

## Innovations in Wastewater Treatment – Harnessing Mathematical Modeling and Computer Simulations with Cutting-Edge Technologies and Advanced Control Systems

Jakub Drewnowski<sup>1</sup>, Bartosz Szela<sup>2</sup>, Fabrizio Sabba<sup>3</sup>, Magdalena Piłat-Rożek<sup>4</sup>, Adam Piotrowicz<sup>5\*</sup>, Grzegorz Łagód<sup>6</sup>

<sup>1</sup> Department of Sanitary Engineering, Faculty of Civil and Environmental Engineering, Gdansk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland

<sup>2</sup> Department of Hydraulics and Sanitary Engineering, Institute of Environmental Engineering, Warsaw University of Life Sciences – SGGW, ul. Nowoursynowska 159 02-797 Warsaw, Poland

<sup>3</sup> Black & Veatch, 11401 Lamar Ave, Overland Park, KS 66211, USA

<sup>4</sup> Department of Applied Mathematics, Faculty of Fundamentals of Technology, Lublin University of Technology, ul. Nadbystrzycka 38, 20-618 Lublin, Poland

<sup>5</sup> Department of Environmental Protection Engineering, Faculty of Environmental Engineering, Lublin University of Technology, ul. Nadbystrzycka 40B, 20-618 Lublin, Poland

<sup>6</sup> Department of Water Supply and Wastewater Disposal, Faculty of Environmental Engineering, Lublin University of Technology, ul. Nadbystrzycka 40B, 20-618 Lublin, Poland

\* Corresponding author's email: [a.piotrowicz@pollub.pl](mailto:a.piotrowicz@pollub.pl)

### ABSTRACT

The wastewater treatment landscape in Central Europe, particularly in Poland, has undergone a profound transformation due to European Union (EU) integration. Fueled by EU funding and rapid technological advancements, wastewater treatment plants (WWTPs) have adopted cutting-edge control methods to adhere to EU Water Framework Directive mandates. WWTPs contend with complexities such as variable flow rates, temperature fluctuations, and evolving influent compositions, necessitating advanced control systems and precise sensors to ensure water quality, enhance energy efficiency, and reduce operational costs. Wastewater mathematical modeling provides operational flexibility, acting as a virtual testing ground for process enhancements and resource optimization. Real-time sensors play a crucial role in creating these models by continuously monitoring key parameters and supplying data to predictive models. These models empower real-time decision-making, resulting in minimized downtime and reduced expenses, thus promoting the sustainability and efficiency of WWTPs while aligning with resource recovery and environmental stewardship goals. The evolution of WWTPs in Central Europe is driven by a range of factors. To optimize WWTPs, a multi-criteria approach is presented, integrating simulation models with data mining methods, while taking into account parameter interactions. This approach strikes a balance between the volume of data collected and the complexity of statistical analysis, employing machine learning techniques to cut costs for process optimization. The future of WWTP control systems lies in “smart process control systems”, which revolve around simulation models driven by real-time data, ultimately leading to optimal biochemical processes. In conclusion, Central Europe’s wastewater treatment sector has wholeheartedly embraced advanced control methods and mathematical modeling to comply with EU regulations and advance sustainability objectives. Real-time monitoring and sophisticated modeling are instrumental in driving efficient, resource-conscious operations. Challenges remain in terms of data accessibility and cost-effective online monitoring, especially for smaller WWTPs.

**Keywords:** wastewater treatment, mathematical modelling, data mining, artificial intelligence, multi-criteria approach, control strategies.

## INTRODUCTION

After joining the European Union (EU), Poland and several other Central European nations embarked on a monumental transformation of their wastewater treatment plants (WWTPs). This extensive overhaul extended beyond equipment and device replacement, incorporating cutting-edge technological solutions that epitomized the forefront of wastewater treatment innovation. This ambitious modernization initiative found its impetus in a dual force – the availability of EU funding opportunities and the rapid evolution of pioneering projects and technologies within the wastewater treatment sector. Consequently, this catalyzed the adoption of state-of-the-art control methods in WWTPs, not confined to Poland but cascading across neighboring nations in the region. This shift carries immense significance, chiefly in its imperative to align with and satisfy the rigorous mandates delineated in the European Union Water Framework Directive [European Commission, 2023].

