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# Assessing control concepts in a full-scale partial nitration-anammox aerobic granular sludge reactor treating reject water

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**Abstract:** In this paper, a set of mathematical tools are developed and assembled to quantify, predict and virtually assess $N_2O$ emission migration strategies in partial nitritation (PN) / anammox (ANX) granular based reactors. The proposed approach is constructed upon a set of data pre-treatment methods, process simulation models, control tools (and algorithms) and key performance indicators to analyze, reproduce, and forecast the behavior of multiple operational variables within aerobic granular sludge systems (AerGSR). All these elements are tested on two full-scale data sets (#D1, #D2) collected over a period of four months (Sept-Dec 2023). Results show that data pretreatment is essential for noise reduction, filling data gaps, and ensuring smooth process simulations. The model accurately predicts (normalized RMSE< 1) multiple N oxidation states ($NH_x$, $NO_2^-$, $NO_3^-$, $N_2O$) and dissolved oxygen (DO), demonstrating its capability to describe bacterial behavior within the studied system. Special emphasis is placed on weak acid-base chemistry where pH is reliably reproduced, and it can be used for control purposes. Both biological and physico-chemical aspects are predicted at different time scales (months, days, minutes). While nitritation mainly occurred in the bulk, biofilm distribution showed inactive inner granule parts and increasing biomass (mostly ANX) towards the surface, with distinct organic concentrations. Gradients for multiple soluble compounds could also be described strongly suggesting nitrifier denitrification (ND) as the main identified $N_2O$ production pathway. The model revealed that the system was suffering from low ANX activity leading to $NO_2^-$ accumulation. The latter produced unusually high EF. The exact cause of this underperformance remains unclear—but it was assumed to be due to excessive granule size. The validation data set also yielded satisfactory results (normalized RMSE< 1). The application of different control concepts revealed the huge impact on EF on different aeration patterns. The presentation will include a discussion on transitioning from process models to digital shadows/ twins for real-time process monitoring. Additionally, it will emphasize the necessity of evaluating reject water (RW) technologies from a plant-wide perspective.
**Keywords**: Climate Change Mitigation, Data science, Digital twins, GHG emissions, Modelling, Net Zero

## Background and Relevance

This abstract summarizes the preliminary scientific outcomes resulting from the digital twining activities for one of the study-sites included within the MUDP funded project NACAT (contract-no: 2021-20015): A partial nitration / annamox aerobic granular reactor (AerGSR) treating reject water at the Ejby Mølle Water and Resource Recovery Facility (EMWRRF) in Odense, Denmark (see **Fig 1**).

## Material and Methods

A mathematical model describing chemical oxygen demand (COD), nitrogen (N) and phosphorus (P) removal is implemented one dimensional (1-d) biofilm framework formulated using spherical coordinates (**Vangsgaard et al., 2012**). The proposed approach considers the three main nitrous oxide ($N_2O$) production pathways: 1) hydroxylamine ($NH_2OH$) oxidation pathway (NN), ammonium oxidizing bacteria (AOB) nitrifier denitrification pathway (ND) and heterotrophic denitrification pathway (DEN) (**Solis et al., 2022, Flores-Alsina et al., 2025**).

The proposed approach is tested using two plant data sets corresponding to different operational periods: September-October 2023 (#D1) and November-December 2023 (#D2). Advanced data treatment routines have been developed to 1) reduce noise from sensor data by signal filtering, 2) increase the frequency of lab-data, 3) filling the gaps by extrapolation when sensor data is not available and 4) automatically adjust cationic/anionic loads to reproduce influent weak-acid base chemistry.

