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Modeling and Simulation of Full-Scale Sequential Batch Reactor Biological Process Using GPS-X

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Abstract: Sequencing Batch Reactors (SBR) are effective for treating reject water and high-strength industrial wastewater. The Knardalstrand wastewater treatment plant in Porsgrunn recently upgraded the plant with two full-scale SBRs with volumes of 115 m³ and 100.4 m³, focusing on simultaneous nitrification and denitrification. This project aimed to model and simulate these processes using GPS-X software to optimizes the municipal wastewater treatment. Two SBR models – simple and advanced – were developed for ammonia nitrogen (NH_4-N) removal. Results indicated that the advanced model outperformed the simple model, achieving a 75% nitrogen removal efficiency at a dissolved oxygen (DO) setpoint of 1.5 mg/L through shortcut partial nitrification-denitrification. The advanced SBR model's ammonia removal efficiency through nitrification increased with an increase in dissolved oxygen (DO) concentration. In all the simulations there was high nitrite (NO_2^-) accumulation in the reactors, which could be due to the partial nitrification coupled with denitrification. The simulation has showed the presence of a simultaneous nitrification-denitrification process in the full-scale SBR plant. Enhancing model accuracy with quality data and optimizing DO levels can significantly reduce operational energy costs.

Keywords: GPS-X, Sequential Bach Reactor, Nitrification, Denitrification, model, Simulation.

1. Introduction

The need for efficient wastewater treatment systems is driven by the rapid growth of world's population, urban development and industrialization (Naidoo and Olaniran, 2013; Singh et al., 2023). Wastewater often has high organic, nitrogen and phosphorus contents and when these wastewater constituents are discharged to water bodies without efficient treatment the consequences can have serious ecological effects (Kesari et al., 2021; Singh et al., 2023). High concentrations of nitrogen and phosphorus in discharged wastewater can lead to eutrophication, resulting in significant blooms of planktonic algae or phytoplankton. This algal blooming increases the quantity of organic matter in the water body and result in depletion of oxygen content in the water. The process of eutrophication can have disastrous impacts in the aquatic ecosystem where certain species may perish because the dissolved oxygen (DO) content in water drops below a critical level (Bhagowati and Ahamad, 2019).

Wastewater treatment technologies have been developed to handle the complex organic and nutrient pollutants and meet the discharge regulatory requirements. The Sequential Batch Reactor (SBR) is one of these novel technologies that has shown to be an effective and flexible method to remove organics and nutrients from wastewater (Azeez et al., 2023). The broad use of SBR system in both municipal and industrial context has been driven by its flexibility to change influent characteristics, high treatment efficiency, small areal footprint, and low energy use (Fernandes et al., 2013).

The SBR processes has mainly five phases (Fig. 1). The first is ***Fill phase*** where raw wastewater is the influent to SBR. The second is ***React phase*** where dissolved oxygen (DO) and mixing starts in SBR process. The third is ***Settle phase*** where the activated sludge is separated from the liquid by the process of settling. The fourth is ***Draw phase*** where clear supernatant is removed using a decanter, and fifth is ***Idle phase*** where a sludge wasting process.

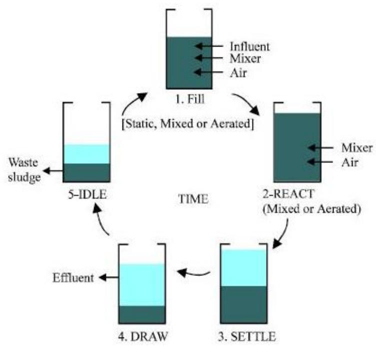

Fig. 1 The five phases of SBR operation for the one cycle periods of fill, react, settle, draw and idle (Irvine and Ketchum, 2004).

Modeling and simulation of full-scale SBR is vital to understand the plant process and control of important process parameters. Several models have been applied in SBR process specially using the activated sludge model (ASM) (Man et al., 2017; Zhou et al., 2013). However, few works have been done in SBR modeling and simulation using a GPS-X modeling platform. GPS-X is a modeling and simulation program, especially for planning and optimizing large-scale or full-scale treatment plants and processes. The biological, chemical, and physical unit activities of wastewater treatment processes can be built into sophisticated models by the software and simulated under different operating situations. In addition, GPS-X provides an extensive library of pre-defined process models and kinetic equations that may greatly accelerate modeling and serve as a strong basis for dynamic simulation and real-time data integration.

