Holistic assessment of management strategies and technological solutions handling anaerobic digester supernatants in wastewater treatment plants

Flores-Alsina, Xavier; Vangsgaard, Anna Katrine; Uri-Carreño, Nerea; Nielsen, Per H.; Gernaey, Krist V.

Published in:
Chemical Engineering Journal

Link to article, DOI:
10.1016/j.cej.2025.160934

Publication date:
2025

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Flores-Alsina, X., Vangsgaard, A. K., Uri-Carreño, N., Nielsen, P. H., & Gernaey, K. V. (2025). Holistic assessment of management strategies and technological solutions handling anaerobic digester supernatants in wastewater treatment plants. *Chemical Engineering Journal*, *508*, Article 160934. https://doi.org/10.1016/j.cej.2025.160934

Chemical Engineering Journal 508 (2025) 160934

Contents lists available at ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Holistic assessment of management strategies and technological solutions handling anaerobic digester supernatants in wastewater treatment plants

Xavier Flores-Alsina [a,*], Anna Katrine Vangsgaard [b], Nerea Uri-Carreño [c], Per H. Nielsen [c], Krist V. Gernaey [a]

[a] Process and Systems Engineering Center (PROSYS), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads Building 228A, Kgs. Lyngby 2800, Denmark

[b] Envidan A/S, Fuglebækvej 1A, Kastrup 2770, Denmark

[c] Vandcenter Syd A/S, Vandværksvej 7, Odense 5000, Denmark

ARTICLE INFO

Keywords:
Anaerobic digester supernatants
Benchmarking
GHG emissions
Net zero
Plant-wide modelling
Reject water
Simulation

ABSTRACT

Effective handling and treatment of anaerobic digestion supernatants (AnDS) in wastewater treatment plants (WWTP) is essential for maintaining effluent quality, minimizing operational costs, and reducing environmental impacts. This study aims to provide a holistic framework to assess management strategies and technological solutions for handling AnDS within the broader context of wastewater operations. The International Water Association (IWA) Benchmark Simulation Model No 2 (BSM2) is used as a testing platform. A new set of models are developed (and adapted) to predict the behavior of storage tanks (ST) with variable volume, aerobic granular sludge reactors (AerGSR) and struvite precipitation units (SPU). Innovative control strategies are implemented and tested under dynamic conditions. Effluent quality (EQi), operational cost (OCi) and greenhouse gas emissions (GHGi) indices are the selected key performance indicators (KPI). Results show that daytime storage of AnDS has a limited impact on plant performance (< 5 % variation in most KPI). The addition of PN/ANX improves nitrogen (N) and phosphorus (P) removal by 20 % but substantially increases total GHGi emissions due to high N_2O production (Emission factors (EF) range between 0.24 % to 3.9 %). The study also reveals that aeration patterns play a crucial role in those emissions and smart dissolved oxygen (DO) control strategies will determine the sustainability of N removal intensification processes. SPU obtained the best P effluent values. Exploration by simulation shows how to balance EQi, OCi and GHGi simultaneously by means of changing the crystallizer dosage (Mg, Na) strategy. Indeed, P recovery can reach up to 30 %. The study reveals synergies and trade-offs between intensified biological nutrient removal and emission minimization, limitations of model-based evaluations and how virtual tools can help narrow down the number of design and operational options at an early stage.

1. Introduction

The management of anaerobic digester supernatants (AnDS), often referred to as reject water (RW), is a critical aspect of modern wastewater treatment plants (WWTPs) [66]. These supernatants often contain elevated levels of ammonia (NH_x), nitrogen (N), and phosphorus (P), which can significantly increase the load on WWTPs and complicate nutrient removal processes [20]. Handling supernatants with high N and P loads also requires additional treatment steps or more intensive operational strategies, leading to increased energy and chemical consumption and, consequently, higher operational costs [50]. Finally, treatment of supernatants, especially through intensified processes with high conversion rates, can lead to the emission of greenhouse gases (GHG) like nitrous oxide (N_2O), contributing to the environmental footprint of the wastewater treatment plant [65,72]. Effective handling and treatment of these streams are essential for maintaining effluent quality, minimizing operational costs, and reducing environmental impacts such as GHG emissions.

In recent years, there has been a growing interest in optimizing the treatment of anaerobic digester supernatants due to their substantial impact on WWTP performance [54]. Various management strategies [38] and technological solutions [35,60,42] have been proposed and implemented ranging from advanced nutrient removal processes [68,36,37] to innovative operational strategies [73,53,70]. However, most existing studies tend to focus on isolated components or specific

* Corresponding author.

https://doi.org/10.1016/j.cej.2025.160934
Received 9 September 2024; Received in revised form 21 February 2025; Accepted 22 February 2025
Available online 25 February 2025

Nomenclature

A	Management and/or technological solution
AD	Anaerobic digester
ADM	Anaerobic digestion model
AE	Aeration energy
AER	Aerobic section in ASR
AerGSR	Aerobic granular sludge reactor
AGSR	Anaerobic granular sludge reactor
A_i	Alternative to be evaluated (Baseline,….)
ANAER	Anaerobic section in ASR
ANOX	Anoxic section in ASR
AmDS	Anaerobic digester supernatants
AOB	Ammonium oxidizing bacteria
ASM	Activated sludge model
AS	Activated sludge reactor
$BIO_{disposal}$	Biosolids to disposal
BSM	Benchmark Simulation Model
Ca	Calcium
CH_4	Methane
$CHEM_I$	Chemicals consumption / production (Na, Mg, struvite)
CO_2	Carbon dioxide
DN	Denitrification pathway
DEW	Dewatering unit
DO	Dissolved oxygen
$E_{consumption}$	Energy consumption
EF	Emission factor
Ei	Energy production / consumption
EQi	Effluent quality index
GHG/ GHGi	Greenhouse gas emission index
H_2	Hydrogen
H_2S	Hydrogen sulfide
HE	Heating energy
IWA	International Water Association
KPI	Key performance indicator
L	Biofilm radial direction
ME	Mixing energy
Mg	Magnesium
N	Nitrogen
N_2	Nitrogen gas
N_2O	Nitrous oxide
ND	Nitrifier denitrification pathway
NHx	Ammonium / ammonia
NH_2OH	Hydroxylamine
NN	Nitrifier nitrification pathway
NO_3^-	Nitrate
NO_2^-	Nitrite
NOB	Nitrate oxidizing bacteria
OCi	Operational cost index
OHO	Ordinary heterotrophic organisms
P	Phosphorus
PAO	Phosphorus accumulating organisms
PCF	Physico-chemical framework
PDE	Partial differential equations
PE	Pumping energy
PN/ANX	Partial nitritation/anammox
PRIM	Primary clarifier
$Q_{i,j}$	Flow-rate
RW	Reject water
SEC	Secondary clarifier
SPU	Struvite precipitation unit
ST	Storage tank
THK	Thickener
TIV	Time in violation
TKN	Total Kjeldahl nitrogen
TN	Total nitrogen
TP	Total phosphorus
V_i	Volume
WWTP	Wastewater treatment plant
Z	Biofilm thickness

aspects of the treatment process, often neglecting importance of the interconnected and multi-objective nature of WWTP operations as stressed by multiple researchers [59,28,52,59,23].

This study aims to provide a holistic assessment of management strategies and technological solutions for handling AnDS within the broader context of WWTP operations. Utilizing the IWA Benchmark Simulation Model No 2 (BSM2) [18,62,63], we evaluate the impact of different strategies on effluent quality, operational costs, and GHG emissions in a comprehensive, plant-wide context.

A significant gap in the existing literature is the limited focus on reject water management within an integrated plant-wide framework. This study addresses this weakness by being the first to assess reject water (management, treatment, recovery) in a holistic, plant-wide context, considering its interactions with the entire WWTP process. Rigorous biological and physico-chemical mathematical models describing transformations and fate of N and P compounds in a plant-wide system have been developed for this purpose. Special emphasis is placed on predicting the behavior of biofilm-based reactors (aerobic granules with partial nitration/ anammox) and P recovery technologies (struvite precipitation). These models allow us to consider the impact of both automatic control (P, PI, cascaded PI, feedforward) and different ways of operating these new units at plant-wide level. Additionally, this research is pioneering in evaluating the impact of various operational and technological solutions on multiple key performance indicators—effluent quality, cost, and GHG emissions—within a unified framework.

By integrating these aspects, we focus on the following research questions:

(i) *How can plant-wide models contribute to optimizing nutrient removal while minimizing GHG emissions and operational costs?*
(ii) *What trade-offs exist between intensified treatment processes, such as partial nitration/anammox (PN/ANX) and struvite precipitation, and their environmental impacts?*
(iii) *What role can advanced control strategies play in mitigating the environmental footprint of AnDS management?*

It also provides a more comprehensive understanding of the implications of reject water management strategies, offering valuable insights for optimizing WWTP operations. This holistic approach is crucial for developing sustainable and efficient wastewater treatment solutions that meet stringent environmental and economic requirements.

2. Materials & methods

2.1. Plant layout

2.1.1. BSM2 flow diagram

The plant layout consists of a primary clarifier (PRIM), an activated sludge reactor (AS), a secondary settler (SEC), a sludge thickener (THK), an anaerobic digester (AD) and a dewatering unit (DW) (see Fig. 1). PRIM has a total volume of 900 m^3. The AS is an A2/O configuration consisting of 7 tanks in series: Tanks 1 and 2 are anaerobic (ANAER1 and ANAER2) with a total volume of 2000 m^3; tanks 3 and 4 are anoxic

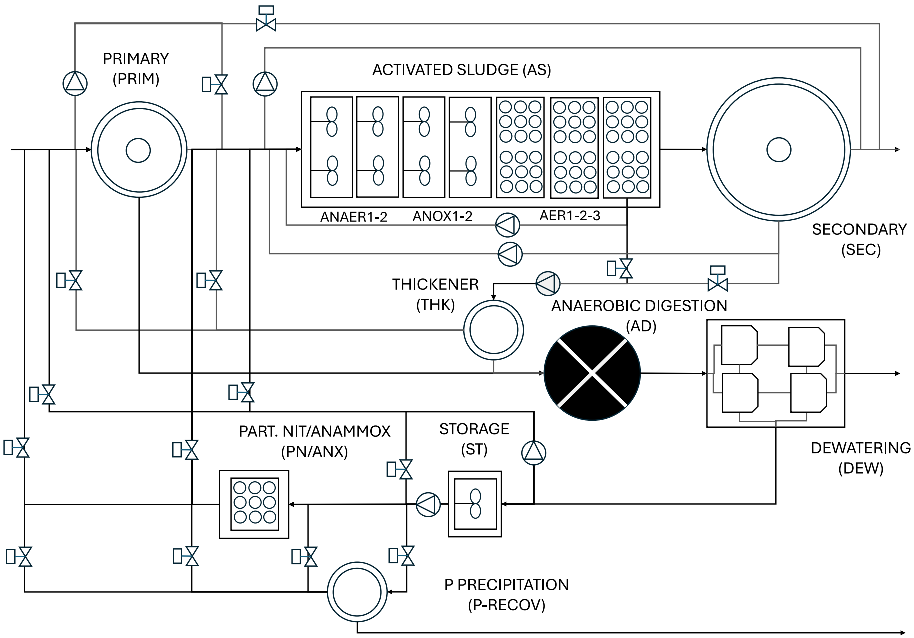

Fig. 1. Schematic representation of the BSM2 layout where management strategies and technological solutions are implemented.