Different *operational strategies* are implemented to a baseline scenario based on increased pH (*S1*), $NH_x$-Based Control (*S2*), $NO_2^-$-Based Control (*S3*) and DO Limit Control (*S4*). While *S1*, *S2* and *S3*

are cascaded PI controllers where aeration is turned ON and OFF based on the sensor (pH / $NH_x$, $NO_2^-$) signals, S4 is a conventional PI-DO controller**.**

**Key Findings**

**1) Fig. 2** illustrates the results of applying advanced data science methods developed within the NACAT project. For illustrative purposes, the effects of applying filtering methods are demonstrated, resulting in a reduction of noise levels in the (influent) $NH_x$ (**B**) sensor signals. Another example is the utilization of extrapolation methods to enhance dynamics (from days to minutes) and fill in missing values for influent, alkalinity (**A**), also $NH_x$ (**B**) and $PO_4^{3-}$ (**C**) (both in sensor and lab data). Finally ionic loads have been adjusted to reflect data pH values (**D**).

**2)** Results show (**Fig. 3**) that the proposed set of tools could realistically reproduce effluent characteristics at different dynamics (days / minutes). Computer simulations also reveal that it is possible to mathematically describe the behaviour of ammonia /nitrite oxidizers (AOB / NOB) + anammox (ANX) bacteria as well as ordinary heterotrophic organism (OHO) within the studied reactor. This is reflected in the good prediction capabilities of dissolved oxygen (**A**), ammonium/a ($NH_x$), (**C**), nitrite ($NO_2^-$) (**D**), nitrous oxide ($N_2O$). The pH dynamics is accurately recreated (**B)**.

**3)** Microscopic predictions reveal that oxidation of ammonium mainly occurs in the bulk and show that the inner part of the granules is mostly inactive, with biomass increasing towards the surface (see **Fig 4**). ANX bacteria are central, while AOB and OHO are more abundant near the surface although in very low concentrations. Gradients in $NH_X$ and $NO_2^-$ indicate ANX activity, with $NO_3^-$ generated centrally. $N_2O$ production primarily comes from the AOB ND pathway, and low biodegradable organics, decreasing $NO_3^-$ gradients, and minimal OHO suggest $NO_3^-$ results mainly from ANX activity, with negligible OHO denitrification. DO levels are not suitable for the NN pathway.

**4)** The high EFs are attributed to abnormal operational conditions (see **Fig 5**). The model predicted higher ANX activity compared to what was reflected in the data. Hence, the $z_{max}$ had to be significantly increased (>2 mm) to match both $NO_2^-$ and $NO_3^-$ profiles. The latter promoted mass transfer limitations not allowing substrates (such as $NH_x$ and $NO_2^-$) penetrating within the inner layers of the granules. The validation dataset of $N_2O$ yields satisfactory results (normalized RMSE <1).

**5)** The detailed behavior of the different controllers is illustrated in **Fig 3** (light blue) and **6** (first column). It is evident how pH, $NH_x$ and $NO_2^-$ levels determine when the aeration is turned on and off and their effect on the overall N removal efficiency. Simulations reveal that higher pH forces the system to operate at a higher NHx concentration (less conversion). Options with more anoxic times (*SC3*) promoting $N_2O$ abatement suffer from loss of nitrification power

**6)** Additional simulations with a "healthier" (lower $z_{max}$, higher VSS) biomass yielded results aligned with what we would typically expect for these types of systems (see **Fig 7**)

