figure 9). The purpose of this model is to map a set of measured inputs (Q, NO_3, NH_4, T, DO) to the output which is the liquid N_2O concentration. The model obtained achieves a coefficient of determination (R^2) of 0.81, 0.70, and 0.70 for the training, validation, and test set respectively. The model prediction performance appears qualitatively low at lower ranges such as 0 – 0.05, while at higher ranges the model fit is better. While the model prediction accuracy is not very high, R^2 of 0.81 is comparable with values reported in the literature for the mechanistic models. Hence we consider the model sufficiently good to perform sensitivity analysis.

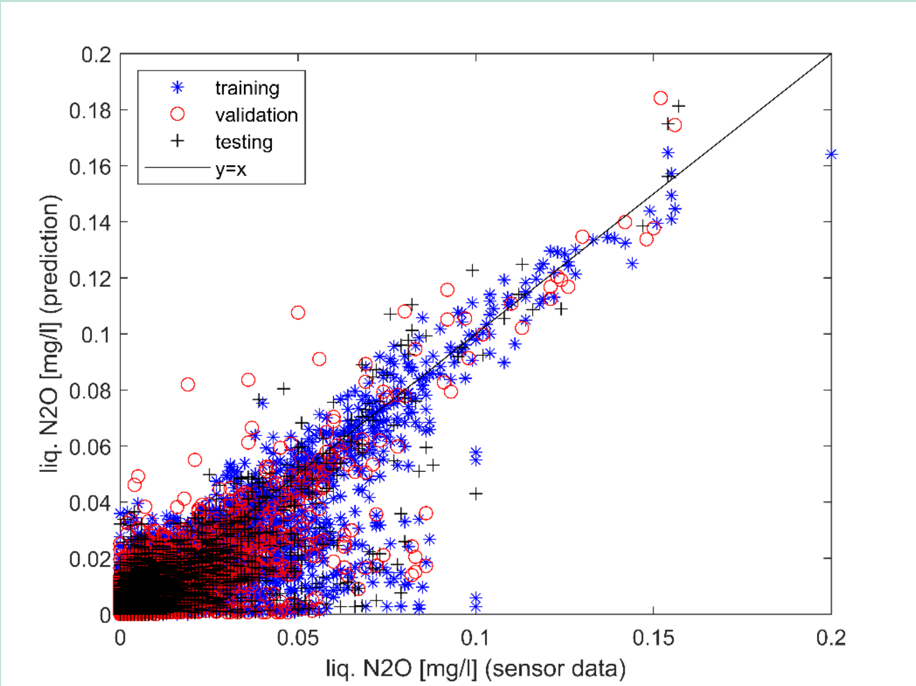

FIGURE 9. Parity plot for the liquid N2O prediction from the DNN model

The global sensitivity analysis is performed using easyGSA toolbox (Al *et al.*, 2019), which provided Sobol's first order (Si) and total (STi) sensitivity indices for model inputs (Q, NO_3, NH_4, T, DO) on model outputs which are liquid N_2O concentration. These can be seen in Figure 10. The interpretation of the results is as follows: sensitivity indices take a value from 0 to 1, which indicates the fraction of the contribution (hence importance) of inputs to the output variance. The low value means the input has zero importance on the output, vice versa high value means higher importance. First-order sensitivity indices indicate the contribution of the inputs to the outputs by itself alone, while the total sensitivity index (STi) indicates the total contribution including interaction effects. In this regard, among the inputs, only DO (dissolved oxygen) has a significant contribution by itself alone meaning a high Si value around 0.4. this indicates that DO is the most important factor explaining the high variability in liquid N_2O concentration by 40% of the output variance. Considering STi, following DO which has the highest contribution (0.8), the other inputs, namely temperature, NH_4, NO_3, and influent flowrate have all significant contributions to liquid N_2O. The main point to emphasize here is that STi is mainly indicating the presence of interaction effects for temperature, NH_4, NO_3, and influent have interaction effects (not single effect). This is not surprising as N_2O emission is an interplay between the AOB denitrification pathway and incomplete hydroxylamine oxidation pathways during aerated periods, and incomplete denitrification during anoxic periods (Sin and Al, 2021). Therefore it is natural to expect that liquid N_2O is influenced by biological activity which is impacted through process control strategy. The control algorithm itself creates dependencies between DO, ammonia, and nitrate (in the plant as well as influent disturbances (temperature and influent load/composition).