(ANOX1 and ANOX2) with a total volume of 3000 m^3 while tanks 5, 6 and 7 are aerobic (AER1, AER2 and AER3) with a total volume of 9000 m^3. The SEC has a surface of 1500 m^2 and a height of 4 m. The AD has a working volume of 3400 m^3 and a headspace volume of 300 m^3. DW is operated continuously. Reject water (RW) is returned to headworks. Cake is sent to disposal. More information about the BSM2 platform can be found in [18,62,61].

2.1.2. New units: Storage tank (ST)

The ST functions as an ideally mixed tank with changing volume topping at 160 m^3. When input ($Q_{ST\text{-}IN}$) and output ($Q_{ST\text{-}OUT}$) flows are the same, the ST volume (V_{ST}) remains constant. Nevertheless, $Q_{ST\text{-}OUTt}$ can be used as control handle, which will cause the V_{ST} to change. When the V_{ST} is too high (> 90 % of maximum volume), a by-pass flow is activated ($Q_{ST\text{-}bypass}$) and the inlet flow ($Q_{ST\text{-}IN}$) is set to zero. When the volume is too low (< 10 %), $Q_{ST\text{-}OUT}$ is closed until the tank is filled again to a higher level. The purpose of the storage tank is to even out variations in the incoming N load caused by diurnal variations in the influent.

2.1.3. New units: Aerobic granular sludge reactor (AerGSR)

A new unit consisting of an anaerobic granular sludge reactor (AerGSR) is added after the storage tank (ST) to treat reject water (RW) ($V_{PN/ANX} = 200$ m^3). The reactor is designed to maintain the microbial community in a granular form, and it is operated to promote partial nitration (PN) / anammox (ANX). PN refers to the conversion of a fraction of the ammonia (NH_x) to nitrite (NO_2^-) through the activity of nitrifying bacteria. This process takes place in the outer layer of the granule, which is characterized by aerobic conditions, where oxygen is available. In the anoxic core of the granule, ANX bacteria thrive. These bacteria are responsible for the anaerobic oxidation of ammonia (NH_x) with nitrite (NO_2^-) to produce nitrogen gas (N_2).

2.1.4. New units: Struvite precipitation unit (SPU)

The P-recovery unit consists of a reactor ($V_{P\text{-}REC}$ = 100) where chemicals are added to: 1) adjust pH to a favorable range (around 7–9); and 2) promote the formation of precipitates. The pH is controlled through the addition of alkaline chemicals (in this case sodium hydroxide). The key component required for phosphorus precipitation is magnesium (added in the form of magnesium chloride). Over time, struvite crystals precipitate out of the solution. Once these crystals have formed, they are separated from the liquid phase. These crystals are stored for later use as a fertilizer or nutrient supplement.

2.2. Process models

2.2.1. Biological and physico-chemical models

Process kinetics and stoichiometries for both AS and AerGSR are based on the Activated Sludge Model No 2d (ASM2d) [22] with eh extensions proposed by [39,60,63] and [13]. The model predicts simultaneous biological C, N and P removal, as well as the chemical and biological processes related to S and Fe, anammox and N_2O production and emission. More specifically, the N_2O biological pathways are:

- NH_2OH oxidation pathway (NN pathway): N_2O is produced from the reduction of NO by the enzyme "Nor" of AOB coupled with the oxidation of NH_2OH to NO_2^- [48].
- AOB nitrifier denitrification pathway (ND pathway): N_2O is produced from NO_2^- reduction to NO and subsequently to N_2O by AOB. These two processes are lumped in one single reaction as in Pocquet et al. [48].
- Heterotrophic denitrification pathway (DEN pathway): N_2O is produced as an intermediate of the denitrification processes either by OHO or PAO [24].

The three biological N_2O production pathways were included in the (bio)chemical model to account for all the known biological N_2O production pathways and to fairly assess the contribution of each pathway under dynamic conditions and under the different control/operational strategies implemented. The ADM1 version, implemented in the plant-wide context provided by the Benchmark Simulation Model No. 2 (BSM2) [4,55] is extended with P, S and Fe interactions [16].

The reader is referred to the original source material [16,62,63] for specific details about model (ASM, ADM) stoichiometry, kinetics and continuity (mass balance) verification.

A common physico-chemical framework (PCF) is implemented to both ADM and ASM [3]. The model simulates the acid-base system and is thereby able to predict pH. It also corrects for ionic strength via the Davies approach to consider chemical activities instead of molar concentrations and hence performs all the calculations under non-ideal conditions. PCF does not account for particle interactions or colloidal properties of the liquid phase. Precipitation of Ca and Mg in the form of carbonates and phosphates is based on saturation index calculations as described in [40]. Fe is described following the principles outlined in [21] (formation of ferrous oxides, P adsorption and co-precipitation). A more simplified approach is used to account for Al and P reactions based on second order kinetics [22]. Part of this PCF is a mass transfer model between the liquid and the gas phase compounds (i = DO, N_2, CO_2, H_2S, NH_3, CH_4 and H_2 in the liquid phase). The transport rates are formulated as a function of the difference between the saturation concentration (based on gas partial pressure) and the actual concentration of the gas dissolved in the liquid.

2.2.2. Model interfaces

The plant-wide model presented in this paper includes two sets of interfaces: First, interfaces between the ADM and ASM (and vice versa) and second, interfaces between both ADM and ASM with the PCF. The first interface is based on the continuous-based interface methodology, and it is used to ensure continuity in the mass balances and avoid component leaks [44]. These interfaces are located between anaerobic and anoxic/aerobic systems. More specifically, between 1) the waste flow from both primary and secondary settler and the anaerobic digester, and 2) the output of the dewatering unit and the storage tank. The ASM/ADM with the PCF interface is codified as a sub-routine, where at each integration step the outputs of the biological models are used to estimate pH and ion speciation and ion pairing. The precipitation/stripping/inhibition equations are embedded within the ADM/ASM ordinary differential equation model structure and are therefore included in the component mass balances. Similar approaches have been used in [2,26].

2.2.3. Ancillary elements

Primary clarification is described according to Otterpohl and Freund [45]. The double exponential velocity function proposed by Takács et al. [65] using a 10-layer is used to represent secondary settling. Thickening (THK) and dewatering (DEW) units are described as ideal solid–liquid separators [28]. Reactor hydraulics and biofilm growth were taken into account for modeling the anaerobic granular sludge reactors (AerGSR) as presented in [11]. The mass balance assumes that the transport of soluble compounds is governed solely by (homogenous) diffusion, whereas movement of particulate compounds takes place by convection [58]. Biofilm thickness (L) is given as the radial distance (z) and varies due to two phenomena: 1) the net growth of the particulate species, and 2) detachment from the biofilm surface [31]. The resulting system of partial differential equations (PDEs) is solved using the method of lines [49]. Influent dynamics follow the principles stated in [19] (see details in supplemental information). Struvite precipitation is described using the same PCF as described above. There is a constant dosage of Mg to promote saturation conditions. The crystalized P is separated from the mainstream in an ideal splitter [28]. More information on how to model P recovery units can be found in [30] and [14].

2.3. Key performance indicators (KPI)

The effluent quality index (EQi) is used to quantify the pollution load leaving the plant. Time in Violation (TIV) represents the degree of compliance with the limits set by regulators (NH_x, TN and TP). The operational cost index is a weighted sum of the plant́s different expenditures: aeration (AE), mixing (ME); heating (HE) and pumping energy (PE) (=$E_{consumption}$). It also includes use of chemicals (carbon source, magnesium & sodium), bio-solids disposal costs ($BIO_{diposal}$) and the potential revenues derived from: 1) methane production ($E_{production}$), and 2) struvite recovery ($CHEM_{production}$ (struvite)). Finally, the GHG_i emission index quantifies both on-site (secondary treatment, sludge processing) and off-site (energy production, consumption of chemicals and sludge disposal). It also accounts for potential GHG stripped in AnDS (centrifuges, before ASR). GHG credits through electricity and heat production are included, but fertilizer substitutions are not accounted for in the GHGi. More information can be found in [60,63] and [12].

2.4. Management strategies and technological solutions

Different types of reject management strategies and technological solutions are simulated using the BSM2 layout (see Table 1). The first set of simulations (= management strategy) involves keeping AnDS in the ST during daytime with subsequent release at night. The main rationale behind this strategy is to reduce the N/P load during the morning when the concentration is higher due to diurnal profile by using ST as buffer (see [19]). The second set accounts for AnDS treatment using PN/ANX (= technological solution). This will enhance the N load biologically [66]. The strategy is further explored by running the plant under different aeration modes: constant DO set-point, time-based DO set-point and pH-based DO set-point and either NH_x or NO_2^- based DO set-point. The impact of controlling PN/ANX load with the ST is also assessed. Different approaches are considered. Constant volume (no control is applied) (load control + 2). Next, constant flow to PN/ANX and sending of the excess (when it occurs) to either headworks (load control 3) or to the same PN/ANX (load control 4). The last strategy involves running the plant with a P-recovery unit. Again, this will capture part of the P load (as struvite) in RW [71]. The strategy here involves the addition of chemicals (Na and Mg) to increase pH and promote precipitation. All alternatives are simulated for 609 days and proceeded with steady state simulations (300 days), but only the last 364 days (52 weeks from day 245 to 609) are used to conduct the assessment [18].

3. Results

3.1. Management of anaerobic digester supernatants with a storage tank (ST)

The wastewater profile represents a general behavior, namely one morning peak, one evening peak, and late night and mid-day minima (see [19]). The morning and the evening peaks represent the residents going to or returning from work. The late-night minimum flow rate corresponds to the sleeping hours with little water consumption. Finally, the daytime flow rate shows a small decline corresponding to the residents' working hours. The main idea behind this strategy is to store RW during daytime, when the plant is highly loaded and release it at night.

Table 2 summarizes the calculated KPIs (see Section 2.3). Unexpectedly, simulations indicate that storing anaerobic digester supernatants (AnDS) has a minimal impact. However, there are some differences in nitrogen (N) and phosphorus (P) removal, as reflected by the time in violation (TIV) for NH_x, TN, and TP indices, which exhibit variations greater than 5 %.

Better values for TIV NH_x values are attributed to lower reactor overload during peak hours. Under normal conditions (i.e., no control), the N and P loads from 8 AM to 8 PM are 1.40 tons per day (T/d) and 473 kg/d, respectively. When load control (1) is activated (see Table 1), these loads decrease to 1.21 T/d and 284 kg/d, respectively. However, the quantity of N and P increases significantly at night (8 PM to 8 AM) (from 580 and 246 Kg /d to 890 and 533 kg /d). This explains the worse values for TIV TN and TP, which are mainly due to the changes in the COD/N and COD/P ratios resulting from the control actions, which change from 11.9 and 29.1 to 8.7 and 16.7, respectively. This fact negatively impacts denitrification and phosphorus removal as these two processes are dependent on organic substate. Fig. 2 illustrates the impact of storing AnDS during the daytime on storage volume on yearly, weekly, and daily time scales (panels A-F). It also shows the effects on nitrogen (N) and phosphorus (P) returning to the headworks (panels G-L). More details on effluent quality and the emissions factor can be found in Fig. 3. This Figure also shows the seasonality (= temperature) effect on both nitrogen and phosphorus removal processes. Simulations start in

Table 1
Scenarios (management / technologies) evaluated within the BSM2 layout.