The operation of wastewater treatment plants inherently unfolds within a complex realm, susceptible to a myriad of external and internal disruptions. These disruptions, characterized by variable flow intensity, temperature fluctuations, dynamic concentration levels, and fluctuating influent compositions, underscore the pressing need for specialized solutions in this domain [Revolzar et al., 2017]. Consequently, the adoption of increasingly sophisticated measurement devices, complemented by advanced control and automation systems, has emerged as a pivotal aspect of modern wastewater treatment processes [Chauhan et al., 2022]. This step is not solely geared towards meeting stringent wastewater quality standards; it is equally driven by the pursuit of heightened energy efficiency and the curtailment of operational costs. In recent times, the wastewater treatment landscape has undergone a profound transformation driven by the visionary principle of “self-sufficiency”. This paradigm shift places a strong emphasis on extracting biogenic and other valuable chemical compounds from wastewater [Battista et al., 2020], transcending the constraints of conventional treatment approaches. It has introduced the innovative concept of “Water Resource Recovery Facilities” [Zhang et al., 2020], redefining the objectives of wastewater treatment to not only purify water but also recover valuable resources. At the heart of this transformative journey lies

the growing reliance on wastewater mathematical modeling. This powerful tool allows wastewater treatment facilities to operate with unprecedented precision, optimizing processes, conserving resources, and achieving sustainable outcomes. Wastewater mathematical modeling entails the creation of intricate mathematical representations of the treatment processes, taking into account the myriad variables that influence wastewater composition and quality.

The integration of real-time sensing, data analysis, and dependable online parameter control, all facilitated by mathematical models, has become integral to contemporary wastewater treatment systems. Real-time sensors continuously monitor key parameters such as flow rates, chemical concentrations, and water quality indicators. This data is then fed into sophisticated mathematical models that predict how the treatment processes will respond to changing conditions. These predictions empower operators to make informed decisions in real-time, adjusting treatment parameters and chemical dosages as needed to maintain optimal performance. One of the primary advantages of wastewater mathematical modeling is its ability to anticipate and mitigate significant process fluctuations and malfunctions. By simulating different scenarios and predicting potential issues, operators can proactively address problems before they escalate, minimizing downtime and costly repairs. This predictive capability is crucial for ensuring the reliability and efficiency of wastewater treatment plants.

Moreover, wastewater mathematical modeling enhances the dexterity of technological operations. It provides a virtual testing ground for experimenting with process improvements and optimizing resource utilization. This means that wastewater treatment plants can continually fine-tune their operations to achieve the highest levels of efficiency and sustainability. In essence, the integration of wastewater mathematical modeling represents a significant leap forward in the field of wastewater treatment. It empowers treatment facilities to not only meet regulatory requirements but also extract valuable resources from wastewater, thereby aligning with the principles of sustainability and self-sufficiency. As this transformative paradigm continues to gain momentum, wastewater mathematical modeling will remain an indispensable tool in shaping the future of wastewater treatment, ensuring that these systems reach their full potential in terms of efficiency, resource



recovery, and environmental stewardship [Solon et al., 2017; Sabba et al., 2023]. The evolution of wastewater treatment practices in Central European countries, subsequent to their EU accession, reflects a dynamic process propelled by a confluence of external and internal factors. The relentless pursuit of excellence in wastewater treatment has triggered a profound shift in focus, centering on sustainability, resource recovery, and operational efficiency. This transformative journey underscores the pivotal role of advanced control systems, real-time monitoring, and wastewater mathematical modeling as bedrock elements in shaping the future of wastewater treatment within the region. The use of simulation software and optimization procedures for designing technological systems is expected to become increasingly prevalent in the near future, rendering simple calculation software obsolete. In this paper previous and current control systems employed in WWTPs were reviewed, and a multi-criteria approach of an integrated system for the optimization of WWTP operation was also presented.