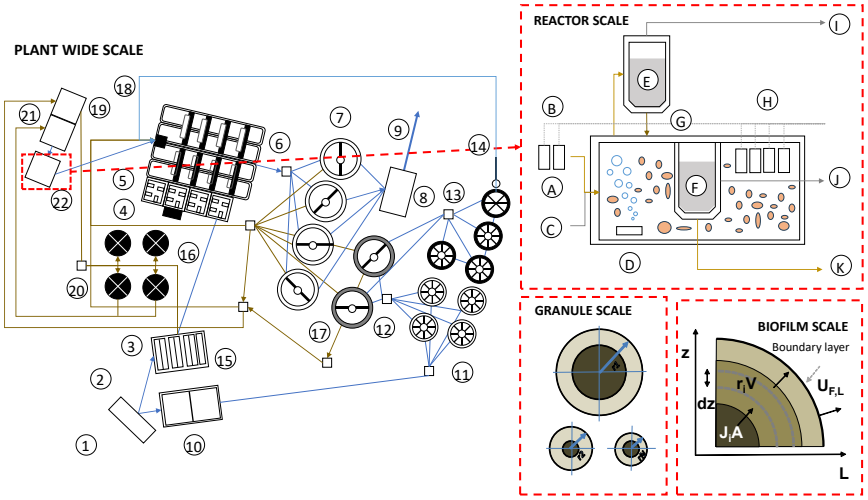


**Fig. 1**. Left: Schematic of the Ejby Mølle WRRF: 1) influent wastewater, 2) grit removal, 3) chemical enhanced primary clarification, 4) membrane aerated biofilm reactors, 5) anaerobic section, 6) oxidation ditches, 7) secondary clarifiers, 8) sand filters, 9) treated effluent,10) storm tanks, 11) trickling filer (first stage), 12) intermediate secondary clarifiers, 13) trickling filter (second stage), 14) treated effluent, 15) primary sludge, 16) thickened secondary sludge, 17) external recirculation, 18) wet weather stream, 19) primary sludge, 20) anaerobic digestion, 21) dewatering sludge (centrifuges), 22) PN/ANX units treating reject water.
Right: Schematic of the PN/ANX process: A) influent wastewater, B) influent sensor (flowrate, NHx,), C) acid-base addition for pH control (no active) l, D) bottom diffuser aeration, E) hydro-cyclone, F) internal settler, G) Anammox return, H) process sensors ($NH_x$, $NO_3$, $NO_2$, pH & $N_2O$)
Bottom: Schematic representation of the granules (left) and the mathematical representation of the biofilm within the granule

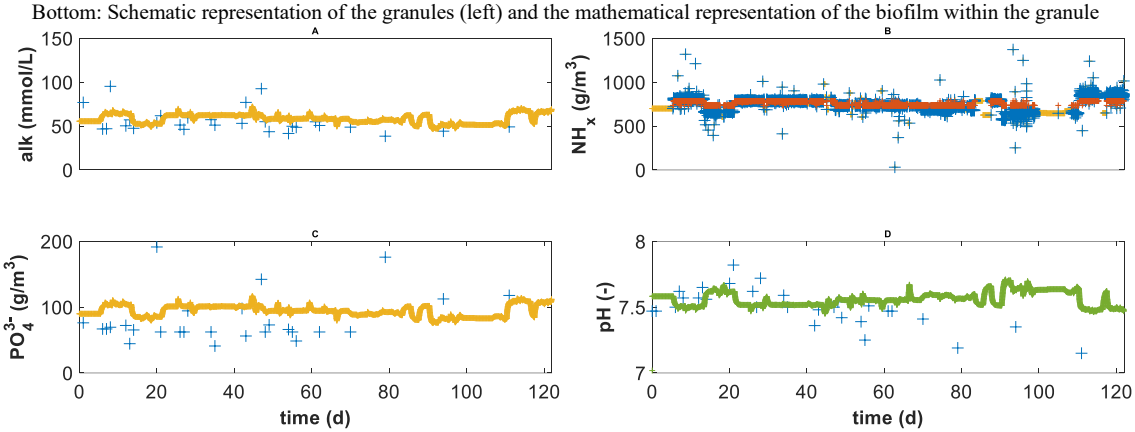


**Fig 2**. Plant measurements (+ blue) and results of data -pretreatment: filtered (+ red) / extrapolated (+ yellow) / calculated from estimated ionic composition (+green)

