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Integrated plant-wide modelling for evaluation of the energy balance and greenhouse gas footprint in large wastewater treatment plants

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Abstract

Modern wastewater treatment plants (WWTPs) should maintain a balance between three combined sustainability criteria, including effluent quality, energy performance and greenhouse gas (GHG) emissions. All of these criteria were considered in the integrated plant-wide model developed in this study. The proposed model incorporates new features, including: (i) the addition of associated facilities to the overall energy balance and GHG footprint and (ii) the implementation and validation of detailed sub-models of heat and power supply and demand. The aim of the study was to investigate the implications of these new extensions on the energy balance and sustainability assessment of the entire facility. The integrated model was evaluated against full-scale data from a large WWTP performing biological nutrient removal in an activated sludge bioreactor and anaerobic digestion of sewage sludge. Upon applying the investigated operational strategies, the potential decreases in the GHG footprint and effluent total nitrogen concentration were estimated to be 20% and 30%, respectively, in comparison with the current conditions. However, only a slight potential for improving the overall energy balance was found. In contrast, with technological upgrades, energy neutrality and the highest reduction in the GHG footprint (by over 30%) were achieved, but the effluent quality remained unchanged in comparison with the current conditions. It was shown that the heat demand of associated facilities could not be neglected in the overall heat balance and GHG footprint. The detailed models of energy demand and supply improved the assessment of energy performance in the full-scale WWTP.

Keywords: Climate Change; Energy Neutrality; Full-scale Wastewater Treatment Plant; Heat Balance; Performance Assessment; Sustainability

1. Introduction

For decades, municipal wastewater treatment plants (WWTPs) have been focused on the efficient removal of pollutants to protect public health and the aquatic environment. In recent years, other aspects have become important, including climate change and the efficient use of resources, especially energy [1]. These two aspects should be considered in conjunction with effluent standards when rethinking the evaluation criteria for sustainability assessment in WWTPs [2].

Energy is one of the most important resources used in wastewater treatment processes and has great potential for recovery from wastewater. Higher energy demands have been observed in response to more stringent effluent standards and increased amounts of wastewater [3, 4]. On the other hand, achieving energy neutrality in WWTPs has become a feasible operational challenge provided that various measures are applied to reduce energy demand and maximize energy recovery from wastewater [3, 5].

WWTPs have been found to be an important source of greenhouse gas (GHG) emissions [6]. Both process-related (direct) and energy-related (indirect) GHG emissions contribute to the overall GHG footprint of a WWTP. In the GHG footprint, the cumulative emissions of different gases, i.e., carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O), are expressed as CO_2 equivalents (CO_{2e}) with respect to their global warming potential (GWP). Among these gases, N_2O has received special attention due to its highest GWP of 265 [7]. However, prediction of the process-related N_2O emissions from WWTPs is not straightforward due to the complexity of N_2O production and consumption mechanisms [8]. Generic N_2O emission factors have shown a high uncertainty of prediction, while mathematical (mechanistic) N_2O models have rarely been applied in full-scale nitrogen and phosphorus removal activated sludge (AS) systems [9, 10].

In medium and large WWTPs, anaerobic digestion (AD) is a commonly adopted process that generates methane-reach biogas from sewage sludge. The heat and power recovered from biogas improve the energy balance of a WWTP and decrease indirect GHG emissions from the combustion of fossil fuels. However, excessive energy savings in the biological stage [11, 12] or co-digestion of external substrates [13] may result in increased process-related GHG emissions .

The complex interactions among effluent quality, energy consumption and GHG emissions require advanced evaluation tools, such as plant-wide modelling [14, 15]. Plant-wide models combine mainstream and sludge treatment lines and take into account interactions between them. The Benchmark Simulation Model No. 2 (BSM2), originally developed to evaluate control strategies in WWTPs [16], has been extended and used as a tool for predicting N_2O production/emission in a few theoretical studies (e.g., [11], [17] and [18]) and a real full-scale facility [19]. Examples of the validated plant-wide models have rarely been presented due to the limited availability of adequate and reliable databases from full-scale facilities [9].

The studies evaluating GHG emissions on a plant-wide scale (Table S1 in Supplementary Information (SI)) revealed different approaches with respect to the following: (i) biokinetic models applied, (ii) sources of GHG emissions and calculation methodology, (iii) evaluated scenarios or strategies for GHG mitigation, and (iv) performance evaluation indicators. The energy-related GHG emissions were primarily based on the assumed energy conversion efficiency and specific emission factors for electricity from the grid in the range 0.25-0.94 kg CO_{2e}/kWh. The GHG emissions, effluent quality and operational cost have been found as potentially conflicting objectives and considered as either separate evaluation criteria (e.g., in the studies of Flores-Alsina et al. [11], Arnell et al. [19]) or integrated performance indicators (e.g., Barbu et al. [20]).

Different approaches have been proposed with respect to the process heat balance. In BSM2, a simplified thermodynamic model of AD is implemented that does not consider heat transfer through the digester walls [16]. In contrast, a detailed methodology for the dynamic prediction of heat produced and consumed in bioreactors was developed in another comprehensive plant-wide modelling approach [21]. However, that approach did not consider GHG emission issues. Until now, plant-wide modelling studies have been process-oriented and have neglected non-process activities inside WWTPs.

Associated facilities, such as space heating and ventilation systems in buildings, affect both the overall energy performance and GHG emissions. In analytical calculations, Panepinto et al. [22] showed the importance of thorough energy balance considerations in WWTPs. Detailed heat and power supply and demand sub-models can provide more realistic energy recovery estimations [23] and give a rationale to further expand plant-wide models [15]. Until now, dynamic calibrations and validations of heat and power demand and supply models in WWTPs have not been reported in the literature.

In response to this gap, an integrated WWTP model was developed in this study. Dynamic process sub-models were combined with a detailed energy balance and GHG emissions. In contrast with previous studies, the proposed model incorporates the following new features: (i) the addition of associated facilities within the plant to the calculations of the overall electrical and thermal energy balance and GHG footprint, (ii) more realistic model predictions, obtained through a detailed thermodynamic AD model and an empirical model of a combined heat and power (CHP) system, and (iii) model calibration and validation using full-scale measurements for the electrical and thermal energy balance. A comparison between the existing plant-wide models and the proposed model is given in Table S2 (in SI). The main difference is that the proposed model changes the energy balance from the process-oriented perspective to the whole plant-oriented view. The integrated model was evaluated against experimental data from a full-scale plant performing biological nutrient removal and AD of sewage sludge. It was also shown how the model could be applied to analyse combined strategies for improving the sustainability of wastewater treatment.

2. Materials and methods

2.1. Study site and plant configuration

The studied WWTP primarily treats domestic wastewater from the city of Slupsk and surrounding communities located in northern Poland. The average pollutant load to the plant corresponds to approximately 250,000 population equivalents. A simplified layout of the studied plant is shown in Fig. 1. The main component of the treatment process is a biological step consisting of three parallel lines. The biological reactor in each line (10,020 m^3) employs an A_2O (anaerobic/anoxic/oxic) process configuration for combined nitrogen and phosphorus removal. After thickening, both raw sludge from the primary clarifier (908 m^2) and waste activated sludge (WAS) from the secondary clarifiers (4 x 1,256 m^2) are directed to anaerobic digesters (8,240 m^3 in total) operated under mesophilic conditions (36-38°C). The dewatered sludge is composted and ultimately disposed of on farmlands. The anaerobic sludge digestion liquor (reject water) returns to the main wastewater train prior to the primary clarifier. Biogas generated in the AD process is kept in a storage tank and subsequently used for either heat generation in a boiler or combined heat and power generation in on-site cogeneration units. The associated facilities include buildings with technological devices, a control centre, a laboratory, and an office.