		Measured variable	Controlled variable	Set-point	Manipulated variable	Control algorithm
BSM2 + ST (A1)	**Load control (1)**	time	$Q_{ST\text{-}OUT}$	0 /500 m^3/d	$Q_{ST\text{-}OUT}$ + $Q_{ST\text{-}bypass}$ in ST	ON/OFF
	Load control (2)	V_{ST} in ST	V_{ST} in ST	–	$Q_{ST\text{-}IN}$ + $Q_{ST\text{-}OUT}$ in ST	No control (input = output)
	Load control (3)	V_{ST} in ST	V_{ST} in ST	200 m^3/d	$Q_{ST\text{-}IN}$ + $Q_{ST\text{-}OUT}$ + $Q_{ST\text{-}bypass}$ in ST	ON/OFF
	Load control (4)	V_{ST} in ST	V_{ST} in ST	200 m^3/d	$Q_{ST\text{-}IN}$ + $Q_{ST\text{-}OUT}$ + $Q_{ST\text{-}bypass}$ in ST	ON/OFF
BSM2 + PN/ANX (A2)	**Constant DO**	DO in PN/ANX	DO in PN/ANX	DO = 0.35 g/m^3	K_La in PN/ANX	PI
	Time based DO	time	DO in PN/ANX	0.45	K_La in PN/ANX	ON/OFF
	PH based DO	pH in PN/ANX	DO in PN/ANX	pH > 6.7 (DO = 0.45 g/m^3) pH < 6.6 (DO = 0 g/m^3)	K_La in PN/ANX	cascaded PI
	NH_x based DO	NH_x in PN/ANX	DO in PN/ANX	NH_x > 14 g/m^3 (DO = 0.45 g/m^3) NH_x < 7 g/m^3 (DO = 0 g/m^3)	K_La in PN/ANX	cascaded PI
	NO_2^- based DO	NO_2^- in PN/ANX	DO in PN/ANX	NO_2^- > 14 g/m^3 (DO = 0.45 g/m^3) NO_2^-< 7 g/m^3 (DO = 0 g/m^3)	K_La in PN/ANX	cascaded PI
BSM2 + SPU (A3)	**Dosage control**	$Q_{SPU\text{-}IN}$	$Q_{SPU\text{-}Mg}$ in SPU	–	$Q_{SPU\text{-}Mg}$ in SPU	Feed-forward
	pH control	pH in SPU	pH in SPU	8.5	$Q_{SPU\text{-}Na}$ in SPU	PI

Table 2
Calculated KPIs for all evaluated reject water management strategies.

	Baseline (A0)	BSM2+ ST (A1)	BSM2 + PN/ANX (A2)	BSM2+ SPU (A3)	Units
TKN	5.3	5.1	3.9	5.6	g/m^3
TN	12.9	12.9	9.1	12.8	g/m^3
TP	2.9	3.2	2.3	1.4	g/m^3
TIV NH_x (= 4 g/m^3)	26.4	23.8	7.1	29.1	%
TIV TN (= 14 g/m^3)	3.4	4.1	0.0	6.2	%
TIV TP (= 2 g/m^3)	48.9	44.6	37.2	8.5	%
EQi	**12575.3**	**13017.8**	**10063.5**	**9586.7**	**Kg/d**
$E_{consumption}$	5638.9	5653.7	5496.6	5545.1	kW.h/d
$E_{production}$	5814.2	5830.6	5781.3	5877.7	kW.h/d
$BIO_{diposal}$	3964.2	3939.4	4025.5	3812.1	Kg/d
$CHEM_{consumption}$ (Mg)	0.0	0.0	0.0	227.8	Kg/d
$CHEM_{consumption}$ (NaOH)	0.0	0.0	0.0	575	Kg/d
$CHEM_{production}$ (struvite)	0.0	0.0	0.0	218.9	Kg/d
OCi	**11691.0**	**11615.7**	**11766.4**	**11443.1**	–
Bio GHG	0.68	0.68	1.50	0.68	$KgCO_2eq/m^3$
Sludge processing GHG	0.21	0.21	0.21	0.21	$KgCO_2eq/m^3$
Energy credit GHG	0.00	0.00	0.00	0.00	$KgCO_2eq/m^3$
Chemicals GHG	0.00	0.00	0.00	0.01	$KgCO_2eq/m^3$
Sludge disposal GHG	0.20	0.20	0.15	0.20	$KgCO_2eq/m^3$
GHGi	1.19	1.19	1.95	1.19	**$KgCO_2eq/m^3$**

June when the T is higher (day 245). The minimum temperature is reached between 400 and 500 days (December- January-February). Simulations finish in May (day 600).

3.2. Treatment of anaerobic digester supernatants with a partial nitrification / anammox reactor

The KPI values obtained from running the BSM2 layout after implementing a partial nitrification (PN) and anammox (ANX) reactor to treat anaerobic digester supernatants (AnDS) can be found in Table 2. Model predictions suggest a substantial improvement in overall nitrogen (N) removal, with improvements with respect to the baseline scenario in TKN, TN, TIV NH_x, TIV TN, and EQi all exceeding 20 %. This improvement is primarily due to the reduced daily N load entering the activated sludge reactor (AS), which decreased from 1.09 tons per day (T/d) to 912 kg per day (kg/d). AnDS accounts for 21.6 % (Baseline) and

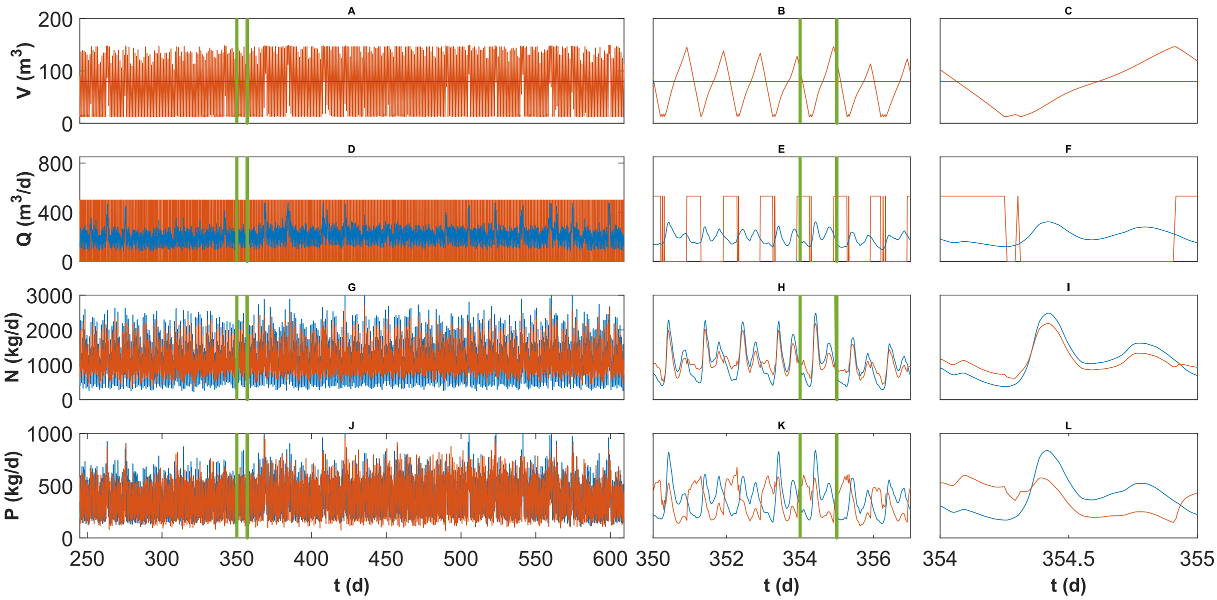

Fig. 2. Comparison of Baseline scenario (blue) and storage load control (1) (red) on: storage volume (row 1) and anaerobic digester supernatants flow (row 2), nitrogen (row 3) and phosphorus (row 4) load. This is depicted at yearly (column 1), weekly (column 2) and daily (column 3) time scales. Green solid lines indicate the part of the time series amplified (= snapshot) to allow to see more details at higher frequency (weeks, days). Long term simulations are supposed to start 1 June. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

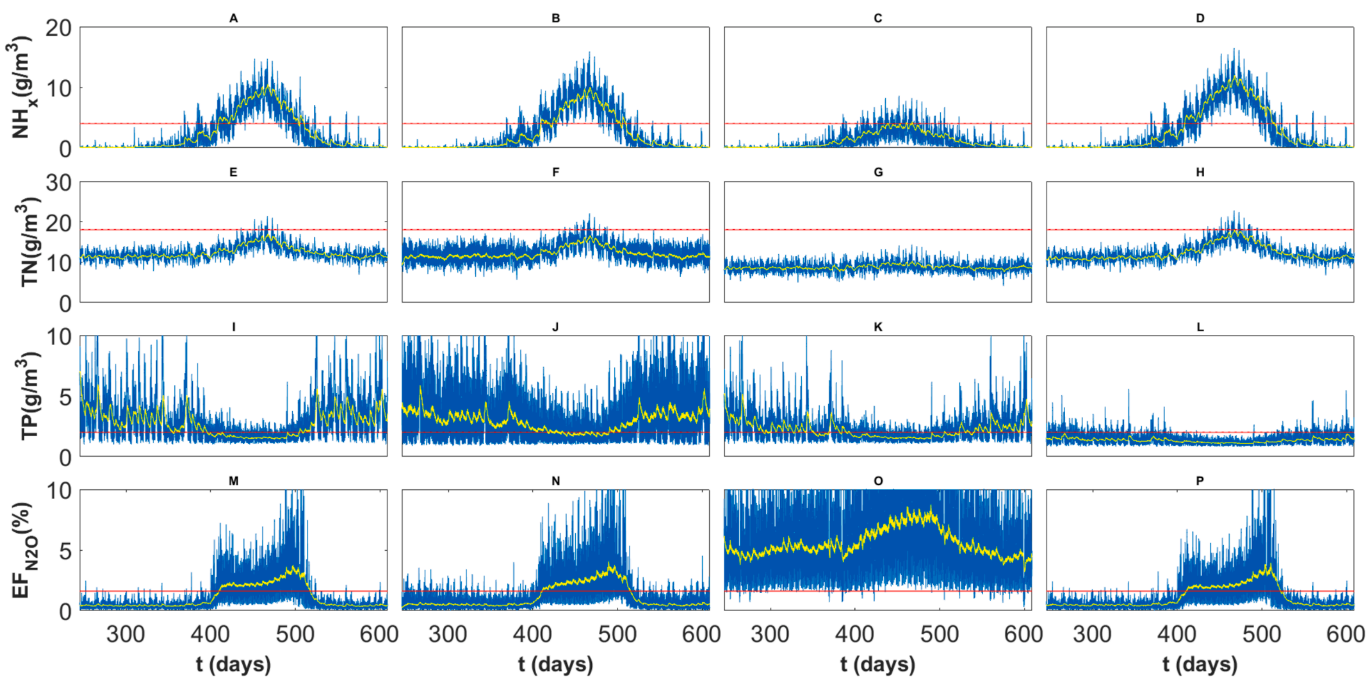

Fig. 3. Predicted dynamic profiles for effluent NH_x (row1), TN (row2) and TP (row3)- Row 4 represents plant emission factors. Red solid lines are recommended limits that are not to be exceeded. Yellow lines are the results of applying a 3-day exponential filter to smoothen the data. This is repeated for all the evaluated alternatives: Baseline (A0) (column1), RW storage (A1) (colum2), PN/ANX (A2) (column 3) and P-recovery (A3) (column 4). Long-term simulations are supposed to start 1 June (day 245). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4.9 % (BSM2 + PN/ANX) of the total incoming N load. In the baseline scenario, 21.9 % of the influent N is denitrified in the AS. In the option with PN/ANX (A2), 30.3 % is removed in both the AS and PN/ANX, with 8.5 % handled within the PN/ANX alone. Further details are provided in the dynamic profiles shown in Fig. 3.