For modeling and simulation of full-scale wastewater treatment plants, GPS-X was applied in the simulation of nitrogen removal, to optimize textile wastewater decision support, for energy consumption and cost minimization of full-scale wastewater treatment plants (Cao et al., 2021; Sadri Moghaddam and Pirali, 2021; Sean et al., 2020; Sid et al., 2017; Wondim et al., 2023). The input data and parameters have significant impact on the accuracy of the simulation outcomes, even though the GPS-X program uses sophisticated mathematical methods and simulation techniques. Hence, validation of the model output with the actual data is vital (Cao et al., 2021; Dolatshah et al., 2024; Łagód et al., 2019). In general GPS-X is a useful tool with an intuitive interface and an extensive library of process models for modeling and simulating wastewater treatment processes in SBR.

Therefore, the aim of this study was to model and simulate the two full-scale SBR plant at Porsgrunn wastewater treatment plant, Norway. The result of the modeling result aims to support process control decisions system and treatment efficiency of SBR for a robust wastewater treatment reactor with small areal footprint and energy use.

2. Materials and Methods

2.1 Simple SBR model setup in GPS-X

The model environment in GPS-X has several unit process objects available for the SBR. The simple SBR model unit has a fixed order of phases, and the user can determine the duration of these phases. The model is simplified and focuses on the side stream treatment using the SBR unit. Therefore, the model only consists of the SBR unit and its inflows and outflows (Fig. 2). The influent flow of the real SBR was a combination of the reject water and the water from thickener. The reject water and its influent characteristics are listed below in table 1, together with the default values in GPS-X. The physical characteristics the full-scale SBR was working volume of 115 m^3, a max water filling height of 4.1 m and a reactor surface area of 28.05 m^2. The simulation was set to simulate for 30 days by setting the stopping time to 30.0 [d] in the GPS-X simulation setup, with a communication interval set to 0.05 [d]. The wastewater temperature was set to 28 °C with a set pH value to 7.7.

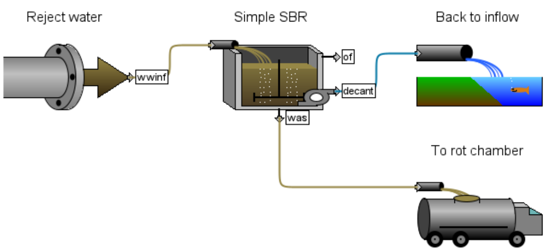

Fig. 2 The model environment of the SBR model in GPS-X with the corresponding side streams reject water influent, effluent and model objects.

2.2 Advanced SBR model setup in GPS-X

To implement a model that is more representative to the real SBR at Knarrdalstrand wastewater treatment plant (WWTP), the advanced SBR model unit in GPS-X was used. The advance model unit allows for more freedom in parameter setup, order and number of phases. Additionally, it allows to decide the phase conditions in terms of aeration, mixing, settling and flowrates. The physical characteristics of the advanced SBR model is identical to the simple SBR model. The aeration set up was using a dissolved oxygen (DO) controller with a proportional-integral-derivative (PID)controller type in velocity form having a derivative kick protection turned off. Fifteen operating phases different in duration (minutes), mixing and DO (mgO_2/L) concentration were setup.

The Knardalstrand WWTP includes more physical, chemical and biological process unit objects. The new process unit objects include a grit chamber, Ferric chloride addition for coagulation, sedimentation tank, thickener, anaerobic digestion (AD) reactor, centrifuge, and buffer tanks. The buffer tanks control the inflow rate since the full-scale SBR did not receive a continuous inflow. Hence, the advanced model environment was developed based on the real WWTP at Knarrdalstrand including the SBR, centrifuge and thickener (Fig. 3).

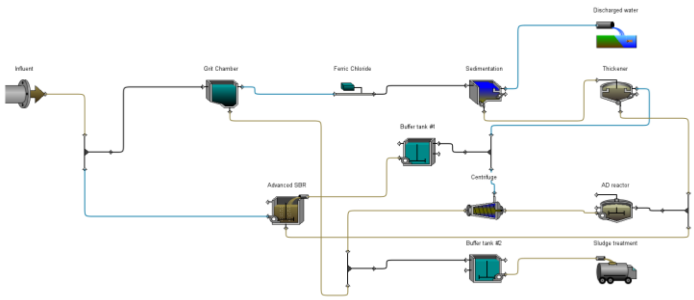

Fig. 3 The model environment of the advanced SBR model in GPS-X with all physical, chemical and biological process unit objects in the main and side streams.