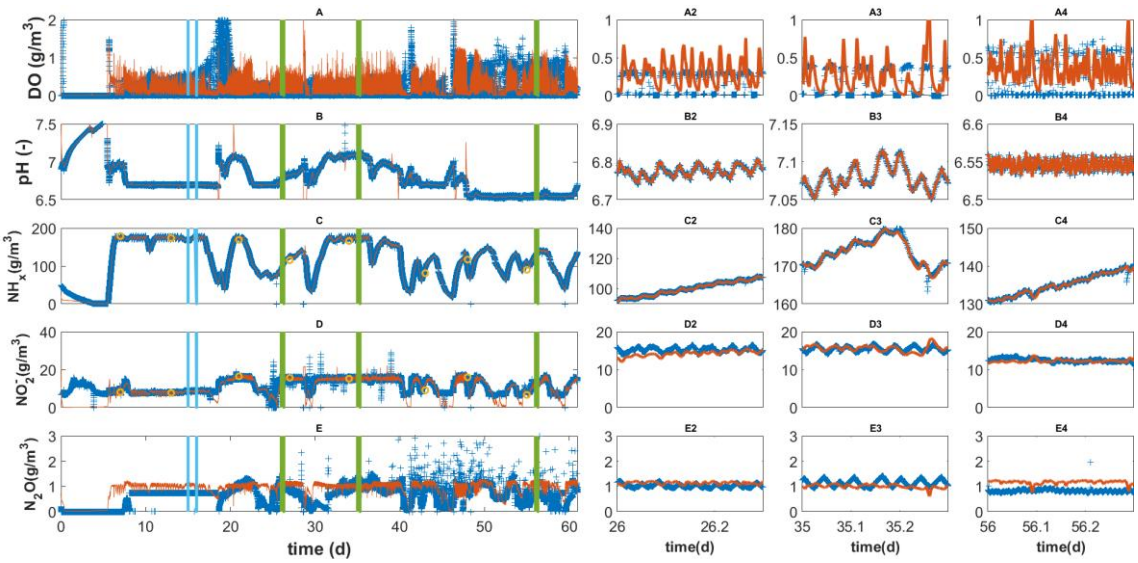


**Fig 3** Three different snapshots showing plant (+) and simulation results (red-solid lines) for #D1. Green lines represent different amplified section of the time series (= snapshots). Snapshot 1= 26.0-26.3, snapshot 2= 35.0-35.3, snapshot 3= 47.0-47.3. Blue lines indicate the part of the time series amplified in Fig 7 to compare control strategy performance.