The reduced quantity of nitrate (NO_3^-) produced in the AS, resulting from the lower N load, gives a competitive advantage to phosphorus-accumulating organisms (PAO) over ordinary heterotrophic bacteria (OHO). Computer simulations indicate that the percentage of PAO relative to total biomass in the AS increases from 33 % to 40 %. This advantage is reflected in the KPIs used to assess phosphorus removal, as seen in the TP, TIV TP, and EQi values in Table 2, as well as Fig. 3C, G and K.

However, as a side effect, GHG emissions are drastically increased (see Table 2). This is attributed to the high N_2O production during bio-treatment in the PN/ANX (see Fig. 3O). The biological model suggests that the low dissolved oxygen (DO) and high nitrite (NO_2^-) concentration in the PN/ANX unit promote high N_2O emissions. Emission factors (EF) escalated from 0.24 % to 3.9 % at the plant-wide level. In the baseline scenario, the EF in the AS is the only operational unit accounted for. However, in the second case, the EFs are 0.1 % (AS) and 25 % (PN/ANX), meaning that almost 3.8 % of the nitrogen entering the BSM2 plant layout is transformed into N_2O. There is a slight reduction in indirect GHG emissions when PN/ANX is operational, mainly due to sludge disposal efficiencies. This is primarily due to the lower quantity of nitrogen contained in dewatered sludge (270 versus 190 Kg / d) resulting from higher removal efficiencies.

3.2.1. Impact of aeration patterns

Figs. 4 and 5 illustrate the dissolved oxygen (row1), pH (row 2), NH_x (row 3), NO_2^- (row 4), and N_2O (row 5) dynamics on both weekly and yearly scales resulting from different aeration patterns: 1) constant (column 1), 2) time-based (column 2), 3) pH-based (column 3), 4) NH_x-based (column 4), and 5) NO_2^- based (column 5) (see Table 1). Weekly simulations (Fig. 5) help to better examine the nature of the different control actions.

Interestingly, the proposed approach predicts no substantial differences in effluent quality (EQi) and operational costs (OCi). Surprisingly, Fig. 6A, B (X-axis) reveals that all strategies with PN/ANX and different DO controllers (Table 1) yield very similar values for OCi / Kg N and/or OCi / Kg P removed. However, there are significant changes in GHG emissions (see Fig. 6A, B Y-axis). Indeed, aeration patterns may have a dramatic effect on N_2O production and the plants overall carbon footprint.

3.2.2. Impact of loading conditions

Fig. 7 depicts three ways of operating the storage tank (ST) changing the load to the PN/ANX: 1) pass through (input = output), 2) constant flow to the PN/ANX and bypass to headworks when overflowing, 3) constant flow to the PN/ANX and by-pass to PN/ANX unit when overflowing. It is very difficult to see a clear pattern in Fig. 6C and D indicating a strong impact derived from storing AnDS. Slight differences can be seen when the ST is operated as depicted in column 2, which sends the excess of untreated R to the headworks Indeed, the effect of managing these streams differently (see Table 1) is disappointingly low.

3.3. Treatment of anaerobic digester supernatants with a struvite precipitation unit

The calculated KPI values of the last technological solution (struvite precipitation unit) are summarized in Table 2. Model predictions suggest a substantial improvement in the overall phosphorus (P) removal, with variation with respect to the baseline scenario in TP and TIV TP exceeding 50 % (see dynamic profiles in Fig. 3). Similar to the effects observed with the implementation of a PN/ANX system, the operation of the SPU markedly reduces the impact of reject water, decreasing the P load entering the activated sludge reactor (AS) by 24 % (from 388 to 295 kg/d). This reduction implies that 30 % of the incoming P is recovered as struvite. Consequently, the COD/N and COD/P ratios shift from 7.9 and 19.2 to 8.12 and 26.5, respectively. OCI values indicate that the costs of chemicals (Mg, NaOH) are effectively offset by the potential revenue from selling struvite as fertilizer. No substantial impact is observed in GHG emissions, with a variation of less than 5 %.

To further demonstrate the usefulness of the developed tool, we reassessed the impact of varying dosages on the removal efficiencies of nitrogen (Kg N) and phosphorus (Kg P) in relation to operational costs (OCi) and greenhouse gas emission intensities (GHGi). The magnesium load is adjusted in proportion to the overflow from the dewatering unit (i.e., reject water) (see Table 1). A higher Q_{DEW}/Q_{Mg} ratio means a lower chemical addition. The dosage of NaOH is required to maintain the pH within the desired range of 8.5 to 9.5 in the struvite reactor (see Table 1). Both Mg and Na streams are assumed to be at a concentration of 25 %. Computer simulations revealed that the potential quantity of N and P recovered as struvite in the BSM2 model depends on the magnesium concentration. Lowering the ratio (i.e., increasing the flow) decreases the cost of N and P removal by increasing the potential revenue derived from selling struvite. Although NaOH and pH levels in the anaerobic digester (AD) might influence the release of free ions from their paired forms, thus facilitating the formation of precipitates[32], the simulations in this case study indicate that these factors do not significantly impact the process. Regarding GHG emissions, similar patterns emerge where higher quantities of recovered struvite correlate

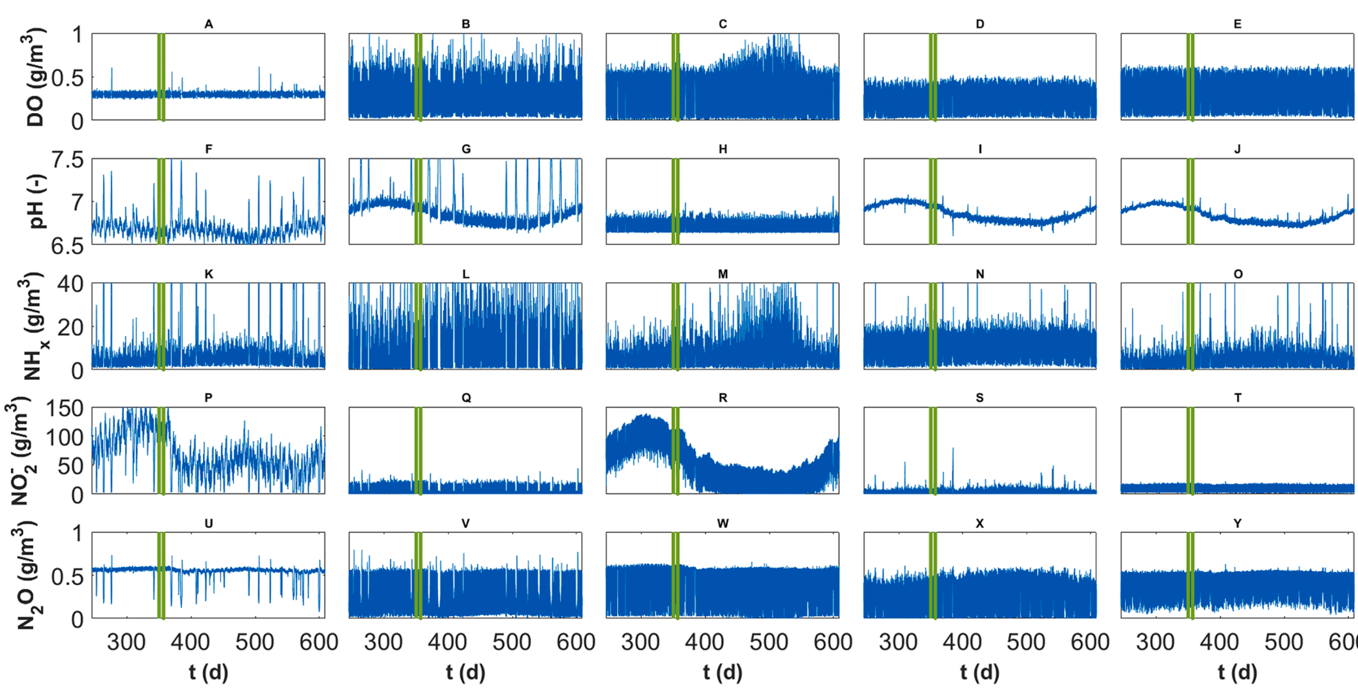

Fig. 4. Effect of aeration mode: constant (column 1), time-based (column 2), pH based (column 3), 4) NH_x based (column 4) and NO_2^- (column 5) on selected BSM2 operational variables. Geen lines indicate the snapshot used in Fig. 5. Long-term simulations are supposed to start 1 June (day 245).

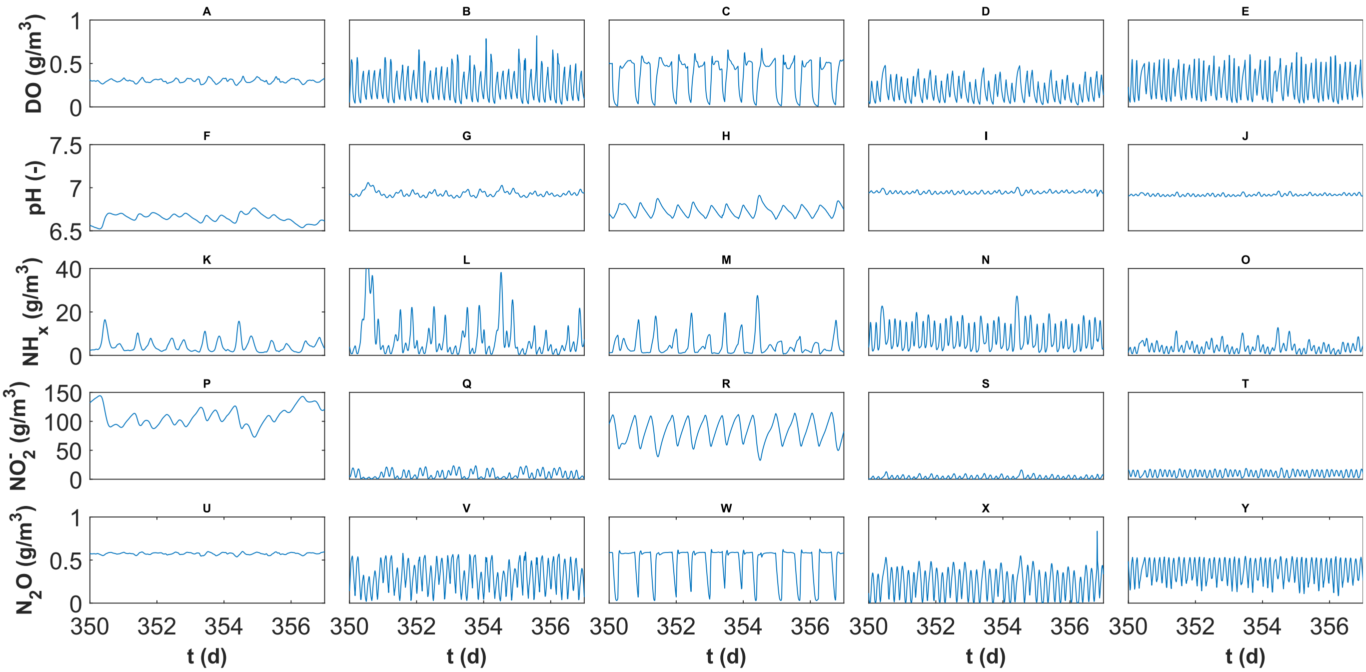

Fig. 5. Effect of aeration mode: constant (column 1), time-based (column 2), pH based (column 3), 4) NH_x based (column 4) and NO_2^- (column 5) on selected operational variables. This is a shapshot taken from Fig. 4 (see green lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