2.3 Equation for nitrogen removal efficiency

The nitrogen removal efficiency in the advanced SBR model was calculated based on the total nitrogen mass balance. It assumed nitrogen is only removed as nitrogen gas through denitrification not other biological processes such as anaerobic ammonium oxidation (ANAMMOX). Therefore, the nitrogen removal efficiency was calculated using equations (1)-(3) (Pathak et al., 2022).

Reject water from AD is commonly characterized for high ammonium nitrogen concentration (568 ±76.7 mg/L) due to mineralization of organic nitrogen, protein degradation, location of nitrification and concentration effect during dewatering. In equation 2 ammonium nitrogen considered as the primary nitrogen species entering to the SBR. In the SBR, nitrification is the major process for the biological oxidation of ammonia into nitrite and nitrate. Besides the ammonium nitrogen, nitrite nitrogen and nitrate nitrogen considered in equation 3 are major nitrogen species in the SBR effluent (Noutsopoulos et al., 2018;).

$$Nitrogen\ Removal\ Efficiency\ (\%) = \frac{C_{N_{in}} - C_{N_{out}}}{C_{N_{in}}} \qquad (1)$$

Where:

$$C_{N_{in}} = C_{NH_4^+{}_{in}} \qquad (2)$$

$$C_{N_{out}} = C_{NH_4^+{}_{out}} + C_{NO_3^-{}_{out}} + C_{NO_2^-{}_{out}} \qquad (3)$$

Table 1. The influent reject water characteristics used for both simple and advanced SBR model and simulation.

Parameter	Default value	Measured value
Total COD	430 $gCOD/m^3$	2500 $gCOD/m^3$
Ammonia nitrogen	25 gN/m^3	600 gN/m^3
TKN*	40 gN/m^3	685 gN/m^3
Total phosphorus	10 gP/m^3	13 gP/m^3
pH	7	7.7
Temperature	20 ºC	28 ºC

*TKN is total Kjeldahl nitrogen which includes organic nitrogen and total ammonia nitrogen

3. Results and Discussion

3.1 Simulating the Simple SBR model

The simple SBR model was used to simulate ammonia removal from the reject water with influent characteristics described in table 1. Figure 4 shows the SBR influent and effluent flow balance for three cycles.

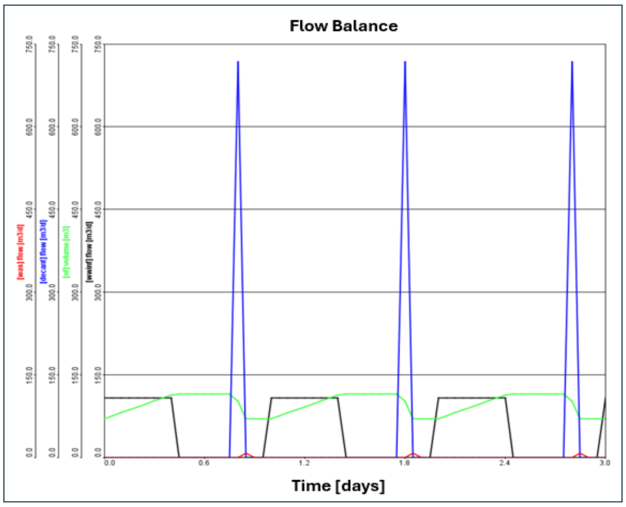

Fig. 4 The simulation environment in GPS-X with the influent and effluent flow balance of the simple SBR model. The plotted black line is the influent flow, the blue plotted line being the effluent (decant) flow and the red plotted line is the sludge waste flow. The green line is the hydraulic volume of the SRR.

The 30-days simulations of the simple SBR model have shown that the average effluent concentrations ammonia nitrogen concentration was 228 mgN/L and the average ammonia removal efficiency found was 62% (Fig. 5). The accumulation of nitrite in the effluent (Fig. 6) could be due to the partial nitrification (PN) where the ammonium oxidizing bacteria (AOB) are dominant over the nitrite oxidizing bacteria (NOB) and the nitrite concentration increases (Duan et al., 2020). The median growth rates for AOB and NOB at 20 °C are 0.74 and 0.65 d^{-1}, respectively. PN is common in SBR as well as operational parameters such as DO, temperature and pH significantly favors PN in SBR (Liu et al., 2020).