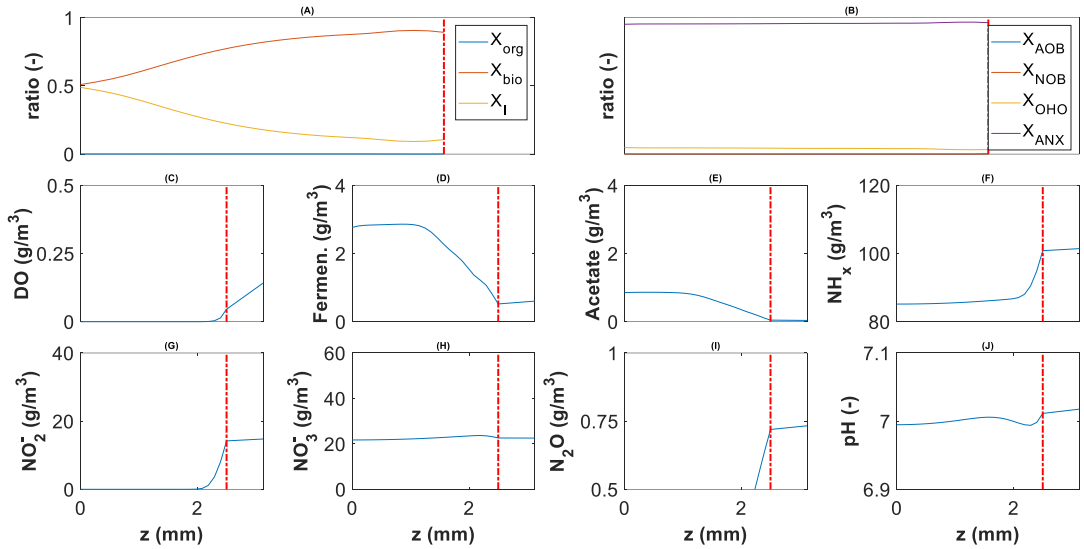


**Fig 4**. Intra-granule model prediction of COD distribution, bacterial composition, and gradients (#D1)

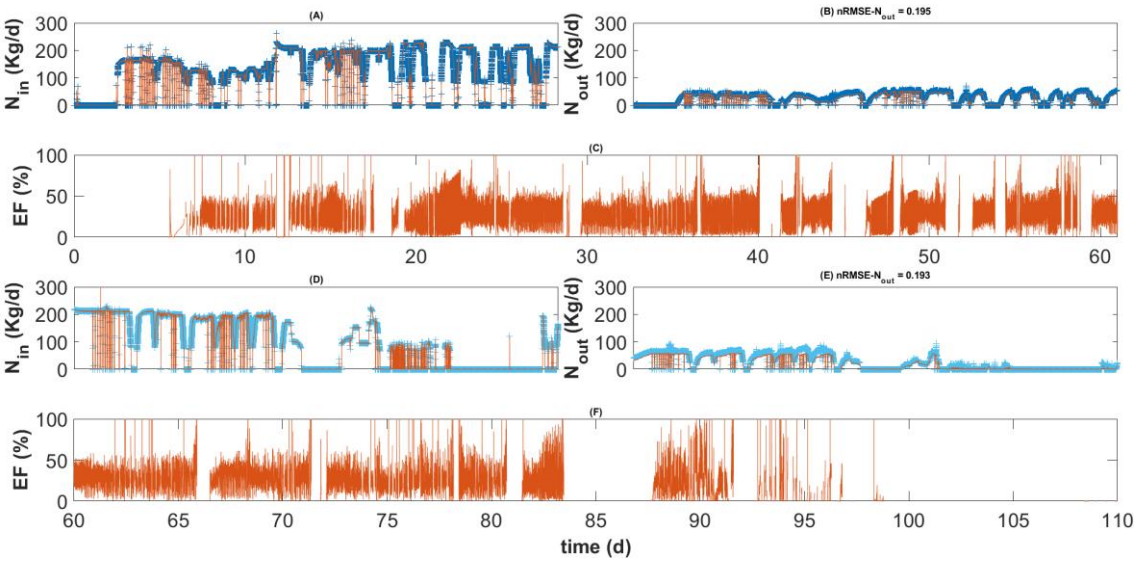


**Fig 5.** Input (A, D) and output (B, E) N load. Calibration (A, B) and validation (D, E) plant data sets (+) are represented in dark and light blue respectively. Simulation results (red-solid lines). Emission factors are calculated from the transfer model and based on the $N_2O$ measurements. X axis units for A and B are the same for C. X axis units for D and E are the same for