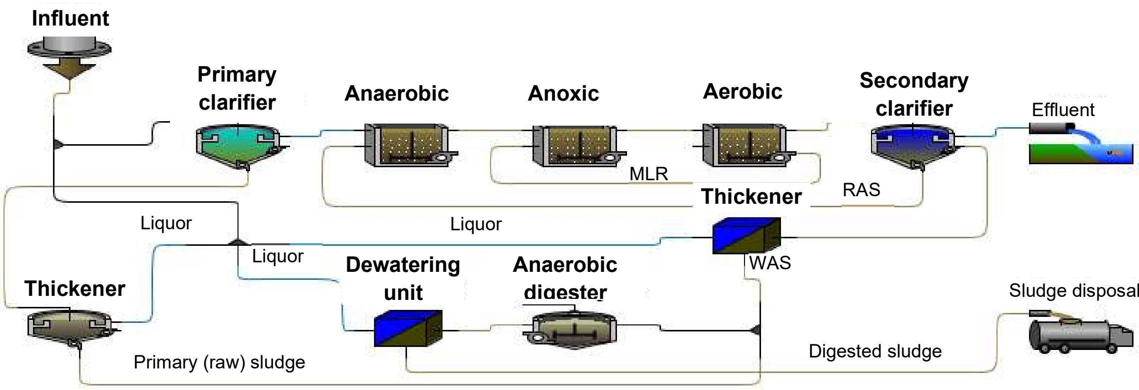

Figure 1. Simplified layout of the studied WWTP; MLR – mixed liquor recirculation, RAS – return activated sludge, WAS – waste activated sludge.

2.2. General concept of the integrated WWTP model

The integrated WWTP model (Fig. 2) incorporates process sub-models related to the core biochemical processes performed in the AS bioreactor and anaerobic digester as well as solid-liquid separation (primary/secondary clarifiers and sludge thickening/dewatering units). The biokinetic process sub-models are used to predict direct GHG emissions. In the extended plant-wide model, the process sub-models are combined with process energy sub-models, including electricity and heat demand. In the overall energy balance, the process-related energy balance is combined with the non-process energy consumption inside the WWTP. The energy conversion and supply sub-models (CHP system and boilers) complete the balance. The overall GHG footprint incorporates energy-related indirect GHG emissions.

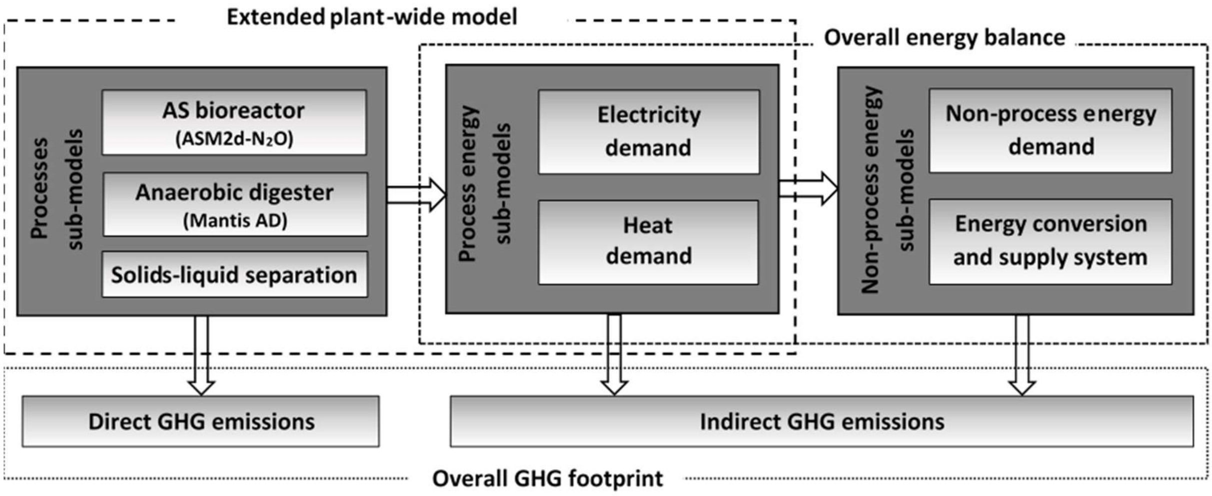

Figure 2. Schematic diagram of the integrated WWTP model developed in the present study.

2.3. Integrated WWTP model components

2.3.1. Processes sub-models

The components of the plant-wide model are described in Table S3 (see SI) and include the following: (i) the modified Activated Sludge Model no. 2d (ASM2d) [24], extended with the N_2O production and emission module (ASM2d-N_2O) [10], and (ii) the Mantis AD model [25]. Both biokinetic models were calibrated and validated during previous studies at the Slupsk WWTP [10, 26]. Solid-liquid separation in the primary/secondary clarifiers is described by a non-reactive 1-dimensional settling model [27]. Empirical models with the assumed solid removal efficiency are used for the thickening and dewatering units. The plant-wide model was implemented in the GPS-X 7.0 simulation platform (Hydromantis/Canada) (Fig. S1 in the SI). In contrast with the previous plant-wide model of the studied WWTP [26], the newly developed model is capable of predicting N_2O production/consumption and emissions from the bioreactor.

2.3.2. Overall energy balance

In the overall energy balance of the WWTP, electricity and heat are considered as two separate components of the process and non-process energy sub-models. The overall electricity demand ($E_{el,\ WWTP}$) is composed of the energy demand for both technological devices and associated facilities. The detailed models for the main types of electricity consumers (blowers and pumps) are shown in Table

S4 (in SI). Other miscellaneous energy components required for various mechanical operations are calculated based on flat energy usage rates. The heat consumption models developed in this study cover the overall heat demand (Q_{WWTP}), including the AD process (Q_{AD}) and the space heating and ventilation systems in the buildings (Table S5 in SI). The energy conversion and supply system, including components such as the CHP plants and gas boilers, enable the operation of electrical devices and maintain set-point temperatures in the anaerobic digesters and inside the buildings. The distribution of electricity and water heating (up to 90°C) throughout the WWTP is shown in Fig. 3.

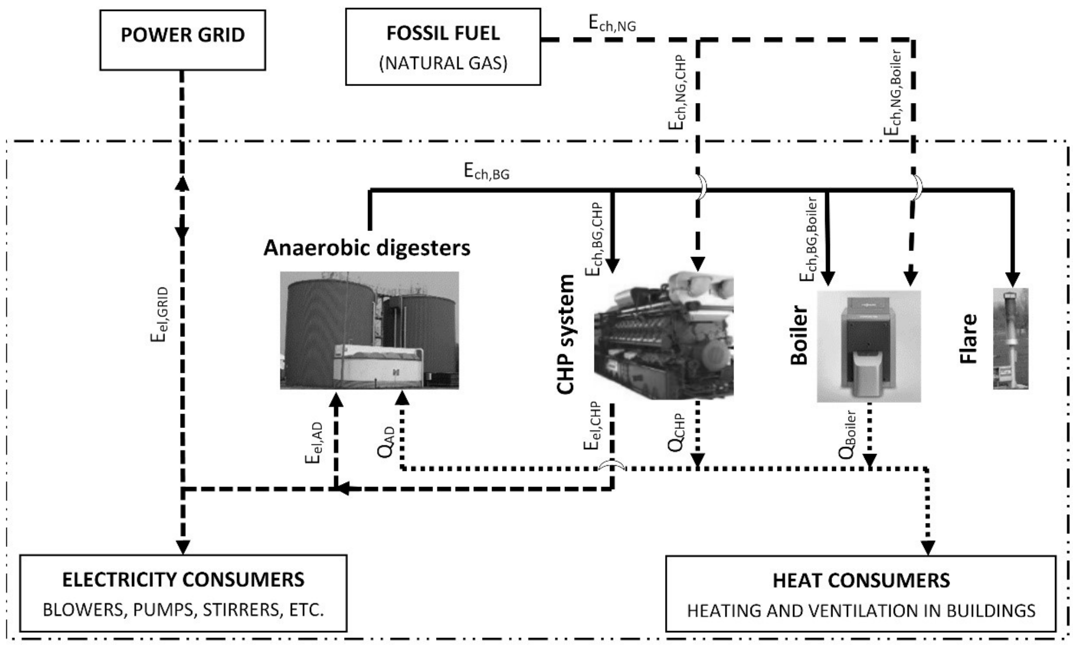

Figure 3. Electricity and heat distribution throughout the studied WWTP.

A general equation for the electricity balance of the WWTP can be expressed as follows:

$$E_{el,WWTP} = E_{el,CHP} + \delta E_{el,GRID,in} + (\delta - 1)E_{el,GRID,out} \quad (1)$$

where $E_{el,CHP}$ is the total electricity supplied from the on-site CHP system, $\delta \langle 0; 1 \rangle$ is a binary variable defining the direction of electricity transfer (to or from the external power grid), $E_{el,GRID,in}$ is the electricity purchased from the external grid, and $E_{el,GRID,out}$ is the excess electricity generated on-site and sold to the external power grid.