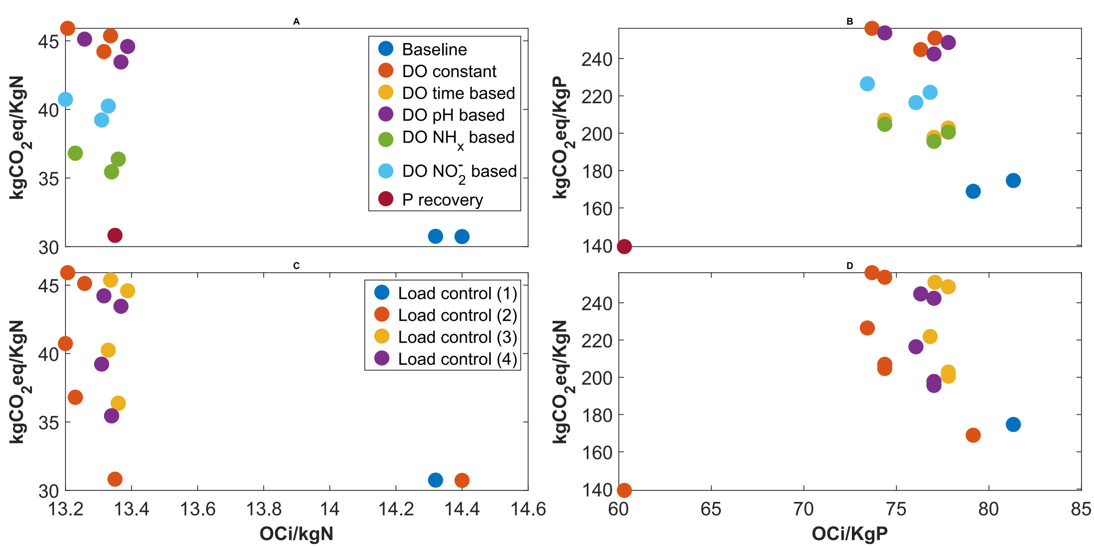

Fig. 6. N and P removal versus OCi and GHGi for ALL reject water management strategies evaluated within the BSM2. Constant aeration, time-based aeration and pH-based aeration include the three ways of operating the storage tank (see Fig. 4).

with better GHG scores. The impact of sodium is similarly minimal.

4. Discussion

4.1. Impact of aeration patterns on the plants carbon footprint

The results presented in Section 3.2 consistently demonstrate the significant impact of aeration patterns on N_2O emissions (see Figs. 4, 5, and 6). This effect is primarily due to the suppression of NO_2^- by both ordinary heterotrophic organisms (OHO) and anaerobic ammonium-oxidizing bacteria (ANX), which substantially reduce the AOB denitrification pathway. Notably, biological emissions during aerobic COD/N conversions account for 76 % of the plant's total carbon footprint (see Table 2). The impact of aeration patterns on N_2O emissions strongly aligns with previous studies published in the scientific literature. Santín et al. [56,57] reported GHG reductions of up to 30 % using smart control strategies using the BSM2 platform. Similarly, [64] found out the profound impact that aeration patterns may have on the overall carbon footprint of a treatment plant. Duan et al., 2020 [10] could reduce N_2O emissions by up to 35 % and operational cost by 20 % by controlling the DO setpoint more tightly in an SBR in Adelaide. Castro-Barros et al. [7] reported that transients from low (or zero) to high aeration favored N_2O emissions. Pijuan et al., 2014 [47] investigated the effect of DO setpoints in a granular airlift reactor, which turned out to decrease emissions from 6 to 2.2 %. More specifically for PN/ANX systems, Domingo-Félez et al. [9] found out that significant decreases in N_2O emissions were obtained

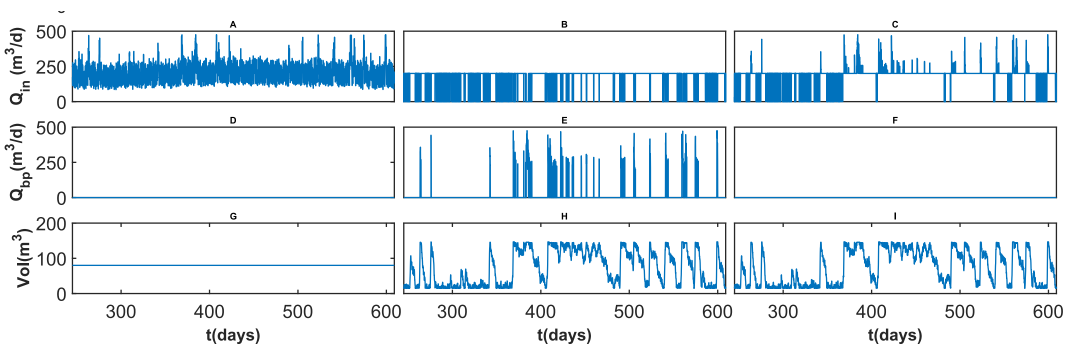

Fig. 7. Dynamics of controlling sorage tank: no control (column 1) (load control 2), constant outflow-bypass excess to headworks (column 2) (load control 3), constant outflow, bypass excess to PN/ANX (column 3) (load control 4). See Table 1 for a detailed description of each strategy. Long term simulations are supposed to start 1 June.

when the frequency of aeration was increased to yield a higher number of shorter aeration periods while maintaining a constant air flow rate. Similar to the findings reported in this study, the authors concluded that N_2O emissions from single stage nitritation/anammox reactors could be reduced by operating under conditions where anaerobic exceeds aerobic ammonium oxidation activity (see columns 2, 4 and 5 in Fig. 5). On the other hand, Wan et al., 2021 [69] reported that ammonium-based aeration control improves nitrogen removal efficiency and reduces N_2O emissions for PN/ANX reactors.

4.2. Nitrogen intensified processes versus N_2O emissions

Previous studies, including Uri-Carreño et al., 2024 [67], have reported a strong correlation between the nitrogen loading rate (NLR, g N/ m^3·d) and emission factors (EF, %). This relationship suggests that higher NLRs lead to increased EF_{N2O}, which can be attributed to increased volumetric specific loading that enhances NH_x turnover or ammonia oxidation rates (AOR), consequently boosting production via NN, DN, and DEN pathways [6]. Within this study, several assessed strategies align with this trend. Specifically, PN/ANX strategies that maximize NO_2^- suppression (time-based DO, NH_x-based DO, and NO_2^- based DO) closely follow this trend. Conversely, strategies aimed at maximizing NH_x conversion—and consequently NO_2^- accumulation—such as constant DO and pH-based DO, are characterized by abnormally high EFs (greater than 15 %). This suggests that more sophisticated control strategies may be necessary to effectively balance nitrogen conversion and N_2O emissions (see Fig. 9).

4.3. Impact of P:Mg ratios

The study highlights the impact of varying phosphorus to magnesium (P:Mg) ratios on phosphorus removal efficiencies within the struvite precipitation unit (SPU), which range from 95 % at a ratio of 0.7 to 17 % at a ratio of 5.1, as depicted in Fig. 8. These results are consistent with findings in the literature. For instance, Aguilar-Pozo et al., 2023 [1], observed that P:Mg molar ratios of 1:1 and 1:2 are optimal for struvite precipitation. Similarly, [8], and [41], recommended ratios between 1.2 and 2.0. The study also explores the broader implications of chemical dosing on effluent quality, operational costs, and greenhouse gas (GHG) emissions. Additionally, the effects of phosphorus recovery on the sludge line have been evaluated using model-based approaches, as detailed in studies by Mbamba et al., 2015 [40] and Flores-Alsina et al., 2021 [14]. This comprehensive analysis underscores the importance of optimizing chemical ratios not only for environmental compliance but

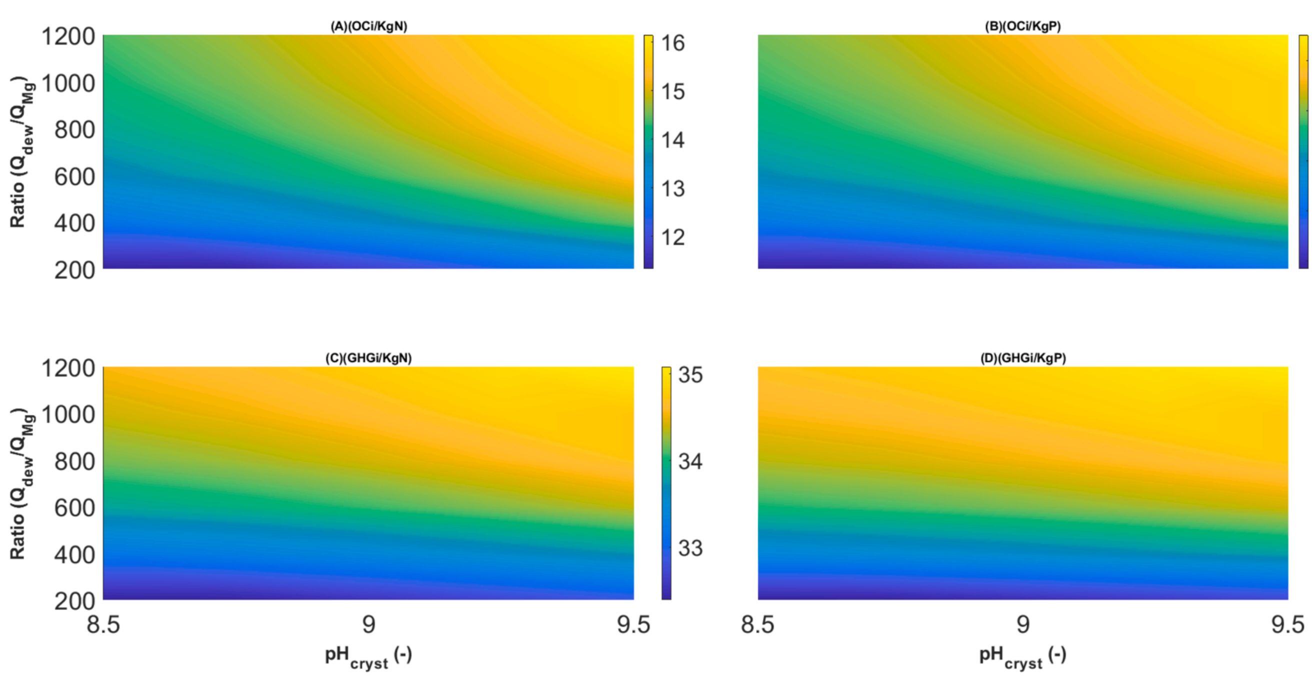

Fig. 8. Impact of chemical dosage (Mg, Na) on the overall plant performance: N (A, C), P (B, D) removal versus OCi (A,B) and GHGi (C,D).