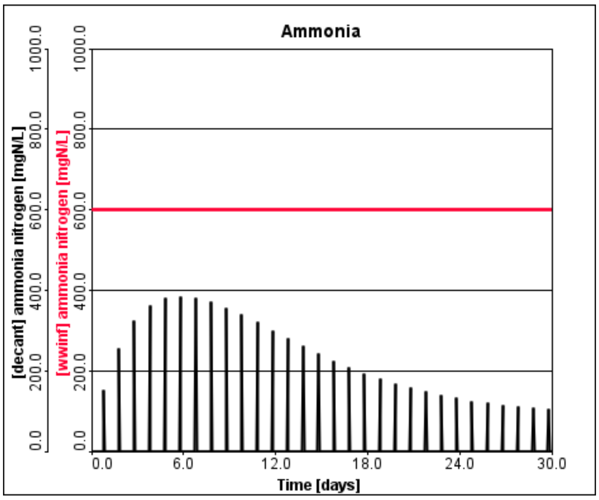

Fig. 5 Simulation of ammonia removal in SBR. The constant influent concentration of ammonia (red line) and the effluent ammonia concentration (black). Simulation was done at DO setpoint of 2.0 mg/L.

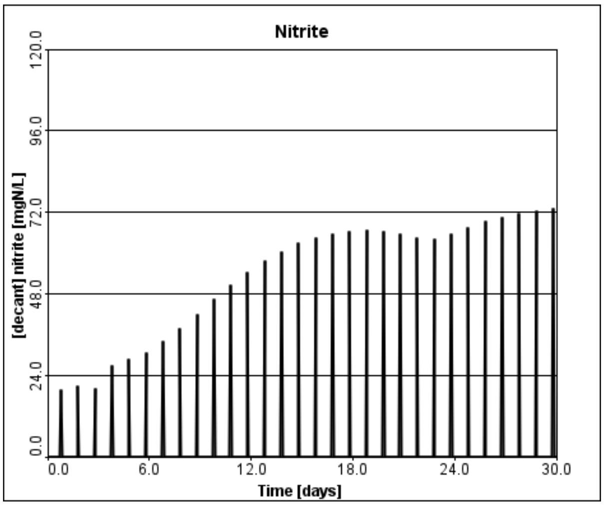

Fig. 6 Simulation ammonia removal where the nitrite [mgN/L] concentration in effluent. Simulation was done at DO setpoint of 2.0 mg/L.

3.2 Simulating the advanced SBR model

The flow balance in the SBR was setup in the simulation environment in such a way that the advanced SBR model was operating according to the cycle settings of fifteen phases different in duration (minutes), mixing and DO (mgO_2/L) concentration were setup. Figure 7 depicts the influent, effluent and sludge wasting flow balance simulated for 3 cycles.

The advanced SBR model was simulated for 30-days with influent ammonia concentration of 600 mgN/L. The average concentration effluent ammonia was 6 mgN/L with ammonia removal efficiency above 90% for all DO concentration setpoints simulated (Fig. 8). Furthermore, the nitrite concentrations in the effluent reach the highest concentration during the third cycle at 222 mgN/L and then after it was decreased and stabilized (Fig. 9).

The advanced SBR model was more accurate replication of the real SBR at Knarrdalstrand WWTP. Where in the model development in the flow balance was successfully set up in the simulation environment to match with the SBR at Knarrdalstrand WWTP with all phases of the cycle. The real plant has an average ammonia removal efficiency of approximately 85%. The simulation result of the advanced SBR model predicted higher with a small margin than the treatment efficiency of the real SBR at Knarrdalstrand WWTP. This was expected when the simulated environment has been considered without disturbance from external factors. However, the advanced SBR model can be improved to the real reactor by experimentally determining the physical characteristics of the reject wastewater and by calibration of the model key process parameters (Sadri Moghaddam and Pirali, 2021).