A general equation for the heat balance of the WWTP can be expressed as follows:

$$Q_{WWTP} = Q_{CHP} + Q_{Boiler} + \delta Q_{in} + (\delta - 1)Q_{out} \quad (2)$$

where Q_{CHP} is the heat supplied from the on-site CHP system (Q_{CHP}) and Q_{Boiler} is the heat supplied from the local boiler. Heat distribution, i.e., imported into the plant (Q_{in}) or exported outside the plant (Q_{out}), is only possible via a district heating network. In the studied case, that option is not available, and the excess heat is dissipated into the environment.

The chemical energy of fuel can be expressed as follows:

$$E_{ch,G} = V_G H_{V,CH} S_{CH} \quad (3)$$

where V_G is the volume of gas (G), i.e., biogas (BG) or natural gas (NG), used for electricity and/or heat generation, $H_{V,CH}$ is the heating value of the combustible component of gas (methane or other hydrocarbons), and S_{CH} is the proportion of the combustible component in the total gas volume. If the biogas installation is equipped with a storage tank, flaring is unlikely to occur.

To account for variations in the electrical and thermal efficiencies of the CHP system (net electrical/thermal energy generated per unit chemical energy consumed) under dynamic biogas flowrates, empirical models were developed based on full-scale measurements (Eq. S11 and S12 in SI). These models were used to predict the electricity and heat recovered via the biogas-driven CHP system in the evaluation of operational strategies and technological upgrades (section 3.3).

2.3.3. Overall GHG footprint

In this study, GHG emissions were classified on the basis of IPCC definitions [28], and the term "GHG footprint," representing equivalent CO_2, CH_4 and N_2O emissions, was adopted from the literature [17]. In the cumulative GHG footprint, the following emissions were included: (i) direct emissions related to biochemical processes in the AS bioreactors (specifically N_2O emission) and anaerobic digesters (specifically CH_4 loss), (ii) indirect emissions related to electricity and heat supply as well as the chemicals used, and (iii) direct and indirect emissions related to the composting, transportation and farmland application of digested sludge. Following IPCC guidelines [29], biogenic CO_2 emissions from wastewater treatment were not taken into account. Energy-related emissions from the combustion of renewable energy sources (biogas) in the CHP system and boiler were also excluded, except for emissions from incomplete combustion.

The direct process emissions, energy balance components and sludge characteristics were derived from the models described in the preceding sections (2.3.1, 2.3.2). The parameters related to the use of coagulants/flocculants in the chemically enhanced primary treatment (CEPT) stage were adopted from previous experiments [26]. In those experiments, the suspended solids removal efficiency was investigated for different doses of ferric (III) sulphate and anionic flocculants. The assumed equivalent CO_2 emission factors are shown in Table S6 (SI).

2.4. Modelling and evaluation procedure for the integrated WWTP model

The modelling and evaluation procedure for the integrated WWTP model was carried out in the following steps (Fig. 4): (i) data collection, (ii) model calibration and validation, and (iii) evaluation of strategies for sustainable wastewater treatment.

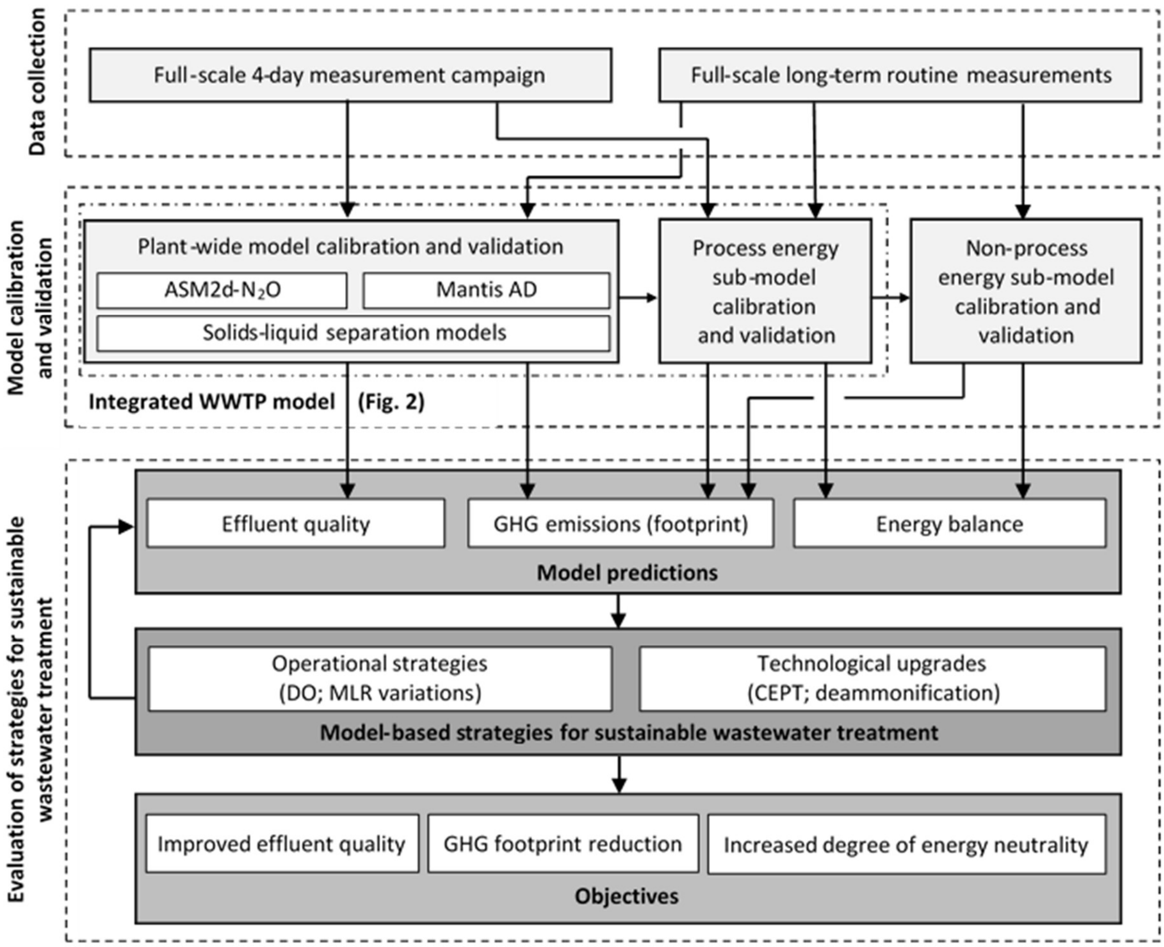

Figure 4. Step-wise modelling and evaluation procedure for the integrated WWTP model.

2.5. Data collection

2.5.1. Full-scale 4-day measurement campaign

An extensive 4-day measurement campaign was carried out at the studied WWTP in summer when the average wastewater temperature was 21°C. In that period, the mixed liquor suspended solids (MLSS) concentration in the biological reactor was 3.9 ±0.4 g/L. The mixed liquor recirculation (MLR) and return activated sludge (RAS) recirculation rates were maintained at approximately 500% and 140% of the influent flowrate, respectively, and the dissolved oxygen (DO) set-points in the aerobic compartments were kept at 2.25 ± 0.5 mg O_2/L.

Wastewater treatment line. Wastewater samples were withdrawn from the plant influent and effluent and the anaerobic, anoxic and aerobic compartments of the bioreactor. The scope of the analyses is shown in Table S7. The N_2O concentration in the liquid phase was measured by a Clark-type microsensor (Unisense, Denmark) placed in a closed mobile reactor continuously fed with mixed liquor from the bioreactor. A Fourier transform infrared (FTIR) gas analyser (Gasmet CX 4000, Finland) coupled with a floating hood was used to measure off-gas N_2O concentrations. More details about the full-scale measurement campaign can be found elsewhere [10].

Sludge handling line. Grab samples of primary sludge and WAS before and after thickening were analysed daily for dry solids (total and organic). Grab samples of digested sludge were additionally analysed for volatile fatty acids (VFA) and alkalinity. Grab samples of sludge digestion liquor were also analysed (Table S7). The biogas production and consumption values were measured online and registered every hour along with the CH_4 content.

Energy balance. Data on electricity, heat and fuel (biogas and natural gas) production/consumption were registered with a frequency of one hour by electricity meters, heat meters and gas meters, respectively (Table S8). Specifically, the energy sources (CHP units and boiler) and main consumers (blowers in the bioreactor aeration system, anaerobic digesters, and buildings) were equipped with measurement devices that allowed a detailed electricity and heat balance of the WWTP to be established. The collected data were comprised of the wastewater temperature and ambient air temperature, as well as the operating times of electrical energy consumers. The rated powers of the heat and power sources and main consumers are listed in Table S9.