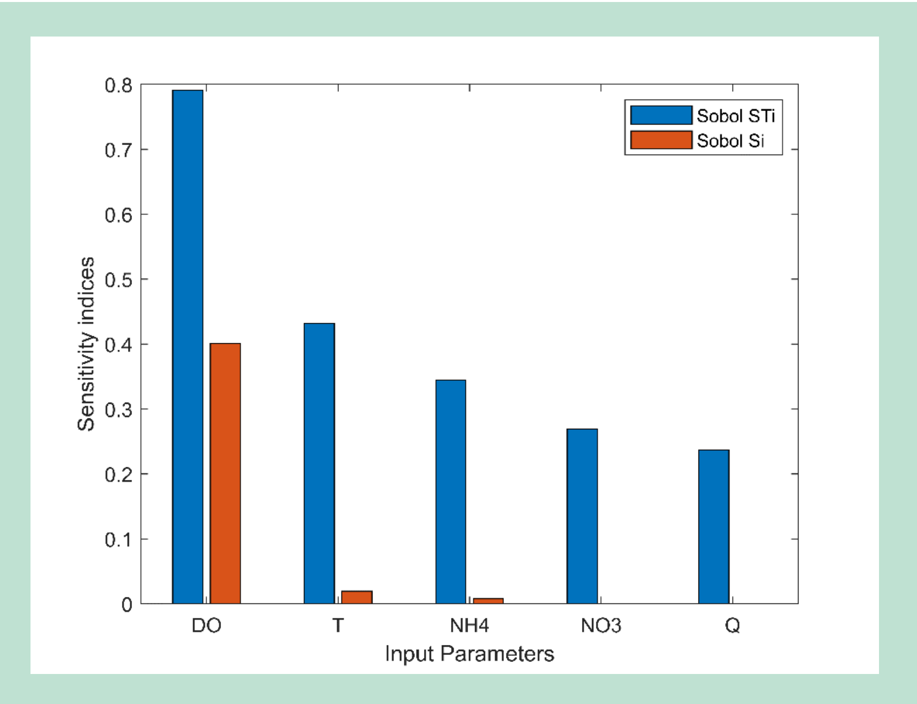

FIGURE 10. Global sensitivity analysis results for model inputs: Sobol's first order (Si) and total sensitivity (STi) indices for DO, Temperature, NH4, NO3, and influent flow rate

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6. Conclusions & perspectives

In this project, we have performed a monitoring campaign for measuring, quantifying, and analyzing N_2O emissions at the Ornum plant for 6 months from March until September 2021. The main conclusions of this project can be summarized in one point: The N_2O emissions from the Ornum plant are found to be **0.06%** on average. This emission factor is quite low compared with the threshold considered in the IPCC 2019 report (**1.6%)** or Danish environmental agency recommendation of **0.84%.** Based on these results, modifying the current process control and operation strategy is not needed at this point. The more specific conclusions are provided below:

- The N_2O concentrations are measured at both aeration tanks at Ornum plants from March 1 until September 30, 2021.
- Mass transfer coefficient for N_2O,k_La_{N2O} is estimated using the Unisense method that relies on a typical oxygen profile from aerated and non-aerated periods. The mean and standard deviation of the calculations were 1.05±0.49 h^{-1} and 1.31±0.32 h^{-1} respectively for LT01 and LT02 tanks. These results are consistent with other reported values for plants with surface aeration (e.g. Ejby Mølle).
- The summary statistics of N_2O emissions as observed during the measurement campaign show that the emission factor is significantly low for Ornum (0.06% kgN_2O/kgN-influent). This calculation is robust against uncertainty in the estimation k_La_{N2O} up to 2 sigma deviation from the mean (that gives a 95% confidence level assuming estimates are normally distributed). In this case, the emission factor was 0.082% kgN_2O/kgN-influent which is still relatively low.
- A deep learning model is trained successfully which provided a training R^2 of **0.81**, which is comparable to N_2O models reported in the literature. The model is deemed qualitative and sufficiently well to perform sensitivity analysis.
- A global sensitivity analysis using the Sobol sensitivity method is conducted with this model. The model indicated that the most important factor is dissolved oxygen, which explains by itself 40% of the variation in the liquid N_2O concentration. The results also showed that all other inputs namely temperature, NH_4, nitrate, and influent flowrate were also important but mainly through their interaction effects. All these inputs are relevant and important to monitor to study N_2O dynamics in the plant.
- There were three peaks observed in N_2O emissions during the monitoring period. These are believed to be caused partly by sensor drift. This point indicates that regular maintenance and recalibration are needed. As a precautionary principle, these peaks were not excluded from the summary analysis to be on the safe side.

As a perspective several suggestions can be made:

- There is no need to modify the process control strategy of the Ornum plant at this moment in time. The current operation strategy works well both with respect to effluent ammonium and N_2O emissions.
- For the Kalundborg utility, it is perhaps more relevant to focus on Kalundborgs Centrale Renseanlæg (KCR) instead of Ornum plant to explore if there is potential for further CO_2 reduction. Among others, one can address the question of whether further CO_2 reduction can be achieved by modifying the operation control strategy at KCR.
- Some empirical observations of the plant design and operation e.g. high COD/N ratio, a good aeration regime (not limited by aeration with DO setpoint around 1 mg/L) which may explain low N_2O emission. However, a better understanding of the underlying biological processes and their interactions with process operating conditions and influent load will require focused multidisciplinary work across microbial community analysis and process engineering/first principles modeling among others (Sin and Al, 2021).

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Nitrous Oxide Emissions from Ornum Waste Water Treatment Plant – Kalundborg Utility

Kalundborg Forsyning har i dette projekt undersøgt udledningen af lattergas (N2O) fra Ornum Renseanlæg.

Hovedformålet har været:
(i) at foretage N2O relaterede målinger gennem en længere periode periode for at bestemme graden af N2O udledningen, (ii) undersøge potentielle faktorer, der bidrager til N2O udledningen ved hjælp af kunstig intelligens baserede modeller udviklet af DTU, og
(iii) baseret på resultaterne afklare om der skal ske ændringer i processer og eksisterende kontrolsystemer.

Rapporten præsenterer resultaterne, som viser, at lattergasemissionen fra Ornum Renseanlæg ligger lavt med en emissionsfaktor på 0,06%, som ligger under den nationalt opgjorte emissionsfaktor.

En følsomhedsanalyse viser, at iltkoncentrationen er den vigtigste procesparameter, idet den har ca. 40% indflydelse på N2O variationen i væskefasen. Øvrige procesparametre som temperaturen, ammoniumkoncentrationen (NH4) og indløbs flow er ydermere indirekte influerende på emissionen af lattergas.

På grundlag af resultaterne anbefales det, at der ikke foretages ændringer i den nuværende operation eller kontrolsystemer.

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