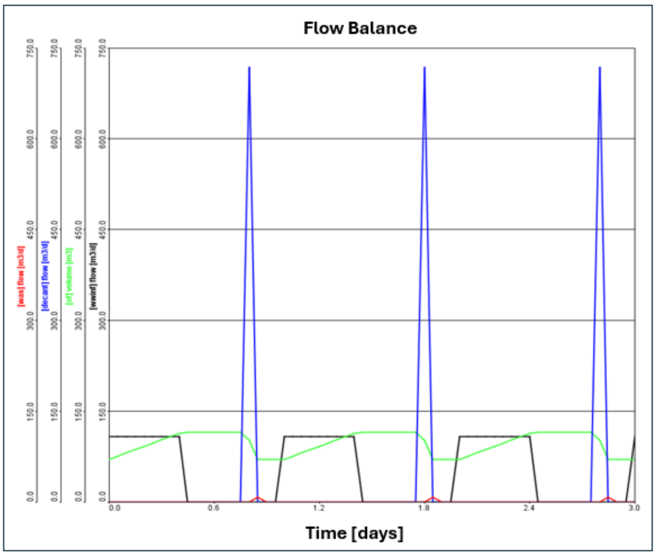

Fig. 7 The flow balance of the advanced SBR model. The black line is the influent flow, the blue line is the decant flow and the red is the waste flow. The green plotted line shows the hydraulic volume of the reactor.

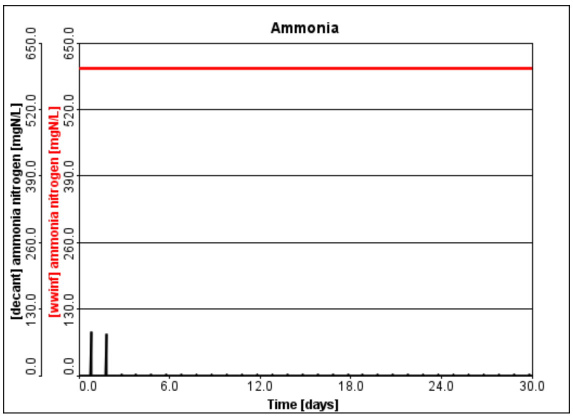

Fig. 8 Simulation of ammonia removal in advanced SBR model. The constant influent concentration of ammonia (red line) and the effluent ammonia concentration (black). Simulation was done at DO setpoint of 2.0 mg/L.

The presence of high concentration of nitrite in the effluent has shown that there was partial nitrification. This indicates that not all of the nitrite has been converted to nitrate where the dominant species in the biological process were the ammonia oxidizing bacteria (AOB) (van Niel et al., 1992).

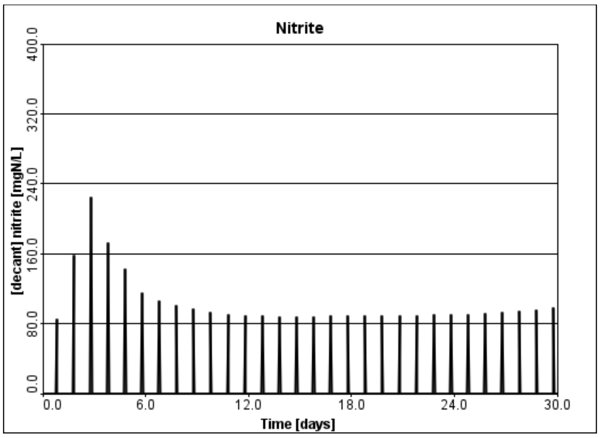

Fig. 9 Simulation of the effluent concentration of nitrite [mgN/L] in the advanced SBR model. Simulation was done at DO setpoint of 1.5 mg/L.

3.3 Simulation of different aeration setpoints in the advanced SBR model

To investigate the impact of dissolved oxygen (DO) concentration on nitrification and denitrification in the advanced SBR model, simulations were done using three DO setpoints. Optimizing the amount of DO required for ammonia removal presents a significant opportunity to minimize operational costs in wastewater treatment by reducing the energy expenses (Sean et al., 2020; Sid et al., 2017).

Particularly, the advanced SBR model has greater flexibility in its aeration settings than the simple model. It allowed to aerate the model more closely to the real SBR at Knarrdalstrand WWTP. Hence, it was able alternate between aerating at 2.0 mg/L DO during the aeration phases and 0.6 mg/L DO during mixing phases. This improved the ammonia removal efficiency from 62% in the simple SBR model to 95% in the advanced SBR model.
The result of the advanced model was validated from the real data from the Knarrdalstrand WWTP. For instance, the ammonia concentration of influent reject water and the effluent decant flow of the real WWTP at Knarrdalstrand was 367.3 mgN/L and 52.3 mgN/L, respectively. Based on these the average ammonia removal efficiency was approximately 85% where the model predicted 10% higher efficiency. Furthermore, the advanced SBR model can be improved to the real reactor by experimentally determining more influent characteristics of the reject and thickener water as well as parameters related with the physical characteristics of the real reactor.