2.5.2. Full-scale long-term routine measurements

Data from two consecutive years (before and after plant retrofitting) were selected for detailed analysis (Set 1 and Set 2, respectively). The main upgrades included a new anaerobic digester and replacement of some electrical devices. The differences between the energy performances of the WWTP (poor vs. satisfactory results) gave a rationale for comparison of the results and confirmation of the robustness of the energy balance model.

Wastewater treatment line. Daily averaged flow-proportional samples of the plant influent and effluent were collected and analysed for the parameters shown in Table S10.

Sludge handling line. Grab samples of the sludge and sludge digestion liquor were collected daily and analysed for several parameters (Table S11). Furthermore, daily biogas production data and quality data were collected.

Energy balance. For the long-term analysis, the daily average data from the electricity, heat and gas meters and thermometers were used (Table S8). Table S12 summarizes the annual energy balance of the studied WWTP.

2.6. Calibration and validation procedure of the integrated WWTP model

The biokinetic sub-models, i.e., ASM2d-N_2O and Mantis AD, were calibrated and validated separately, as described in detail in [10] and [26]. A multi-step procedure was used for ASM2d-N_2O calibration and validation using laboratory-scale and full-scale experiments [10]. Specifically, for N_2O production and emission, a two-step calibration was applied as proposed by [30]. The estimation of the most sensitive parameters was performed in GPS-X using the Nelder-Mead simplex method with the maximum likelihood objective function. To calibrate the Mantis AD model, full-scale measurements were applied [26].

In the present study, the kinetic parameters related to the biochemical processes in the bioreactor and anaerobic digester were adopted from previous studies without further modifications. The plant-wide model was calibrated by adjusting the flowrates in the sludge handling line and the solid-liquid separation efficiency (in the primary clarifier, thickeners and dewatering units) using dynamic data from the full-scale 4-day measurement campaign (Section 2.5.1). The primary objective was to achieve good fits for the concentrations of nutrient compounds in the bioreactor. For the AD process, which is much slower than the AS processes, the objective was to achieve consistency between model predictions and measurements for the daily average concentrations of dry solids, VFA and alkalinity in the digested sludge, as well as the biogas production. The efficiency of solid-liquid separation was evaluated with respect to the dry solids concentration in thickened/dewatered sludge, as well as organic and nitrogen compounds in the sludge digestion liquor. At this stage, the process energy demand sub-models for aeration and pumping were calibrated by adjusting the pressure loss and efficiency of the devices (blowers and pumps). In general, the 4-day measurement campaign was used to calibrate the process energy sub-models, such as the electricity demand and energy recovery from wastewater (biogas production), while the full-scale long-term routine measurements were used for model validation.

The long-term routine operational data (Section 2.5.2) before and after plant retrofitting were used to calibrate (Set 1) and validate (Set 2), respectively, the heat demand sub-models of the anaerobic digesters (process) and buildings (non-process). To ensure reliable performance of the energy conversion and supply system, the proposed empirical models of the CHP plant (Eq. S11-S12 in SI) were calibrated and validated using the data from the two sets.

The coefficient of determination (R^2) was adopted as a measure of consistency between the model predictions and measurements; values > 0.81 were assumed to be very highly correlated, values > 0.49 were highly correlated and values > 0.25 were moderately correlated. Moreover, the measured data were compared with the dynamic predictions (average values) and steady-state predictions by means of the relative difference.

2.7. Analysis of strategies for sustainable wastewater treatment

Sustainability is defined as a multi-dimensional concept aimed at balancing economic, environmental and societal objectives which are quantified by means of different indicators. The indicators should be able to show progress towards or away from sustainability [12]. In WWTPs, sustainability can be measured in terms of the key performance indicators (KPIs), including effluent quality, operational costs, and GHG emissions. The key factors affecting the KPIs are related to operational strategies and applied technologies (Table S2 in SI). Specifically, the energy balance is significantly affected by the

DO concentration in the bioreactor (energy for aeration), circulation flow rates (energy for pumping), and biogas production (energy recovery). However, modifications focused on reduction of the energy demand and improvement of energy recovery can have a negative effect on the effluent quality and GHG emissions [11, 18].

Assumptions for the strategies. Following the findings of the previous studies, four strategies were selected for analysis, including different operational modes and technological upgrades. Both the DO set-point in the aerated compartments and MLR ratio were recognized as significant operational parameters affecting energy consumption and GHG emissions at WWTPs. The two possible technological upgrades comprised CEPT and deammonification for nitrogen removal in the sidestream treatment line. The first upgrade (CEPT) benefits from the increased energy recovery in the anaerobic digester and decreased oxygen demand for carbon oxidation in the bioreactor. The deammonification process requires no organic carbon source and less than half of the aeration energy required in conventional nitrification-denitrification [5]. In the present study, the assumed TSS removal efficiency from the primary clarifier ranged from 20 to 80%. To set changes in the total nitrogen (TN) removal efficiency from the sludge digestion liquor (0-90%), a "black-box" model was used.

A series of steady-state simulations in each scenario was carried out automatically using the special "Analyze" utility in GPS-X. The applicability of steady-state predictions for the model-based analysis of different scenarios was evaluated based on a comparison with average values from dynamic simulations (Table S13 in SI). In the previous study [10], this approach was found to be reliable, useful and time-effective for the multi-criteria analysis of combined strategies.

Three reference states representing the actual operational conditions and process performance were considered separately in each scenario: (i) average summer (RS), (ii) average winter (RW), and (iii) extreme winter (RWE) (the characteristics are shown in Tables S14-S17 in SI). During those periods, the average ambient air temperatures were 17.2°C, 1.9°C and -16.0°C, respectively. The average wastewater temperatures were 20.4°C, 11.6°C and 10.0°C, respectively.

Evaluation of the strategies. The model predictions were evaluated with respect to the following sustainability criteria: (i) effluent quality, (ii) degree of energy neutrality (for electricity and heat), and (iii) GHG footprint of the WWTP (Fig. 4). To achieve energy neutrality, the overall energy demand must be met by the energy recovered as biogas from wastewater. The proportion of energy recovered via biogas-driven devices, i.e., the CHP plant and boiler, in the overall WWTP energy demand was defined as the degree of energy neutrality for electricity (EN_E) and heat (EN_H), respectively. The following sources were considered to cover the energy deficit: (i) an external power grid for electricity and NG-driven boiler for heat or (ii) a NG-driven CHP system for electricity and heat supported by a NG-driven boiler.

Three objectives were formulated: (i) to improve effluent quality by decreasing the effluent TN concentration, (ii) to improve the electricity/heat balance by increasing $EN_E/_H$, and (iii) to reduce the GHG footprint in comparison with the reference states (RS, RW, and RWE; see Table S18 in SI). The goal was to achieve at least one of the objectives while not deteriorating the other two indicators. The results that meet this condition shift the WWTP closer to sustainability. The proposed performance assessment could be recommended for practical applications in full-scale WWTPs as it offers flexibility in balancing the different sustainability indicators without assumption of any arbitrary weighting factors. Bearing in mind that regulations require a maximum annual average effluent TN of 10 mg N/L, an option of discharging higher amounts of TN is winter and lower amounts in summer could possibly be considered. However, the aim of this study was to explore whether sustainable wastewater treatment could be achieved under unfavourable temperature conditions without a loss in actual effluent quality.

3. Results and Discussion

3.1. Preliminary analysis of the overall energy balance of the WWTP

The electricity balances in the years before and after retrofitting were significantly different (Table S12 in SI). The 22% increase in the observed energy intensity (0.50 kWh/m^3 vs. 0.61 kWh/m^3) could be attributed to the newly implemented electricity-driven devices. However, EN_E also increased from 0.41 to 0.60. The WWTP was upgraded by adding a new digester, which increased the total active digester capacity by over 40%. That upgrade resulted in a higher hydraulic retention time (33 d vs. 22 d), enhanced destruction of dry organic solids (55% vs. 38%) and increased biogas production (by 47%) in comparison with those in the preceding year.

The total annual heat demand was comparable in both years (Table S12 in SI). Due to the poor biogas production before retrofitting, the EN_H of the WWTP was only 0.8. On the other hand, after retrofitting, the surplus heat recovered from biogas (19%) was dissipated in ambient air, and over 40% of the total heat generated on-site (from both biogas and NG) was lost due to the excess supply in the summer.