## OPTIMIZATION AND CONTROL METHODS FOR WASTEWATER TREATMENT PLANTS: INSIGHTS THROUGH MATHEMATICAL MODELING AND COMPUTER SIMULATIONS

Continuous progress in the field of mathematical modeling of biochemical processes related to wastewater treatment has led to the development of comprehensive activated sludge models (ASM). Among the ASM models, ASM1 stands out as the most notable, providing a framework for understanding the removal of carbon and nitrogen compounds in wastewater. Subsequent models, including updated versions like ASM2 and modifications like ASM2d or ASM3, have been introduced [Henze et al., 2000]. These models have become instrumental in optimizing wastewater treatment processes, especially in the context of Central Europe, and particularly in Poland, where their adoption has been rapidly increasing, driven by various objectives outlined earlier. Both mathematical modeling and computer simulation methods hold immense potential to make substantial contributions to the design, operation, and optimization of wastewater treatment processes, ultimately leading to the development

of highly efficient wastewater treatment systems. However, it's essential to recognize that the extent and application of these methods can vary significantly based on their intended purposes and the specific needs of each wastewater treatment facility [Mąkinia et al., 2002; Brdys et al., 2008; Piotrowski et al., 2023].

Hauduc et al. [2009] have shed light on the multifaceted roles that ASM models predominantly serve. These models are primarily employed for process optimization (59%), process design (42%), and forecasting corrective measures for wastewater treatment processes (21%). The diverse goals and applications of these models hinge on the preferences and requirements of the users. In Europe, these models find their primary utility among scientists engaged in research endeavors aimed at optimizing process efficiency and energy consumption. On the other hand, in North America, particularly in the United States and Canada, private companies primarily employ ASMs for process design [Mazurkiewicz, 2016].

Notably, private enterprises have recently introduced novel models and treatment technologies with a common overarching objective: enhancing the sustainability of wastewater treatment processes [Sabba et al., 2017; Cerruti et al., 2021]. Concurrently, advancements in information technology and the rapid enhancement of computational capabilities within available hardware have paved the way for the application of more sophisticated computational tools in the optimization of biochemical processes, particularly those rooted in activated sludge systems [Drewnowski and Szeląg, 2020]. This transition is driven not only by formal and legal requirements, such as the necessity to conduct simulation studies during the process design phase employing appropriate data acquisition and processing methods but also by economic factors, including the decreasing costs of hardware and software [Mazurkiewicz, 2016].

Presently, more than three decades after the groundbreaking publication by Henze et al. [1987], the ASM1 model continues to stand as the standard for describing activated sludge processes [Gernaey et al., 2004; Mąkinia, 2010; Khalaf et al., 2021]. It serves as a reference point for a multitude of scientific and practical projects, often being adapted or extended within commercially available software packages like GPS-X, WEST, SUMO, BIOWIN, DESASS, AQUASIM, and SIMBA [Rieger et al., 2013; Kirchem et al., 2020; Nadeem et al., 2022]. These software tools