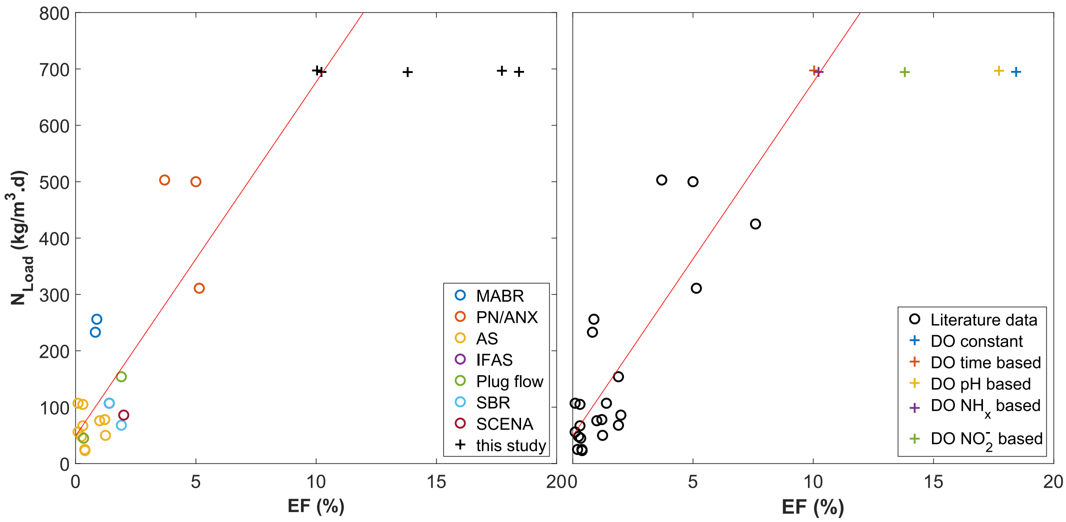

Fig. 9. Comparision of different types of biological N removal technologies according to the % of N load emitted as N_2O-N (y-axis) and the nitrogen loading rate (g N / m^3 d) (x-axis).(Original data extracted from **Uri-Carreno et al., 2024**).

also for economic efficiency and sustainability in wastewater treatment processes.

4.4. Alternative modes of operation / technologies

This paper has presented, for exemplary purposes, the (plant-wide) impacts of very few management strategies (ST control) and technological solutions (PN/ANX, SPU). Nevertheless, the list of potential options that could be implemented and simulated in the proposed platform is far from being complete. Ammonia stripping could be integrated with struvite precipitation for improved efficiency [25]. Other options could be precipitation + adsorption [43], stripping + adsorption [34]. The authors refer to [71] for a comprehensive list of technologies. Additional work will be necessary to adapt modelling approaches and develop and integrate KPI.

This study has demonstrated the potential of partial nitration/anammox (PN/ANX) reactors and SPU in enhancing nitrogen and phosphorus removal while addressing greenhouse gas (GHG) emissions. Importantly, the technologies assessed are already available on the market and are successfully implemented in multiple wastewater treatment plants worldwide. For example, PN/ANX reactors, provided by Paques (Netherlands) and AnoxKaldnes (Veolia, France), are operational in full-scale facilities like the Dokhaven WWTP in Rotterdam. These facilities have reported significant reductions in nitrogen loads and operational costs. Similarly, struvite precipitation units offered by Ostara Nutrient Recovery Technologies (Canada) and NuReSys (Belgium), including the Pearl® and NuReSys processes, are implemented in the Stickney WWTP in Chicago, USA, and the Durham Advanced WWTP in Ontario, Canada. These technologies have demonstrated high phosphorus recovery efficiencies, while producing marketable struvite fertilizers. The adoption of these technologies indicates their cost-effectiveness, scalability, and environmental benefits, making them viable alternatives to conventional treatment approaches at specific sities. The operational success of these systems in diverse global contexts further supports the feasibility of the solutions proposed in this study.

5. Uncertainties and limitations

Despite the comprehensive nature of the proposed framework for managing anaerobic digestion supernatants (AnDS) in wastewater treatment plants (WWTP), several uncertainties and limitations must be acknowledged [5]. Firstly, the predictive models developed for storage tanks, aerobic granular sludge reactors (AerGSR), and struvite precipitation units (SPU) rely on numerous parameters that may vary significantly across different WWTPs. Variability in influent characteristics, operational conditions, and local environmental factors can affect the accuracy of these models. For instance, the models' sensitivity to changes in influent composition, such as variations in chemical oxygen demand (COD), nitrogen (N), and phosphorus (P) concentrations, could lead to discrepancies between predicted and actual performance [15,51].

Another limitation stems from the assumptions made in the simulation environment. The International Water Association (IWA) Benchmark Simulation Model No 2 (BSM2) provides a standardized testing platform, but real-world WWTPs often exhibit complexities that are difficult to capture fully in a simulation. These complexities include microbial community dynamics, unmodeled biochemical interactions, and the potential for unforeseen operational challenges. Moreover, the control strategies tested under dynamic conditions in the simulations may not translate to real-world applications due to differences in plant infrastructure and automation capabilities [46].

Uncertainty also arises from the innovative control strategies proposed for managing AnDS. While these strategies have demonstrated potential in simulations, their implementation in practice may face hurdles related to technology integration, staff training, and maintenance requirements. The real-time adjustment of dissolved oxygen (DO) setpoints and other parameters necessitates robust monitoring and control systems, which may not be readily available in all WWTPs [27].

Despite the comprehensive nature of the proposed framework, several scalability and implementation barriers must be acknowledged. For instance, while the modular design of PN/ANX reactors and struvite precipitation units supports their scalability, the reliance on advanced control systems and the need for site-specific adaptations may limit their feasibility in certain contexts. As discussed in Section 3.3, maintaining optimal operating conditions, such as P:Mg ratios, is critical for maximizing phosphorus recovery and minimizing costs. Moreover, economic feasibility and training requirements could pose challenges, particularly for smaller WWTPs or those with limited resources. Addressing these barriers will be essential to ensure broader adoption of these technologies.

5.1. Potential benefits for other WWTP and decision tool towards net zero

The presented set of tools have demonstrated its utility in developing and evaluating net zero strategies for water infrastructures, while balancing these strategies with effluent quality and cost considerations. It includes: 1) a comprehensive simulation model that accounts for all relevant emissions, including N_2O from activated sludge and CH_4 from anaerobic digesters, and 2) sophisticated emission calculation algorithms that consider chemical dosages and energy usage. The study has highlighted the significant impact of operational changes, technological interventions, and optimization algorithms on emissions.

The framework's adaptability to different WWTP configurations enhances its applicability. The models can be tailored to specific plant conditions, allowing for the exploration of customized solutions that address local challenges. For instance, BSM tools have been successfully exported to multiple set-ups: see studies in Brisbane [30], Stockholm [29] Cape Town [14] and Pretoria [51].

Additional validation studies have been conducted to test model credibility under various conditions. Flores-Alsina et al. [17] quantified, predicted, and mitigated nitrous oxide emissions in a full-scale partial nitritation/anammox reactor treating reject water. The model accurately predicted multiple nitrogen oxidation states (NH_x, NO_2^-, NO_3^-, N_2O) and dissolved oxygen (DO), with a normalized RMSE < 1, demonstrating its ability to effectively describe bacterial behavior within the studied system. Similarly, Lei et al. [33] dynamically predicted nitrous oxide emissions in a full-scale industrial activated sludge reactor for a range of aeration patterns and COD/N ratios. A deviation of 8.6 % (plant data versus computer simulations) is achieved over a six-week measuring campaign. Their study illustrated how to generate response surfaces that highlight variations in key performance indicators (KPIs) such as emission factors (EFs), nitrification capacity, effluent quality, and aeration energy consumption as functions of different aeration setpoints (DO and NO_2^-). Based on the model outputs, it is feasible to develop automated control systems that adjust WWTP operations in real-time to optimize GHG emission reductions. Additionally, the model can serve as a decision-support tool, aiding plant manager and operators in understanding the implications of changes in plant layout and operation on GHG emissions and guiding them toward net zero objectives. It also enables the creation of reports that document emissions and the effectiveness of implemented strategies. Ultimately, insights gained from ongoing operations and model predictions will continuously refine and enhance these strategies.

6. Conclusions

The main findings of this manuscript can be summarized in the following points:

- A plant-wide model benchmarking anaerobic digester supernatants' (AnDS) management strategies and technological solutions is presented. The proposed approach is constructed upon rigorous biological and physico-chemical models. The latter allowed to predict the behavior of storage tanks, an aerobic granular sludge reactor (partial nitration/ anammox) and struvite precipitation units (P recovery) and how their mode of operation propagated to the rest of the plant. This study goes beyond the state of the art by accounting both the interconnected and the multi-objective nature of WWTP operations.
- Simulations revealed that management of AnDS with a storage tank in the BSM layout had a low improvement in the overall process performance. N load reduction during daytime (8 AM to 8 PM) reduces NH_x effluent peaks (= TIN NH_x). On the other hand, nighttime (8 PM to 8 AM) changes in the COD/N and COD/P ratios negatively impact denitrification and phosphorus removal.
- PN/ANX substantially decreases the cost (OCi /kg N and OCi / kg P) of N and P removal. Nevertheless, low DO and high NO_2^- concentration promoted high N_2O emissions, increasing the global GHGi. These emissions can be substantially reduced by adopting innovative aeration patterns. Management input AnDS with streams with a storage tank has a poor effect on PN/ANX performance.
- The addition of a struvite precipitation unit (SPU) substantially reduces the quantity of P returning from the sludge. This substantially changes the COD/N and COD/P improving both denitrification and biological phosphorus removal. Exploration by simulation reveals that EQi, OCi and GHGi are extremely dependent on the addition of chemicals (Na and Mg).
- The set of models presented herein (process models, evaluation criteria) are easily exportable and will allow process engineers in water utilities to evaluate different technological solutions for sludge treatment in a plant-wide context. The models should be complemented with additional experiments to determine important model parameters in order to achieve more accurate predictions in the scenario analysis.
- This research advances chemical engineering and wastewater management knowledge by providing a novel, holistic plant-wide modeling framework that integrates multi-objective optimization, innovative technologies, and advanced control strategies. This study equips engineers and decision-makers with tools to optimize nutrient removal, reduce GHG emissions, and improve the cost-effectiveness of WWTP operations. The findings also contribute to the growing body of knowledge required to develop sustainable, net-zero wastewater treatment solutions.