Moreover, the average ammonia removal efficiency of the advanced SBR model simulation at 1.5 mg/L and 1.0 mg/L DO setpoints while maintaining 0.6 mg/L DO setpoint during mixing was 94% and 90%, respectively. Although these are averaged values of the ammonia removal efficiency, the overall trend for all these DO scenarios was reduced efficiency in the first few cycles before it eventually stabilized at higher efficiencies. Our simulation shows that the main difference observed between the model running at the different DO setpoints were the amount of time the model needs to stabilize. The simulation at 2.0 mg/L DO had the lowest time needed for the model to stabilize with only two cycles. Whereas the simulation at 1.5 mg/L DO and 1 mg/L DO have taken three and five cycles to stabilize, respectively. Study reported that different DO concentrations have shown effect on the long-term stability of partial nitrification process at room temperature. Where AOB activity was significantly higher than NOB activity at DO of 2.5 mg/L (Cui et al., 2020). Table 2 summarizes the simulation results of the three DO setpoints in the advanced SBR model.

Table 2 The simulation result in the three DO simulated with the advanced SBR model. The average ammonia concentration in the effluent, average ammonia removal efficiency, the average COD concentration in the effluent and the average COD removal efficiency for all scenarios.

DO setpoint (mg/L)	Av. Effluent ammonia (mg/L)	Av. Ammonia removal efficiency (%)	Av. Effluent COD (mgCOD/L)	Av. COD removal efficiency
2.0	5.9	95	123	95
1.5	9.9	94	123	95
1.0	19.9	91	123	95

When compared with the influent ammonia concentration of 600 mgN/L, the ammonia concentration in the effluent were significantly lower in all DO setpoint scenarios. Moreover, the presence of high nitrite concentration than nitrate in the effluent has shown there was partial nitrification. The simulation at 2.0 mg/L DO had an effluent with high concentration of nitrite and with small concentration of nitrate. The average concentration of nitrite and nitrate were 102 mgN/L and 23 mgN/L, respectively. Hence, this indicates that not all of the nitrite has been being converted to nitrate through nitrification where the process was partial nitrification (Duan et al., 2020). Partial nitrification is common in SBR reactors when operation parameter such as DO, pH and temperature favors the process (Liu et al., 2020). Moreover, in the partial nitrification the dominant species in process are AOB that has higher bacterial growth rate (Liu et al., 2020; van Niel et al., 1992). The growth of NOB was decreasing with each cycle, while the growth AOB as well as the denitrifies remained stable and dominated in the process. Studies shows that the NOB suppression occurring due to nitrite competition between NOB and denitrifiers instead of oxygen competition (Xu et al., 2021).

The analysis of nitrogen removal efficiency through denitrification based on the nitrogen mass balance (equation 1-3) as well as the simulation result of nitrification and denitrification rates (Fig. 10) strongly confirm that denitrification process has occurred in the SBR. From the nitrogen mass balance analysis, the nitrogen removal efficiency through denitrification in the advanced SBR model simulated with 2.0 mg/L DO was 72%. Which means that 72% of the influent ammonia across the 30-day simulated period has been converted to nitrogen gas (N_2) through the denitrification process. Comparatively, simulations conducted with 1.5 and 1.0 mg/L DO setpoints had the nitrogen removal efficiency of 75% and 72% through denitrification, respectively. The results were not significantly different, although simulations with the 1.5 mg/L DO setpoint had higher amount of nitrogen removed through denitrification. Since denitrification is anoxic process it is known that denitrifying bacteria (heterotrophs) thrive best in anoxic conditions (Song et al., 2021).

Moreover, simultaneous nitrification and denitrification (SND) is an advantageous bioprocess that allows the complete removal of ammonia nitrogen (Di Capua et al., 2022; Janka et al., 2022). From the nitrogen mass balance study and the simulation result it can be concluded that nitrification and denitrification process occurred in the Knardalstrand WWTP SBR and the process is the SND process.