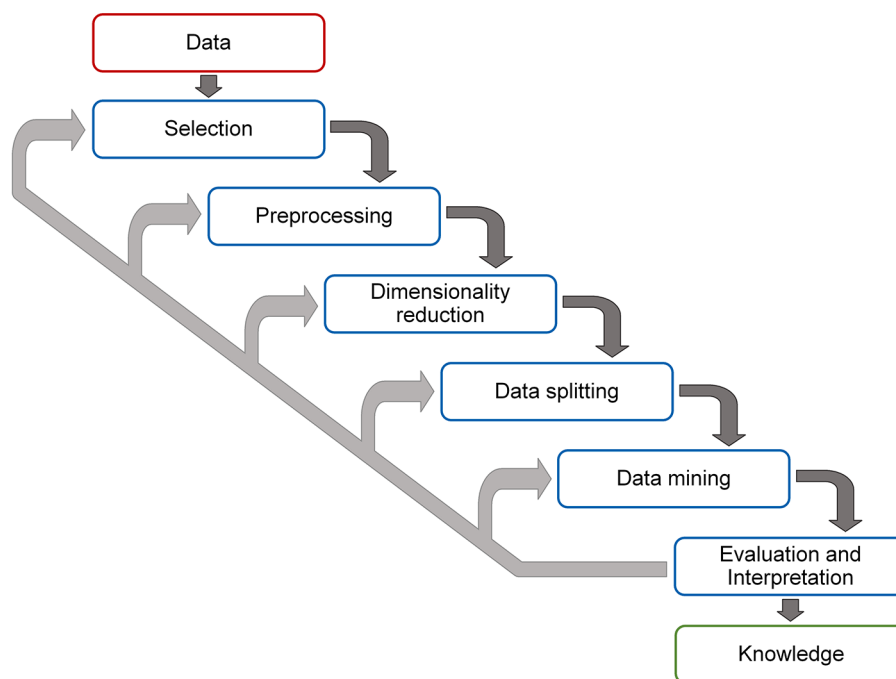
are widely used for modeling and simulating the operations of wastewater treatment plants, with a particular focus on nitrogen removal [Copp, 2002; Eldyasti et al., 2011; Cao et al., 2021]. This is further evidenced by the extensive adoption of these models across various platforms [Mąkinia, 2010; Jafarnejad, 2020], as well as by the research findings in Hauduc et al. [2009] and Henze et al. [2000]. Consequently, for modeling purposes, the biokinetic ASM1 model [Henze et al., 1987] is employed in 57% of cases, while ASM2d [Henze et al., 1999] is utilized in 32% of cases. Recently, ASM3 [Gujer et al., 1999] has gained comparable popularity among all stakeholders, including scientists, local authorities, and the commercial industry. Additionally, ASM2d and TUD [Smolders et al., 1995], as well as New General [Barker and Dold, 1997], have garnered widespread adoption, particularly among governmental organizations, spanning regions like the United States, Canada, Switzerland, as well as several EU countries such as the Netherlands, Germany, and Belgium. These models collectively represent a robust toolkit for addressing the complexities and challenges inherent in wastewater treatment processes, offering valuable insights and solutions for a more sustainable and efficient future in the wastewater treatment sector.

## USE OF DATA MINING METHODS FOR MODELING WASTEWATER TREATMENT PLANTS

In addition to the mechanistic models discussed earlier, statistical models employing data mining methods can also be utilized for modeling wastewater treatment processes. In this approach, models are constructed based on long-term measurement series that encompass the quality of wastewater at the outlet, the quality of wastewater at the inlet, and operational parameters of the bioreactor. Data mining represents a set of data analysis techniques aimed at extracting and organizing knowledge from raw data. It encompasses various computational methods, including the computation of descriptive statistics, exploration of multivariate data, and the use of linear models such as time series analysis. Additionally, data mining involves data visualization techniques, artificial intelligence, and machine learning models [Gorunescu, 2011; Scott-Fordsmand and Amorim, 2023]. The process of knowledge

discovery in databases can be outlined as follows: (1) selection of the dataset to be analyzed, which may involve working with a subset of raw data; (2) dataset preparation, including data cleaning and addressing missing data through imputation; (3) dimensionality reduction and data transformation; (4) splitting of the data to learning, test and optionally validation sets; (5) application of the chosen data mining technique; (6) interpretation and evaluation of the correctness of the results obtained, with the possibility of revisiting earlier steps; (7) implementation of the acquired knowledge. The individual steps of the process are shown in Figure 1 [Fayyad et al., 1996; Mirraftabzadeh et al., 2023].