The detailed inventory and measurements showed dynamic variations in the energy balance components and helped identify the most significant consumers (Fig. S2 and Fig. S3 in SI). The daily balances of the bioreactor and whole WWTP were strongly affected by the electricity consumption for aeration, with contributions of 59-78% and 26-51%, respectively (Fig. S2 in SI). The pumps were the second largest energy-consuming devices in the WWTP (~22%), followed by the centrifuges (~6%). The contribution of the blowers to the total annual electricity demand decreased from 84% (before retrofitting) to 55% (after retrofitting). The former value is out of the typically reported range of 42-77% [5]. In the heat balance of the WWTP, the contribution of the AD process to the total daily heat demand varied in the range of 49-98%, depending on the weather conditions. The non-process heat consumption in buildings contributed approximately 25% to the total annual heat balance.

3.2. Calibration and validation of the integrated WWTP model

3.2.1. Biokinetic sub-models in the plant-wide model

When modelling only the biological step [10], the ASM2d-N_2O model predictions for nitrogen and phosphorus compounds, i.e., ammonium (NH_4^+-N), nitrates (NO_3^--N), nitrites (NO_2^--N), N_2O-N, and orthophosphates (PO_4^{3-}-P), were consistent with the measurements from laboratory-scale experiments (R^2 = 0.88-0.98) and full-scale data (R^2 = 0.41-0.83). After the implementation of ASM2d-N_2O in the plant-wide model and adjustment of the sidestream flowrates and solid-liquid separation efficiency, the model predicted the behaviour of nitrogen and phosphorous compounds with a satisfactory accuracy (Fig. 5a-c). The measured data and model predictions were very highly correlated (R^2 = 0.78-0.93) for nitrogen and moderately correlated (R^2 = 0.36-0.52) for phosphorus. The N_2O emission rates from the first aerobic compartment, where the highest emissions had been detected in the preceding longitudinal profile, followed the trend of the measured data (Fig. 5d). For N_2O, the relative difference between the average values of the model predictions and measured data was only 7.2% in the studied period (Table

S13 in SI). For comparison, in the studies of Arnell et al. [19] and Blomberg et al. [31], the models could not fully capture the dynamics and the level of the measured N_2O emissions, respectively.

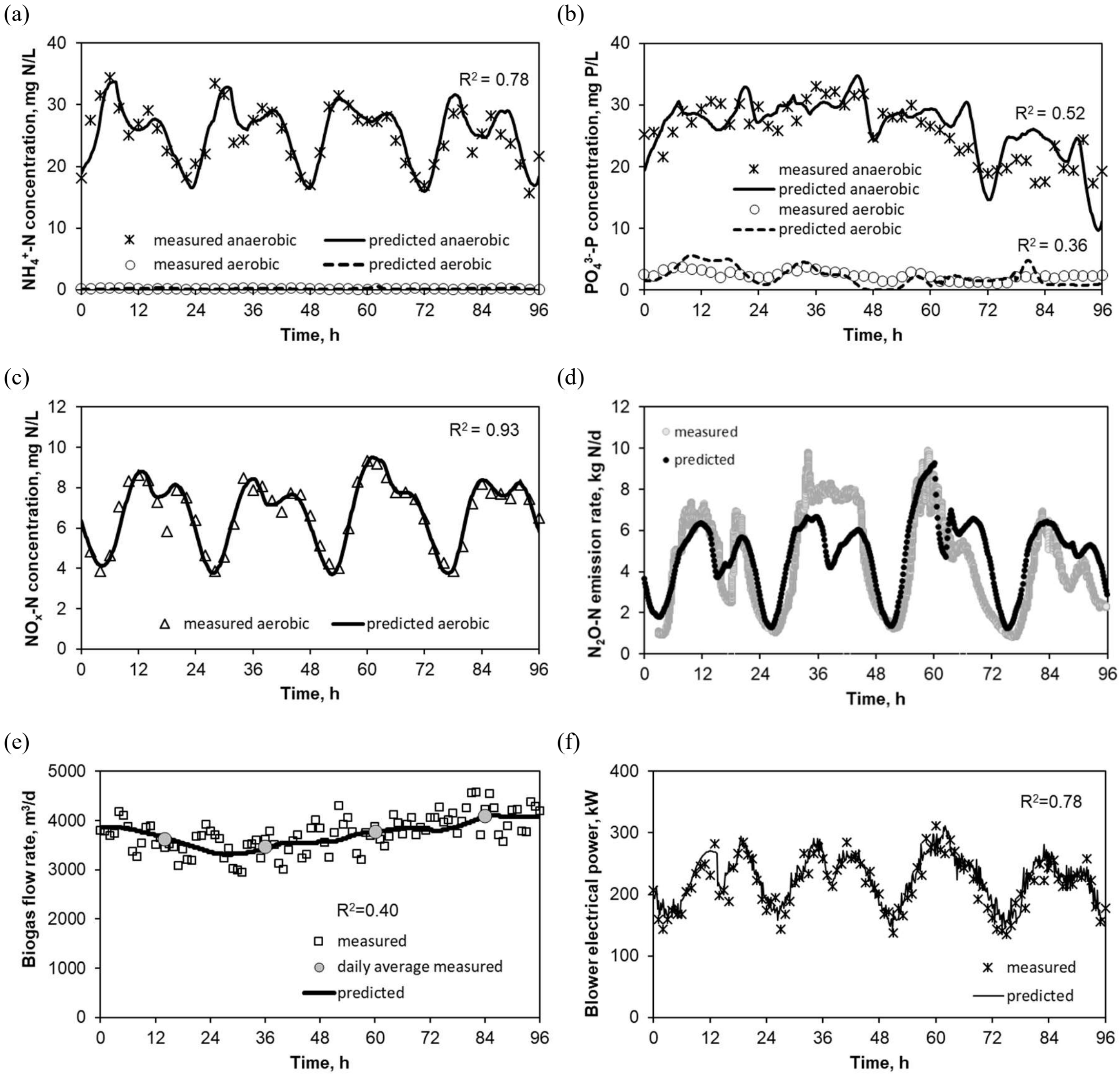

Figure 5. Model predictions vs. measured data in the bioreactor during the 4-day measurement campaign: NH_4^+-N concentration in the anaerobic and aerobic zone effluents (a), PO_4^{3-}-P concentration in the anaerobic and aerobic zone effluents (b), NO_x-N (NO_3^--N + NO_2^--N) concentration in the aerobic zone effluent (c), N_2O-N emission rate from the aerobic compartment (d), biogas flowrate (e), and blower electrical power (f).

For the Mantis AD model, the full-scale model predictions were consistent with the measured data for the AD substrates and product characteristics during the model calibration. For the biogas yield, the relative difference between the measured daily average and the model prediction did not exceed 3.7%

[26]. After incorporating Mantis AD into the plant-wide model in this study, the predicted biogas volumetric flowrates followed the trend of the measured data (Fig. 5e), while the methane content in the biogas volume was stable (61±0.7%). The long-term observations showed a very strong correlation between the daily biogas production and consumption for useful energy recovery (R^2 = 0.85). These values were slightly shifted in time due to the buffering capacity of the gas storage tank.

3.2.2. Process and non-process energy sub-models in the extended plant-wide model

Process electricity demand. The oxygen transfer model, which is a core component of the aeration system model, was calibrated simultaneously with ASM2d-N_2O to maintain the DO set-point in the aerobic zone. This study extended the plant-wide model considerations by incorporating the energy consumption for aeration. The predicted electrical power for the blowers supplying air to the aerobic compartments of the bioreactor was consistent with the measured data (R^2 = 0.78, Fig. 5f).

Process heat demand. The model predictions and the data representing the daily heat demand for the AD process were highly correlated (Fig. 6a for Set 1 and Fig. S3a for Set 2). The heat demand was primarily affected by the amount of sludge feedstock and the temperature difference between the raw and digested sludge. The heat transfer through the walls of the digester accounted for 7 to 18% of the total heat demand. The observed difference between the predictions and measured data can be attributed to the thermal inertia of the digester and the influence of solar irradiation and convection due to wind.

Non-process heat demand. The proposed simplified model accurately predicted the heat demand in the associated buildings (R^2 = 0.50). Differences between the model inputs and actual internal temperatures could result in either overestimation or underestimation of the actual heat demand. Moreover, it was a practice in the WWTP to partially dissipate the surplus heat from the CHP system via space heating systems to limit engine cooling. Regarding the overall energy balance, the measured data representing the total heat demand at the studied WWTP were consistent (R^2 = 0.70-0.84) with the model predictions, as shown in Fig. 6b and Fig. S3b.