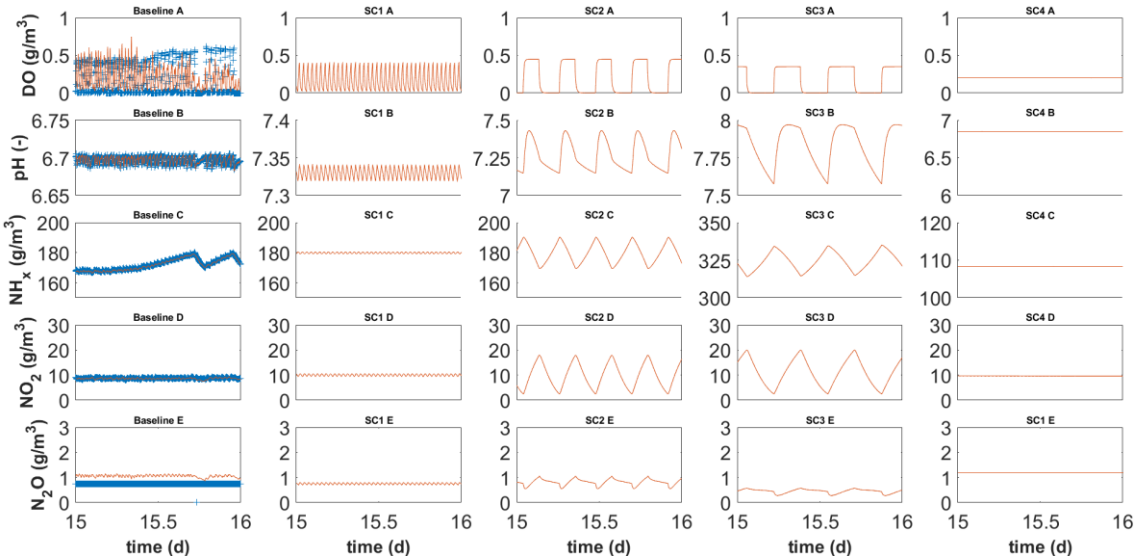


**Fig 6.** Snapshots extracted from #D1 showing plant (+) and simulation results (red-solid lines) (column 1) (see Figure 3, blue lines). The results of implementing the control strategies summarized in **Fig 7**.

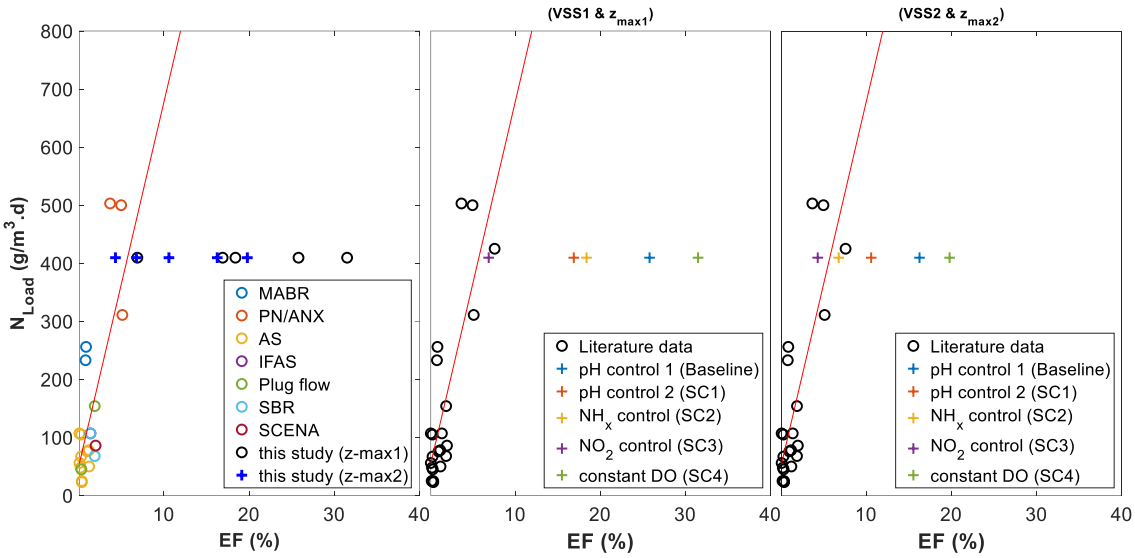


**Fig 7.** Comparison of the correlation between emission factors and N load for literature data and the results obtained in this study (column 1 = detailed literature data + results in this study, column 2 = literature data + first set of simulations, column 3 = literature data +second set of simulations)

## References

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Solis et al., 2022**. Water Research.** 215:118223
Vangsgaard et al., 2012. **Bioresour Technol**. 123. 230-41.