Artificial intelligence plays a role in developing systems designed to achieve intelligence equal to or even surpassing that of humans. Consequently, AI, by certain definitions, is associated with the notion of behaving or thinking rationally to mitigate human systematic errors [Russell and Norvig, 2010]. This is further reinforced by the fact that machine learning is employed to create precise regression or classification models, positioning this scientific domain as an integral component of artificial intelligence. The fundamental categorization of machine learning models falls into two main groups: supervised and unsupervised models. In unsupervised learning, the dependent variables play no role in constructing the model, while supervised learning involves the inclusion of output variables within the model domain. In supervised learning methods, the process of model creation occurs in two stages: in the initial stage, the model's parameters are estimated using the learning dataset, and in the subsequent stage, the model is tested using the test dataset [Hastie et al., 2009]. This latter stage is crucial for assessing the predictive capabilities of the mathematical model under development. In more contemporary learning scenarios, additional model types have emerged, including semi-supervised learning. In semi-supervised learning, the learning process involves observations with known information about the dependent variable alongside those for which this information is missing, with predictions made during the learning process [Mohri et al., 2018]. A diverse range of machine learning methods has been employed for modeling wastewater treatment plants. These methods encompass multiple regression and its variations, such as MARS (Multivariate Adaptive Regression Splines), neural networks and



**Figure 1.** Individual steps comprising the process of knowledge discovery in databases

their adaptations, fuzzy models, and regression tree methods and their enhancements [Güçlü and Dursun, 2010; Abba and Elkiran, 2017; Santín et al., 2018]. In the realm of regression tree models, improvements have been achieved through the introduction of methods such as random forests or gradient boosting. These modifications have significantly enhanced the predictive capabilities of the regression tree model [Zhou et al., 2019; Wang et al., 2022; Wodecka et al., 2022]. The random forest model has also found utility in classification tasks, demonstrating nearly flawless accuracy when categorizing observations into the relevant stages of wastewater treatment [Piłat-Rożek et al., 2023]. An illustrative instance is provided by the publication of Szeląg et al. [2020], which serves as an exemplar of constructing a sludge bulking simulation model within WWTP using a range of machine learning models, including random forest, boosted trees, support vector machine, multilayer perceptron neural networks, and logistic regression.

A critical phase in the development of a statistical model for modeling processes within wastewater treatment plants is the performance of sensitivity analysis and simulation analyses. These analyses aim to evaluate the impact of alterations in the numerical values of input data on simulation outcomes. This aspect is of utmost importance as the developed model must accurately reflect the

influence of selected independent variables and bioreactor operational parameters on the quality of sewage at the wastewater treatment plant's inflow.

## ADVANCEMENTS IN WWTP CONTROL SYSTEMS AND DEVELOPMENT OF MATHEMATICAL MODELS BASED ON EMERGING TREATMENT TECHNOLOGIES

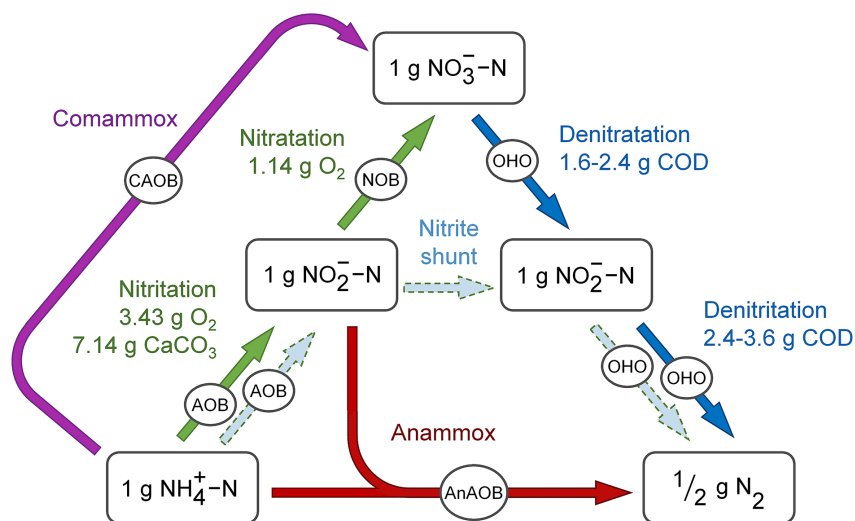
In the 21<sup>st</sup> century, mathematical models have continued to evolve, with the introduction of innovative tools such as ASDM and Mantis [Elawwad et al., 2019; Moragaspitiya et al., 2019; Mu'azu et al., 2020]. Initially, these models found primary usage in governmental organizations and private companies, rather than scientific research units. However, recent years have witnessed an expansion of research efforts focused on discovering novel methods for nitrogen removal from wastewater. This research aims to reduce treatment costs and has led to the modification of standard ASM models into more intricate frameworks that incorporate anammox bacteria and other emerging nitrogen metabolisms, exemplified by Mantis2 [Faris et al., 2022; Mehrani et al., 2022a; Pryce et al., 2022]. These methodologies are rooted in the partial nitrification (nitritation) and anammox processes depicted in Figure 2 [Sobotka et al., 2018; Drewnowski et al., 2021]. Notably, while the