Software Availability

The Matlab/Simulink implementation are available on request. To express an interest for obtaining the code, please contact Dr. Xavier Flores-Alsina (xfa@kt.dtu.dk) or Prof. Krist V. Gernaey (kvg@kt.dtu.dk) at the Department of Chemical and Biochemical Engineering at the Technical University of Denmark. The authors will also make the code available through the GitHub platform (www.github.com/wwtmodels).

CRediT authorship contribution statement

Xavier Flores-Alsina: Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Anna Katrine Vangsgaard:** Writing – review & editing, Writing – original draft, Methodology, Investigation, Conceptualization. **Nerea Uri Carreno:** Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis. **Per H. Nielsen:** Supervision. **Krist V. Gernaey:** Writing – review & editing, Writing – original draft, Visualization, Supervision, Software, Project administration, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors gratefully acknowledge the financial support received by MUDP (Miljøteknologisk Udviklings- og Demonstrationsprogram) under the project NACAT (contract number: 2021-20015). The GENOCOV research group (Juan Baeza, Albert Guissasola and Borja Solis) at the Autonomous University of Barcelona is also acknowledged for providing the basis upon the simulation framework used in this study has been constructed.

Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.cej.2025.160934.

Data availability

Data will be made available on request.

References

[1] V.B. Aguilar-Pozo, J.M. Chimenos, B. Elduayen-Echave, K. Olaciregui-Arizmendi, A. López, J. Gómez, S. Astals, Struvite precipitation in wastewater treatment plants anaerobic digestion supernatants using a magnesium oxide by-product, *Sci. Total Environ.* 890 (2023) 164084, https://doi.org/10.1016/j.scitotenv.2023.164084.

[2] **R. Barat, J. Serralta, M.V. Ruano, E. Jiménez, J. Ribes, A. Seco, J. Ferrer,** Biological Nutrient Removal Model No. 2 (BNRM2): a general model for wastewater treatment plants, Water Sci. Technol. 67 (2013) 1481-1489. https://doi.org/10.2166/wst.2013.004.

[3] D.J. Batstone, X. Flores-Alsina, Generalised physicochemical model - PCM for wastewater processes, IWA Scientific and Technical Report 29 (2022), https://doi.org/10.2166/9781780409832.

[4] D.J. Batstone, J. Keller, I. Angelidaki, S.V. Kalyuzhnyi, S.G. Pavlostathis, A. Rozzi, V.A. Vavilin, The IWA anaerobic digestion model no 1 (ADM1), *Water Sci. Technol.* 45 (2002) 65–73, https://doi.org/10.2166/9781780403052.

[5] E. Belia, Y. Amerlinck, L. Benedetti, B. Johnson, G. Sin, P.A. Vanrolleghem, K. Villez, Wastewater treatment modelling: dealing with uncertainties, *Water Sci. Technol.* 60 (2009) 1929–1941, https://doi.org/10.2166/wst.2009.225.

[6] J.M. Blum, Q. Su, Y. Ma, B. Valverde-Pérez, C. Domingo-Félez, M.M. Jensen, B. F. Smets, The pH dependency of N-converting enzymatic processes, pathways and microbes: effect on net N2O production, Environ. Microbiol. 20 (5) (2018) 1623–1640.

[7] C.M. Castro-Barros, M.R.J. Daelman, K.E. Mampaey, M.C.M. Van Loosdrecht, E.I. P. Volcke, Effect of aeration regime on NO emission from partial nitritation-anammox in a full-scale granular sludge reactor, *Water Res.* 68 (2015) 793–803, https://doi.org/10.1016/j.watres.2014.10.056.

[8] D. Crutchik, N. Morales, J.R. Vázquez-Padín, J.M. Garrido, Enhancement of struvite pellets crystallization in a full-scale plant using an industrial grade magnesium product, *Water Sci. Technol.* 75 (2017) 609–618, https://doi.org/10.2166/wst.2016.527.

[9] C. Domingo-Félez, A.G. Mutlu, M.M. Jensen, B.F. Smets, Aeration strategies to mitigate nitrous oxide emissions from single-stage nitritation/anammox reactors, *Environ. Sci. Tech.* 48 (2014) 8679–8687, https://doi.org/10.1021/es501819n.

[10] H. Duan, B. van den Akker, B.J. Thwaites, L. Peng, C. Herman, Y. Pan, et al., Mitigating nitrous oxide emissions at a full-scale wastewater treatment plant, Water Res. 185 (2020) 116196.

[11] H. Feldman, X. Flores-Alsina, P. Ramin, K. Kjellberg, U. Jeppsson, D.J. Batstone, K. V. Gernaey, Modelling an industrial anaerobic granular reactor using a multi-scale approach, *Water Res.* 126 (2017) 488–500, https://doi.org/10.1016/j.watres.2017.09.033.

[12] X. Flores-Alsina, L. Corominas, L. Snip, P.A. Vanrolleghem, Including greenhouse gas emissions during benchmarking of wastewater treatment plant control strategies, *Water Res.* 45 (2011) 4700–4710, https://doi.org/10.1016/j.watres.2011.04.040.

[13] X. Flores-Alsina, H. Feldman, V.T. Monje, P. Ramin, K. Kjellberg, U. Jeppsson, K. V. Gernaey, Evaluation of anaerobic digestion post-treatment options using an integrated model-based approach, *Water Res.* 156 (2019) 264–276, https://doi.org/10.1016/j.watres.2019.02.035.

[14] X. Flores-Alsina, E. Ramin, D. Ikumi, T. Harding, D. Batstone, C. Brouckaert, K. V. Gernaey, Assessment of sludge management strategies in wastewater treatment systems using a plant-wide approach, *Water Res.* 190 (2021) 116714, https://doi.org/10.1016/j.watres.2020.116714.

[15] X. Flores-Alsina, I. Rodríguez-Roda, G. Sin, K.V. Gernaey, Multi-criteria evaluation of wastewater treatment plant control strategies under uncertainty, *Water Res.* 42 (2008) 4485–4497, https://doi.org/10.1016/j.watres.2008.05.029.

[16] X. Flores-Alsina, K. Solon, C.K. Mbamba, S. Tait, K.V. Gernaey, U. Jeppsson, D. J. Batstone, Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes, *Water Res.* 95 (2016) 370–382, https://doi.org/10.1016/j.watres.2016.03.012.

[17] X. Flores-Alsina, N. Uri-Carreño, A.K. Vangsgaard, P.H. Nielsen, K.V. Gernaey, Quantification, prediction and mitigation of nitrous oxide emissions in a full-scale partial nitrification/anammox reactor treating reject water, Water Res. (2025), https://doi.org/10.1016/j.watres.2025.123200.

[18] K.V. Gernaey, J.B. Copp, U. Jeppsson, I. Nopens, M.N. Pons, P.A. Vanrolleghem, Benchmarking of control strategies, in: Benchmarking of Control Strategies for Wastewater Treatment Plants, IWA Publishing, London, 2014, pp. 55-58. https://doi.org/10.2166/9781780401171F.

[19] K.V. Gernaey, X. Flores-Alsina, C. Rosen, L. Benedetti, U. Jeppsson, Dynamic influent pollutant disturbance scenario generation using a phenomenological modelling approach, *Environ. Model. Softw.* 26 (2011) 1255–1267, https://doi.org/10.1016/j.envsoft.2011.06.001.

[20] C.L. Grady Jr., G.T. Daigger, N.G. Love, C.D. Filipe, *Biological Wastewater Treatment*, third ed., CRC Press, Boca Raton, 2011.

[21] H. Hauduc, T. Wadhawan, B. Johnson, C. Bott, M. Ward, I. Takács, Incorporating sulfur reactions and interactions with iron and phosphorus into a general plant-wide model, *Water Sci. Technol.* 79 (2019) 26–34, https://doi.org/10.2166/wst.2018.482.

[22] M. Henze, W. Gujer, T. Mino, T. Matsuo, M.C. Wentzel, G.V.R. Marais, M.C. Van Loosdrecht, Activated sludge model no. 2d (ASM2d), Water Sci. Technol. 39 (1999) 165-182. https://doi.org/10.1016/S0273-1223(98)00829-4.

[23] Y. He, Y. Li, X. Li, Y. Liu, Y. Wang, H. Guo, Y. Liu, Net-zero greenhouse gas emission from wastewater treatment: mechanisms, opportunities and perspectives, *Renew. Sustain. Energy Rev.* 184 (2023) 113547, https://doi.org/10.1016/j.rser.2023.113547.

[24] W.C. Hiatt, C.L. Grady, An updated process model for carbon oxidation, nitrification, and denitrification, *Water Environ. Res* 80 (2008) 2145–2156, https://doi.org/10.2175/106143008X304776.

[25] H. Huang, J. Liu, C. Xu, F. Gao, Recycling struvite pyrolysate obtained at negative pressure for ammonia nitrogen removal from landfill leachate, *Chem. Eng. J.* 284 (2016) 1204–1211, https://doi.org/10.1016/j.cej.2015.09.080.

[26] D.S. Ikumi, T.H. Harding, Kinetics of biological and chemical processes in anoxic-aerobic digestion of phosphorus rich waste activated sludge, *Water Res.* 170 (2020) 115333, https://doi.org/10.1016/j.watres.2019.115333.

[27] P. Ingildsen, G. Olsson, Smart Water Utilities: Complexity Made Simple, IWA Publishing, London, 2016. https://doi.org/10.2166/9781780407586.

[28] U. Jeppsson, M.N. Pons, I. Nopens, J. Alex, J.B. Copp, K.V. Gernaey, P. A. Vanrolleghem, Benchmark simulation model no. 2: general protocol and exploration case studies, *Water Sci. Technol.* 56 (2007) 67–78, https://doi.org/10.2166/wst.2007.604.

[29] C. Kazadi-Mbamba, E. Lindblom, X. Flores-Alsina, S. Tait, S. Anderson, R. Saagi, U. Jeppsson, Plant-wide model-based analysis of iron dosage strategies for chemical phosphorus removal in wastewater treatment systems, *Water Res.* 155 (2019) 12–25, https://doi.org/10.1016/j.watres.2019.01.048.

[30] C. Kazadi-Mbamba, X. Flores-Alsina, D.J. Batstone, S. Tait, Validation of a plant-wide phosphorus modelling approach with minerals precipitation in a full-scale WWTP, *Water Res.* 100 (2016) 169–183, https://doi.org/10.1016/j.watres.2016.05.003.

[31] S. Lackner, A. Terada, B.F. Smets, Heterotrophic activity compromises autotrophic nitrogen removal in membrane-aerated biofilms: results of a modeling study, *Water Res.* 42 (2008) 1102–1112, https://doi.org/10.1016/j.watres.2007.08.025.

[32] M.A. Latif, C.M. Mehta, D.J. Batstone, Low pH anaerobic digestion of waste activated sludge for enhanced phosphorous release, *Water Res.* 81 (2015) 288–293, https://doi.org/10.1016/j.watres.2015.05.062.

[33] T. Lei, J. Whale-Obrero, S.B. Larsen, K. Kjellberg, K.V. Gernaey, X. Flores-Alsina, Dynamically predicting nitrous oxide emissions in a full-scale industrial activated sludge reactor under multiple aeration patterns and COD/N ratios, Water Research (2025). https://doi.org/10.1016/j.watres.2025.123379.

[34] J. Lubensky, M. Ellersdorfer, Pilot scale experiments for ammonium recovery from sludge liquor at a municipal wastewater treatment plant, *J. Sustain. Dev. Energy Water Environ. Syst.* 9 (2021) 1–11. https://doi.org/10.13044/j.sdewes.d8.0349.