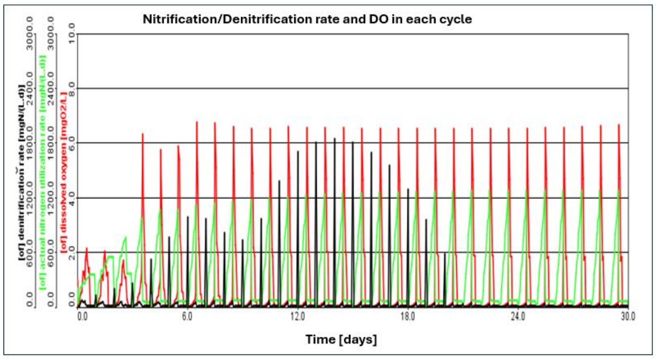

Fig. 10 The simulation of denitrification and nitrification rates for 30-days simulation period in the advanced SBR model at DO 2.0 mg/L

Hence, in the SND process, there is a huge possibility to reduce the carbon and energy consumption with a simultaneous removal of both nitrogen and phosphorus. In general, SND is cost-effective due to low DO and energy requirements (Di Capua et al., 2022; James and Vijayanandan, 2023).

3.4 Energy cost reduction

GPS-X allow for wastewater treatment plant operational cost estimation in the model and simulation environment (Sadri Moghaddam and Pirali, 2021; Sean et al., 2020; Sid et al., 2017). Therefore, simulation was done at different DO setpoints to investigate the energy requirement of the SBR model. In full-scale wastewater treatment plant, the major cost of the treatment process is aeration, which occupies 49% the operational cost (Pryce et al., 2022). In our simulation, the cost estimation was based on the use of blower only. The study found that the cumulative energy required for the blower running at 2 mg/L DO setpoint over 30 days simulation period was 1641 kWh. In the model the energy cost of 1 kWh was assumed 0.1$ which resulted in the cumulative energy cost for the SBR blower was 164.1$.

When further simulations were conducted with the DO setpoints 1.5 mg/L and 1 mg/L, respectively. The cumulative energy required for the blower operating at 1.5 mg/L DO setpoint for 30 days simulation period was 1512 kWh. With the same energy cost the cumulative energy cost for the blower has reduced to 151.2$ which was 7.8 % energy cost reduction. For the blower operating at 1 mg/L DO setpoint for 30 days simulation period, the cumulative energy required was 1378 kWh which has reduced the energy cost to 137.8$ which was 16% energy cost reduction.

Hence, the energy cost reduction simulated at different DO setpoint has shown that there is a substantial opportunity to reduce the energy cost of full-scale SBR plant. The overall operation cost can be minimized by optimizing the amount of DO used for the SBR process, while maintaining the treatment efficiency. Our simulation study showed that switching the blower operation from 2 mg/L to 1.5 mg/L DO saves approximately 12% energy cost, yearly. However, the choice should be compensated with the process efficiency in removing nitrogen and organics constituents in the wastewater. For instance in similar study optimization of the SBR model process parameters such as optimum air flow into the aeration tank saved 91.5% of energy in the process that enable decision makers for the best course of action (Wondim et al., 2023).

4. Conclusions

The biological process in SBR can be model and simulated using the GPS-X software. In this study SBR models have been developed for ammonia removal of the reject water at Knarrdalstrand WWTP. The advanced SBR model in GPS-X was found to be the most robust and efficient model that predicted the actual process condition of the real SBR at treatment plant. However, the advanced SBR model with the complete wastewater treatment process units needs more validation work to improve the model accuracy. Even though, the SBR model environment developed in GPS-X functions properly regarding aeration cycle and phase operations.

The advanced SBR model simulation with a DO setpoint of 2.0 mg/L has shown the highest average ammonia removal efficiency while the efficiency decreased slightly as the DO setpoint decreased. The simulated three DO setpoint scenarios and simulation of nitrification and denitrification in the advanced SBR model has shown that DO at 1.5 mg/L had the higher nitrogen removal efficiency through denitrification.

Generally, the model validation shows that the advanced SBR model was more effective in ammonia removal with a little higher than the ammonia removal efficiency of the real full-scale SBR plant at Knarrdalstrand. Hence, further research on sufficient data on reject waster physical and biochemical characteristics and accurate assumptions of the physical characteristics of the real SBR is vital to make the model more representative and robust in the predictive capability. Furthermore, sensitivity analysis of model parameters with different operational settings i.e. dissolved oxygen levels, pH, sludge retention time, and temperature are needed. Further work is also needed to optimize energy consumption.

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