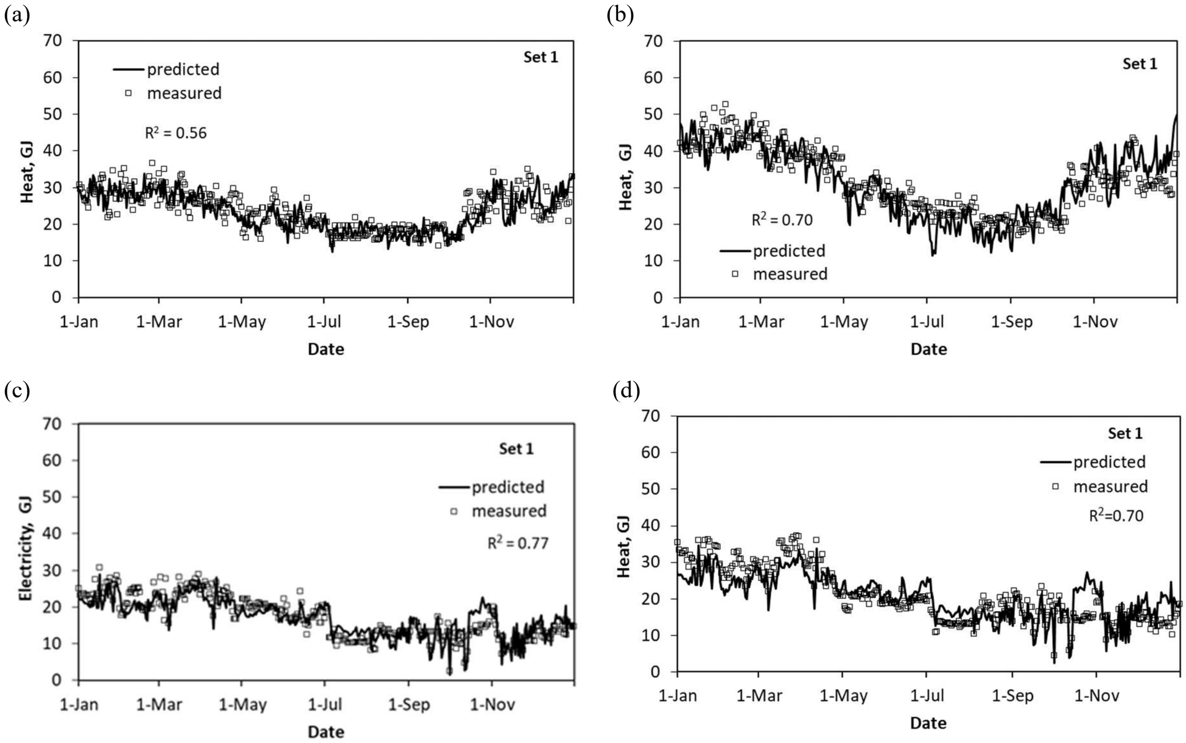

Figure 6. Long-term model predictions vs. measured data before retrofitting of the studied WWTP (Set 1) representing the daily heat demand for AD (a), overall daily heat demand (b), electricity generation via the biogas-driven CHP system (c), and heat recovery via the biogas-driven CHP system (d).

Energy conversion and supply system. Before retrofitting, due to poor biogas production, the CHP system was underloaded (17-39%) and showed a lower operational performance than expected. The annual average efficiency of electricity generation from combusted biogas was 0.27±0.05. Similar to the electrical efficiency, the effective thermal efficiency (excluding the heat dissipated via the fan coolers) was not constant (0.33±0.07). A strong correlation (R^2 = 0.81) was found between the actual electrical output and heat recovery of the CHP system. The model predictions were consistent with the measured data during both periods of operation (Set 1 and Set 2) (Fig. 6c-d and S4c-d). For comparison, the average efficiency of the CHP system after retrofitting was estimated to be 0.31±0.03 and 0.38±0.02 for electricity and heat, respectively. The opposite annual trends in energy recovery in Sets 1 and 2 were affected by the trends in biogas production during those periods.

3.3. Improving the sustainability of wastewater treatment through operational strategies and technological upgrades

3.3.1. Operational strategies

The simulation results for different DO set-points and MLR ratios are shown in Fig. 7 with respect to the effluent TN, EN_E and relative GHG footprint reduction under the average summer, average winter and extreme winter operational conditions. The recommended operational areas are limited by lines representing the results of simulations equal to those of RS, RW and RWE, respectively (see Table S18 in SI).

Effluent quality. Both decision variables (DO and MLR) affected the effluent TN. The results showed the potential for decreasing the DO set-point in the aerobic zone of the bioreactor from 2.5 mg O_2/L (as in RS/RW) down to 1.0 mg O_2/L in the summer period (Fig. 7a) and 1.5 mg O_2/L in the winter period (Fig. 7b, c). Lowering the DO set-point primarily affected the effluent NH_4+-N concentration, while increasing MLR resulted in a reduction in the effluent NO_3^-N concentration. A strategy focused solely on reducing the aeration intensity could be effective in WWTPs with respect to NH_4+-N ammonia discharge limits [32]. In view of sustainability goals, both operational parameters should be considered due to their interrelations with the energy balance and direct GHG footprint.

Electricity balance. The overall electricity demand was primarily affected by the blowers (accounting for 35-50% within the entire analysed area). Therefore, by decreasing the DO set-point, a relatively high EN_E could be achieved (up to 0.62-0.72, depending on the temperature conditions) without compromising the actual effluent quality. These results confirm the findings of previous studies that technological upgrades would be needed in conventional AS systems to reach $EN_E = 1$ [5, 33]. Increasing the MLR pumping energy to improve effluent quality could easily be compensated for by reducing the energy for aeration [32]. In the present study, the maximum potential improvement in the overall electrical energy balance was estimated to be 12% relative to actual conditions, which suggests that the WWTP was operated close to the optimum energy performance and that changes could be implemented to improve other sustainability indicators.