[35] A. Magrí, F. Béline, P. Dabert, Feasibility and interest of the anammox process as treatment alternative for anaerobic digester supernatants in manure processing – an overview, *J. Environ. Manage.* 131 (2013) 170–184, https://doi.org/10.1016/j.jenvman.2013.09.021.

[36] S. Malamis, E. Katsou, S. Di Fabio, D. Bolzonella, F. Fatone, Biological nutrients removal from the supernatant originating from the anaerobic digestion of the organic fraction of municipal solid waste, *Crit. Rev. Biotechnol.* 34 (2014) 244–257.

[37] A. Malovanyy, J. Trela, E. Plaza, Mainstream wastewater treatment in integrated fixed film activated sludge (IFAS) reactor by partial nitritation/anammox process, *Bioresource Technology* 198 (2015) 478–487, https://doi.org/10.1016/j.biortech.2015.08.123.

[38] N. Martí, R. Barat, A. Seco, L. Pastor, A. Bouzas, Sludge management modeling to enhance P-recovery as struvite in wastewater treatment plants, *J. Environ. Manage.* 196 (2017) 340–346, https://doi.org/10.1016/j.jenvman.2016.12.074.

[39] T.M. Massara, S. Malamis, A. Guisasola, J.A. Baeza, C. Noutsopoulos, E. Katsou, A review on nitrous oxide (NO) emissions during biological nutrient removal from municipal wastewater and sludge reject water, *Sci. Total Environ.* 596 (2017) 106–123, https://doi.org/10.1016/j.scitotenv.2017.03.191.

[40] C.K. Mbamba, S. Tait, X. Flores-Alsina, D.J. Batstone, A systematic study of multiple minerals precipitation modelling in wastewater treatment, *Water Res.* 85 (2015) 359–370, https://doi.org/10.1016/j.watres.2015.08.041.

[41] M. Muys, R. Phukan, G. Brader, A. Samad, M. Moretti, B. Haiden, M. Spiller, A systematic comparison of commercially produced struvite: quantities, qualities and soil-maize phosphorus availability, Sci. Total Environ. 756 (2021) 143726, https://doi.org/10.1016/j.scitotenv.2020.143726.

[42] E.V. Musvoto, M.C. Wentzel, G.A. Ekama, Integrated chemical–physical processes modelling—II. Simulating aeration treatment of anaerobic digester supernatants, Water Res. 34 (2000) 1868–1880, https://doi.org/10.1016/S0043-1354(99)00335-8.

[43] A. Muhmood, J. Lu, R. Kadam, R. Dong, J. Guo, S. Wu, Biochar seeding promotes struvite formation, but accelerates heavy metal accumulation, *Sci. Total Environ.* 652 (2019) 623–632, https://doi.org/10.1016/j.scitotenv.2018.10.302.

[44] I. Nopens, D.J. Batstone, J.B. Copp, U. Jeppsson, E. Volcke, J. Alex, P. A. Vanrolleghem, An ASM/ADM model interface for dynamic plant-wide simulation, *Water Res.* 43 (2009) 1913–1923, https://doi.org/10.1016/j.watres.2009.01.012.

[45] R. Otterpohl, M. Freund, Dynamic models for clarifiers of activated sludge plants with dry and wet weather flows, *Water Sci. Technol.* 26 (1992) 1391–1400, https://doi.org/10.2166/wst.1992.0582.

[46] G. Olsson, ICA and me – a subjective review, *Water Res.* 46 (2012) 1585–1624, https://doi.org/10.1016/j.watres.2011.12.054.

[47] M. Pijuan, J. Torà, A. Rodríguez-Caballero, E. César, J. Carrera, J. Pérez, Effect of process parameters and operational mode on nitrous oxide emissions from a

nitritation reactor treating reject wastewater, *Water Res.* 49 (2014) 23–33, https://doi.org/10.1016/j.watres.2013.11.009.
[48] M. Pocquet, Z. Wu, I. Queinnec, M. Spérandio, A two pathway model for NO emissions by ammonium oxidizing bacteria supported by the NO/NO variation, *Water Res.* 88 (2016) 948–959, https://doi.org/10.1016/j.watres.2015.11.029.
[49] W.H. Press, Numerical Recipes 3rd Edition: The Art of Scientific Computing, Cambridge University Press, New York, 2007.
[50] S.R. Qasim, G. Zhu, Wastewater Treatment and Reuse, Theory and Design Examples, Volume 1: Principles and Basic Treatment, CRC Press, Boca Raton, 2017.
[51] E. Ramin, X. Flores-Alsina, C. Gaszynski, T. Harding, D. Ikumi, C. Brouckaert, K. V. Gernaey, Plant-wide assessment of alternative activated sludge configurations for biological nutrient removal under uncertain influent characteristics, *Sci. Total Environ.* 822 (2022) 153678, https://doi.org/10.1016/j.scitotenv.2022.153678.
[52] S. Revollar, R. Vilanova, P. Vega, M. Francisco, M. Meneses, Wastewater treatment plant operation: simple control schemes with a holistic perspective, *Sustainability* 12 (2020) 768, https://doi.org/10.3390/su12030768.
[53] Á. Robles, D. Aguado, R. Barat, L. Borrás, A. Bouzas, J.B. Giménez, A. Seco, New frontiers from removal to recycling of nitrogen and phosphorus from wastewater in the Circular Economy, *Bioresource Technology* 300 (2020) 122673, https://doi.org/10.1016/j.biortech.2019.122673.
[54] G. Rodriguez-Garcia, N. Frison, J.R. Vázquez-Padín, A. Hospido, J.M. Garrido, F. Fatone, G. Feijoo, Life cycle assessment of nutrient removal technologies for the treatment of anaerobic digestion supernatant and its integration in a wastewater treatment plant, *Sci. Total Environ.* 490 (2014) 871–879, https://doi.org/10.1016/j.scitotenv.2014.05.077.
[55] C. Rosén, D. Vrecko, K.V. Gernaey, M.N. Pons, U. Jeppsson, Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink, *Water Sci. Technol.* 54 (2006) 11–19, https://doi.org/10.2166/wst.2006.521.
[56] I. Santín, M. Barbu, C. Pedret, R. Vilanova, Control strategies for nitrous oxide emissions reduction on wastewater treatment plants operation, *Water Res.* 125 (2017) 466–477, https://doi.org/10.1016/j.watres.2017.08.056.
[57] I. Santín, M. Meneses, C. Pedret, M. Barbu, R. Vilanova, Nitrous oxide reduction in wastewater treatment plants by the regulation of the internal recirculation flow rate with a fuzzy controller, *J. Water Process Eng.* 53 (2023) 103802, https://doi.org/10.1016/j.jwpe.2023.103802.
[58] V. Saravanan, T.R. Sreekrishnan, Modelling anaerobic biofilm reactors—a review, *J. Environ. Manage.* 81 (2006) 1–18, https://doi.org/10.1016/j.jenvman.2005.10.002.
[59] A.G. Sheik, E. Tejaswini, M.M. Seepana, S.R. Ambati, M. Meneses, R. Vilanova, Design of feedback control strategies in a plant-wide wastewater treatment plant for simultaneous evaluation of economics, energy usage, and removal of nutrients, *Energies* 14 (2021) 6386, https://doi.org/10.3390/en14196386.
[60] L. Shu, P. Schneider, V. Jegatheesan, J. Johnson, An economic evaluation of phosphorus recovery as struvite from digester supernatant, *Bioresource Technology* 97 (2006) 2211–2216, https://doi.org/10.1016/j.biortech.2005.11.005.
[61] S. Skogestad, Plantwide control: the search for the self-optimizing control structure, *J. Process Control* 10 (2000) 487–507, https://doi.org/10.1016/S0959-1524(00)00023-8.
[62] B. Solís, A. Guisasola, X. Flores-Alsina, U. Jeppsson, J.A. Baeza, A plant-wide model describing GHG emissions and nutrient recovery options for water resource recovery facilities, *Water Res.* 215 (2022) 118223, https://doi.org/10.1016/j.watres.2022.118223.
[63] K. Solon, X. Flores-Alsina, C.K. Mbamba, D. Ikumi, E.I.P. Volcke, C. Vaneeckhaute, U. Jeppsson, Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies, *Water Res.* 113 (2017) 97–110, https://doi.org/10.1016/j.watres.2017.02.007.
[64] C. Sweetapple, G. Fu, D. Butler, Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment, *Water Res.* 62 (2014) 249–259, https://doi.org/10.1016/j.watres.2014.06.002.
[65] I. Takács, G.G. Patry, D. Nolasco, A dynamic model of the clarification-thickening process, *Water Res.* 25 (1991) 1263–1271, https://doi.org/10.1016/0043-1354(91)90066-Y.
[66] G. Tchobanoglous, H.D. Stensel, R. Tsuchihashi, F. Burton, M. Abu-Orf, G. Bowden, W. Pfrang, Wastewater Engineering: Treatment and Resources Recovery, Metcalf and Eddy Inc., New York, 2014.
[67] N. Uri-Carreño, P.H. Nielsen, K.V. Gernaey, C. Domingo-Félez, X. Flores-Alsina, Nitrous oxide emissions from two full-scale membrane-aerated biofilm reactors, *Sci. Total Environ.* 908 (2024) 168030, https://doi.org/10.1016/j.scitotenv.2023.168030.
[68] J. Vázquez-Padín, I. Fernádez, M. Figueroa, A. Mosquera-Corral, J.L. Campos, R. Méndez, Applications of Anammox-based processes to treat anaerobic digester supernatant at room temperature, *Bioresource Technology* 100 (2009) 2988–2994, https://doi.org/10.1016/j.biortech.2009.01.028.
[69] X. Wan, J.E. Baeten, M. Laureni, E.I. Volcke, Ammonium-based aeration control improves nitrogen removal efficiency and reduces N_2O emissions for partial nitritation-anammox reactors, *Chemosphere* 274 (2021) 129720, https://doi.org/10.1016/j.chemosphere.2021.129720.
[70] P. Wu, J. Chen, V.K. Garlapati, X. Zhang, F.W.V. Jenario, X. Li, X. Zhang, Novel insights into Anammox-based processes: a critical review, *Chem. Eng. J.* 444 (2022) 136534, https://doi.org/10.1016/j.cej.2022.136534.
[71] H. Wu, C. Vaneeckhaute, Nutrient recovery from wastewater: a review on the integrated Physicochemical technologies of ammonia stripping, adsorption and struvite precipitation, *Chem. Eng. J.* 433 (2022) 133664, https://doi.org/10.1016/j.cej.2021.133664.
[72] L. Ye, J. Porro, I. Nopens, Quantification and modelling of fugitive greenhouse gas emissions from urban water systems, IWA Publishing, London, 2022. https://doi.org/10.2166/9781789060461.
[73] Q. Zhang, H. De Clippeleir, C. Su, A. Al-Omari, B. Wett, S.E. Vlaeminck, S. Murthy, Deammonification for digester supernatant pretreated with thermal hydrolysis: overcoming inhibition through process optimization, Appl. Microbiol. Biotechnol. 100 (2016) 5595–5606, https://doi.org/10.1007/s00253-016-7368-0.