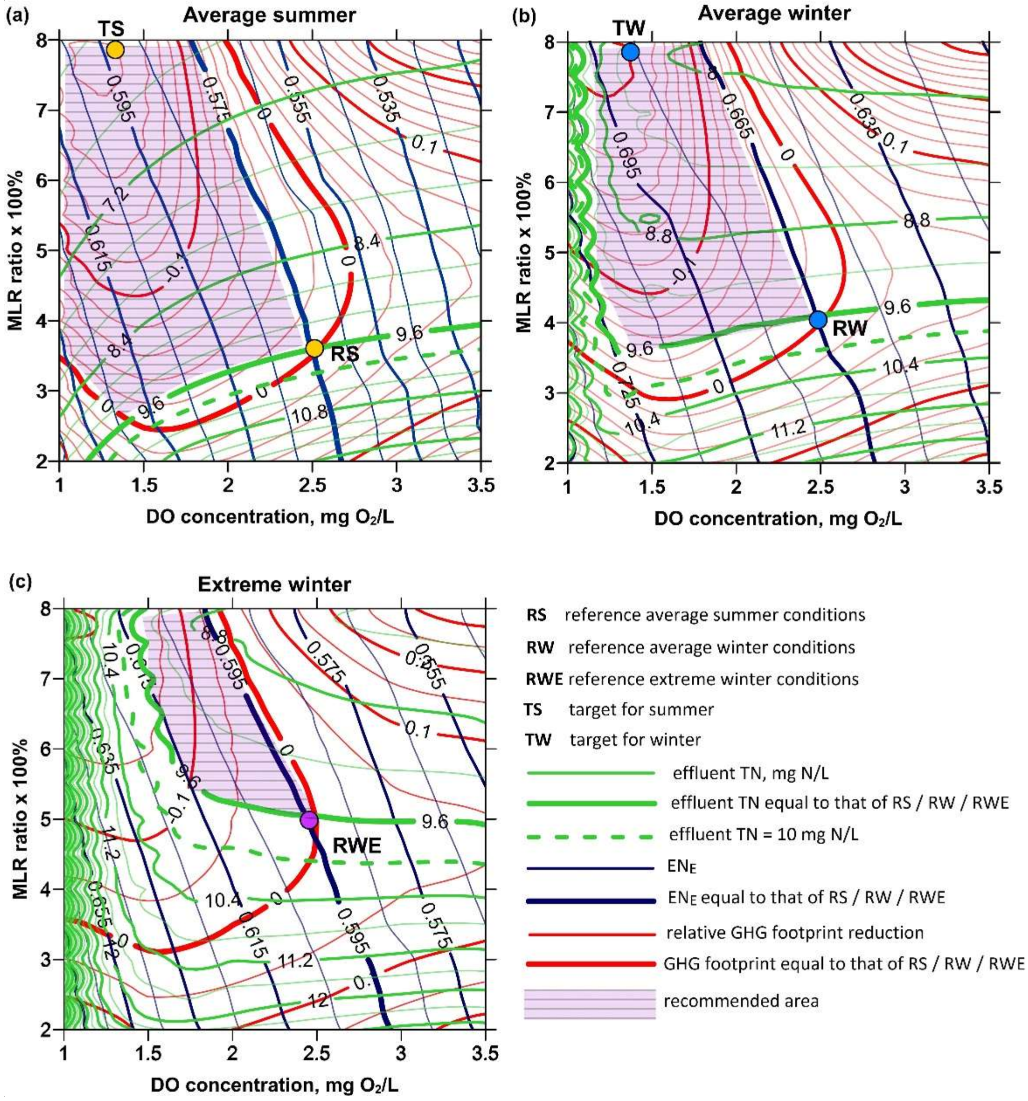

Figure 7. Effluent TN, EN_E and relative overall GHG footprint reduction under different DO set-points and MLR ratios under average summer conditions (a), average winter conditions (b), and extreme winter conditions (c).

Heat balance. The WWTP heat demand and biogas production were not affected by variations in the DO set-point and MLR. The associated facilities (buildings) contributed substantially to the overall heat demand, i.e., ~30% and ~45% under average and extreme winter conditions, respectively. It is worth noting that the overall heat balance was positive in the summer period, and the recovered heat exceeded the demand by 70%. However, under average and extreme winter conditions, the EN_H was estimated to be 0.97 and 0.63, respectively. Thus, covering both electricity and heat deficits needed to be considered in the studied WWTP with respect to the indirect GHG footprint.

GHG footprint. Under varying DO set-points and MLR ratios, the area within which the total GHG footprint improved in comparison with the reference state was larger than those obtained under the other two constraints. Specifically, under extreme winter conditions, the effluent TN strongly limited the operational range. Thus, the recommended areas in Fig. 7a-c were primarily limited by the reference effluent TN and EN_E. The results demonstrated that sustainable operation is possible even under unfavourable temperature conditions.

The overall GHG footprint was affected by both direct and indirect GHG emissions. Within all of the analysed ranges of DO set-points and MLR ratios, the contribution of process emissions to the overall GHG footprint was estimated to range from 26-70%, depending on the assumed energy sources. In the optimum scenario with respect to the overall GHG emissions (shown in Fig. 7), the electricity and heat deficits from biogas were covered by the NG-driven CHP system. A higher GHG footprint (by up to 20%) was achieved in the scenario assuming that electricity was imported from the power grid and heat was obtained from the NG boiler. When increasing the share of renewables or NG relative to that of coal, the focus shifts from indirect to direct emissions. When applying the sustainability concept (the recommended areas in Fig. 7), the share of direct N_2O emissions was > 45% in summer and > 58% in winter. Similar to previous studies [10, 19, 34], these emissions were dominated by N_2O released from the aerobic compartments of the bioreactor due to the stripping effect. However, the reduction in GHG emissions related to decreased aeration energy could be counterbalanced by increased process N_2O emissions. This was shown in the studies of Flores-Alsina et al. [11], Massara et al. [35], Puchongkawarin et al. [36]. A similar effect was observed in this study, but at DO < 1.5 mg O_2/L, i.e., beyond the recommended area. The influence of an increased MLR ratio on N_2O emissions and the overall GHG footprint switched the trend from descending to ascending upon changes in the nitrogen compound concentrations. Following the findings of Mannina et al. [37], Puchongkawarin et al. [36] and Zaborowska et al. [10], these results can be affected by local conditions, such as the influent characteristics, mixing intensity, DO concentration, and process configuration.

At the target points (TS and TW in Fig. 7a-b), the overall GHG footprint could be reduced by up to 20% while reducing the effluent nitrogen load by 15-30%. The simultaneous improvement in electricity balance would not be significant (1-2%).

3.3.2. Technological upgrades

The simulation results for different TSS removal efficiencies in the primary clarifier and TN removal efficiencies from the sludge digester liquor are shown in Fig. 8 with respect to the WWTP effluent TN, EN_E, EN_H and relative GHG footprint reduction under the three specific operational conditions (average summer, average winter and extreme winter). The recommended operational areas are limited by lines representing the results of simulations equal to those of RS, RW and RWE, respectively (see Table S18 in SI).

Effluent quality. The effluent TN was very sensitive to both manipulated variables (Fig. 8). Upon increasing the quantity of TSS removed in the primary clarifier, the effluent TN tended to rise due to the reduction in the amount of carbon available for denitrification. Moreover, additional AD feedstock increased the NH_4^+-N loads returned to the main line in the sludge digester liquor (by 4-20% in comparison to the influent load). Thus, increasing the efficiency of TN removal in the sidestream treatment line resulted in a descending trend in the effluent TN. This effect was achieved without dosing external carbon for denitrification in the bioreactor.

Electricity balance. EN_E was predominantly affected by primary sludge removal (almost horizontal lines in Fig. 8a-c) due to its contribution to enhanced biogas production. A 60% increase in biogas recovery accompanied the changes in the TSS removal efficiency from the reference values of 30/40% (RW/RS) to 80%. This result was supported by the energy savings associated with oxidation of the carbon loads entering the bioreactor. In the study of [32], a change in the solid capture efficiency from 30% to 55% improved the electricity balance by 15%. In the present study, better energy performance was achieved by applying an energy-efficient sidestream deammonification process. The potential electricity savings due to the implementation of the combined upgrades were estimated to reach 38% in comparison with the reference state without compromising the effluent quality. To reach $EN_E = 1$, removal efficiencies of at least 55-65% and at least 80% for TSS in the primary clarifier and TN in the sludge digester liquor, respectively, would be necessary (Fig. 8a-b). The slightly better energy performance in winter can be explained by the specific wastewater composition. The influent chemical oxygen demand (COD) load was 16% higher in winter than in summer; in the same time periods, the soluble COD to TKN ratio increased from 3.4 to 3.9. In effect, the organic load in the digester influent could be 20% higher, which would contribute to higher biogas production. Indeed, the EN_E is closely related to the influent COD concentration and COD/N ratio [33]. Maximizing energy recovery from wastewater is primarily recommended provided that the carbon flows to the bioreactor (for denitrification) and to the anaerobic digester (for biogas recovery) are balanced. To improve the energy performance of the WWTP, co-digestion of sewage sludges with food wastes or harvesting other renewable energy sources could be proposed as the next step (as recommended by Macintosh et al. [38], Maktabifard et al. [13] and Solon et al. [15]).

Heat balance. The strong effect of the considered upgrades on the overall heat balance is demonstrated in Fig. 8d-f. It was found that achieving EN_H =1 was almost impossible under extreme winter conditions (Fig. 8f). However, RW is located close to EN_H =1 (Fig. 8e). In contrast, the excess heat in summer might be more than twice the heat demand (Fig. 8d). The associated facilities contributed 24-34% and 36-48% to the overall heat demand under average and extreme winter conditions, respectively. This result confirms the importance of performing thorough heat balance considerations with respect to both covering the heat deficit and estimating the potential for utilizing excess heat. These decisions would affect the assessment of the overall WWTP performance. In the studied case, exporting heat outside the facility was found to be reasonable due to the location of an aqua park in the neighbourhood.

GHG footprint. The optimum considered scenario with respect to the GHG footprint included energy recovery from biogas supplemented by the NG-driven CHP system and, to a lesser degree, by the NG boiler. The overall GHG footprint reduction (up to 39%, Fig. 8h) was accompanied by an increase in the TSS removal efficiency by approximately 65% above the reference value (Fig. 8g-i). Subsequently, the opposite trend was observed, which could be attributed to the increasing N_2O emissions from the bioreactor. The contribution of process-related N_2O emissions to the total GHG footprint was ≥ 55% and ≥ 65% in summer and winter, respectively. Lower temperatures could increase process N_2O emissions due to reduced biochemical activities hindering complete nitrification and denitrification. On the other hand, lower N_2O emissions have been reported under such conditions by Daelman et al. [39] and Guo and Vanrolleghem [40], which may reflect different site-specific operational strategies in summer and winter.

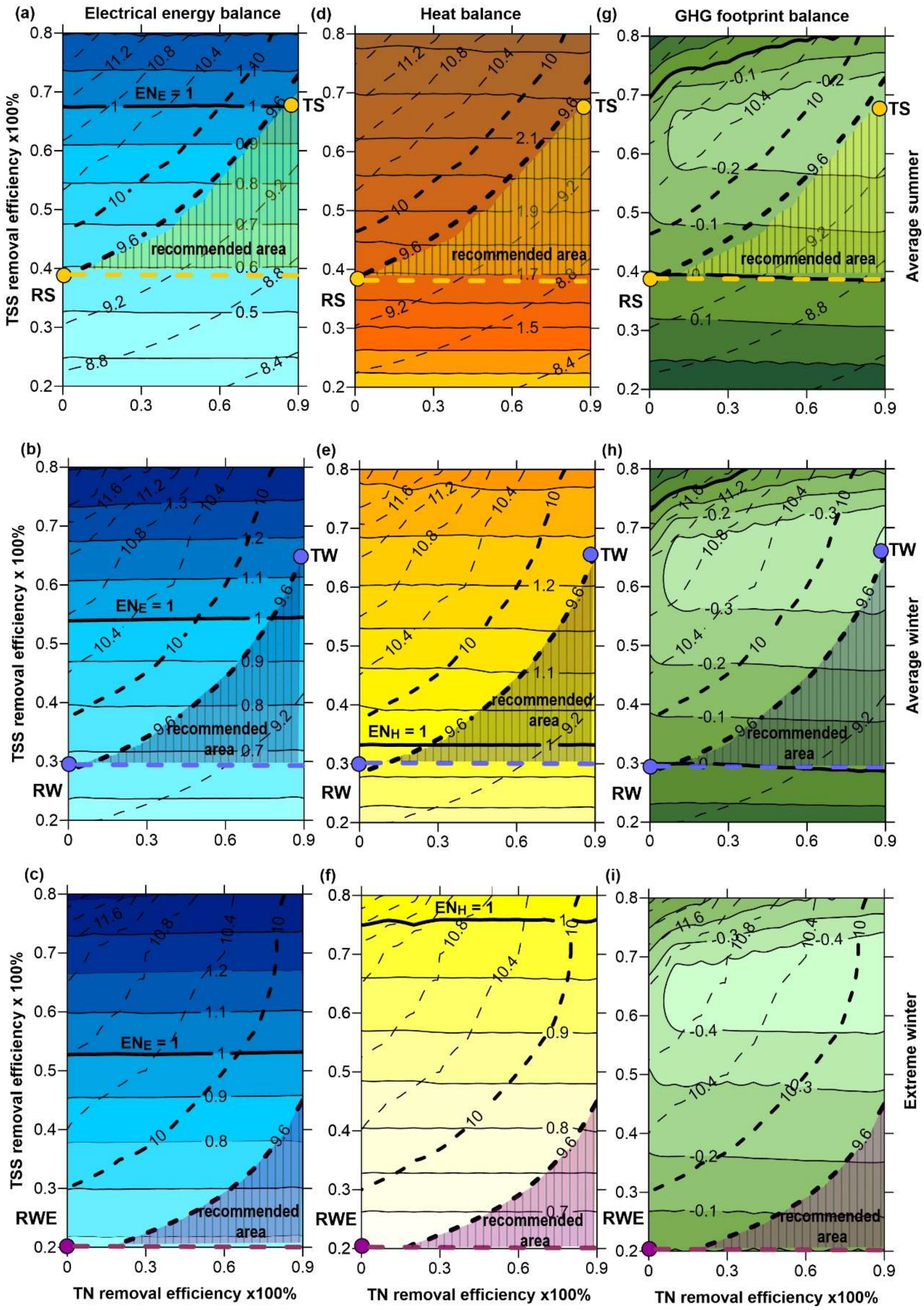

Figure 8. WWTP effluent TN in mg N/L (dashed lines), EN_E (a-c), EN_H (d-f) and relative overall GHG footprint reduction (g-i) under different TSS removal efficiencies in the primary clarifier and TN removal efficiencies from digester liquor under average summer (top), average winter (middle) and extreme winter conditions (bottom).

The GHG footprint credit gained from the increased energy recovery from biogas was consumed by the elevated process-related emissions. In contrast to the present study, Flores-Alsina et al. [11] did not show a substantial change in the predicted total quantity of GHGs emitted from a WWTP under TSS removal efficiencies ranging from 33% to 66%. That prediction was strongly influenced by increased N_2O emissions from the bioreactor due to inadequate COD/N ratios and off-site GHG emissions from the production of a supplemental carbon source for denitrification. The difference between the results of [11] and the present study demonstrates the positive influence of combining CEPT with sidestream deammonification and applying less carbon-intensive heat and power sources.

At the target points (TS and TW in Fig. 8a-b, d-e, g-h), the WWTP could be energy neutral or positive while reducing the overall GHG footprint by over 30%. However, the improvement in effluent quality achieved at the same time would be insignificant.

3.4. Advantages and limitations of the developed model

The proposed extensions of the plant-wide model increased the reliability of model predictions and its usability for practical applications in real WWTPs. The results confirmed the importance of introducing the new model elements in the overall energy balance. At both the design and operational stages, accompanying facilities need to be considered to select and properly manage energy sources. In a broader context, the approach presented in this study assesses the sustainability of the management of WWTPs. The accuracy of this assessment was improved by implementing the empirical model of the CHP plant, which prevented an overestimation of energy recovery compared to the commonly used fixed energy efficiency. In the analysed WWTP, the annual overestimation would be 7-24% for electricity and 24-38% for heat.

Both the wastewater treatment processes and energy conversion were found to contribute significantly to the overall GHG footprint of the WWTP. The improved energy balance allowed for a better estimate of energy-related GHG emissions. However, predicting N_2O emissions has been challenging since the mechanisms of N_2O production are complex and still under debate [8, 9]. Three known N_2O production pathways were used in this study together with the stripping effect. The observed inaccuracy of model predictions can be attributed to other mechanisms not included in the production model, imperfections of the emission model and measurement inaccuracies. Accordingly, the N_2O model can be further improved as research advances. However, the mechanistic N_2O model already demonstrates higher accuracy under dynamic conditions than generic emission factors.

The temporary fluctuations in biogas production were predicted by the model with moderate accuracy. In terms of the 1-hour results, the actual variations could reflect the potential effects of imperfect mixing, gas stripping and intermittent substrates feed to the digester. However, the short-term fluctuations in biogas production had a minor effect on the daily energy balance of the system equipped with the gas storage tank. The maximum relative difference between the predicted and measured daily volume of biogas was only 0.8%.

In practical applications, the limitations can be found in the complexity of the integrated plant-wide model and extensive full-scale campaigns in WWTPs. In each specific case, the model calibration and validation procedure requires additional effort due to extended electricity and heat measurements. This study demonstrated the benefits of the proposed approach to support energy management in WWTPs while considering the effluent quality, operational cost and sustainability.

4. Conclusions

In this study, an integrated plant-wide model extended with new energy balance elements was investigated and evaluated with respect to the effluent quality, energy performance and GHG footprint. It was shown that to perform a comprehensive sustainability assessment of WWTPs, both process and non-process activities need to be considered. The results confirmed that the heat demand for associated facilities could not be neglected in the overall heat balance. The detailed models of energy demand and supply improved the assessment of energy performance in the full-scale WWTP by enabling a realistic estimation of energy neutrality.

The examined operational strategies showed that the WWTP could simultaneously improve two of the three sustainability criteria considered. Application of these operational strategies could potentially decrease the GHG footprint and effluent total nitrogen concentration by 20% and 30%, respectively, in comparison with the current conditions. However, only a slight potential for improving the overall energy balance was found. In contrast, technological upgrades enabled energy neutrality and the highest reduction in the GHG footprint (by over 30%) to be reached, but the effluent quality did not improve compared to the current conditions.

The proposed model and methodology may support and encourage engineers, operators and managers to implement sustainable operational or technological solutions in WWTPs that simultaneously meet high effluent standards, reasonable energy performance of the entire facility and reduced GHG emissions.

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Declaration of interest: none.

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