anammox process is commonly found in natural environments such as oceans [Arrigo, 2005], it was only discovered in the late 1990s [Jetten, 1998; Strous, 1999a; Strous, 1999b]. Most of the previous studies mainly focused on ammonia-oxidizing microorganisms, while ignoring the important role of nitrite-oxidizing microbes (Meng et al., 2017; Gao et al., 2018; Zhang et al., 2018). Results of recent studies show that in addition to ammonia oxidation activity, activated sludge exhibits strong nitrite oxidation activity that has to be taken into consideration (Lu et al., 2021). In wastewater treatment systems involving anammox, suppression of the growth of nitrite-oxidizing bacteria (NOB) is one of the most important determinants of highly efficient nitrogen removal [Lotti et al., 2014]. Co-occurrence of NOB oxidizing  $\text{NO}_2^-$  to  $\text{NO}_3^-$  under aerobic conditions with anammox bacteria may lead to rapid consumption of nitrite by NOB. As a result, due to an insufficient supply of  $\text{NO}_2^-$ , the growth of anammox bacteria will be restricted [Ma et al., 2015]. This becomes a serious problem because controlling the growth of NOB is not an easy task, especially during simultaneous nitrification and anammox processes [De Clippeleir et al., 2011; De Clippeleir et al., 2013].

The concept of the nitrite ( $\text{NO}_2^-$ ) shunt is rooted in inhibiting the nitrification process at the  $\text{NO}_2^-$  stage by suppressing the growth of bacteria responsible for oxidizing  $\text{NO}_2^-$  to  $\text{NO}_3^-$  (i.e. NOB) [Cerruti et al., 2021]. This strategy aims to reduce costs associated with aeration during the nitrification process and the expense of adding organic carbon during denitrification carried

out by ordinary heterotrophic organisms (OHO). By converting ammonia nitrogen into  $\text{NO}_2^-$ , it reduces oxygen demand by approximately 25%, and the conversion of  $\text{NO}_2^-$  to nitrogen gas ( $\text{N}_2$ ) decreases the demand for organic carbon by about 40% [Roots et al., 2020].

The Anammox process (Anaerobic Ammonium Oxidation) involves the removal of nitrogen compounds from wastewater using autotrophic microorganisms known as *Planctomycetales*. These bacteria, known as anaerobic ammonia-oxidizing bacteria (AnAOB), convert ammonia and  $\text{NO}_2^-$  (in a ratio of 1:1.3) into  $\text{N}_2$  (approximately 90%) and  $\text{NO}_3^-$  (around 10%) without requiring an external source of organic carbon. Consequently, the anammox process proves especially useful for nitrogen removal from wastewater with a low  $\text{BOD}_5:\text{N}$  ratio, which often arises in water from sludge dewatering processes after anaerobic digestion [Kaewyai et al., 2022]. Deammonification combines nitrification and anammox and can be executed as a single-step process in SBRs (e.g., the DEMON process) [Wett, 2007; Podmirseg et al., 2022] or in hybrid systems (e.g., AnitA<sup>TM</sup> Mox process) [Christensson et al., 2011; González-Martínez et al., 2021]. As mentioned above, deammonification offers significant advantages, including reduced electrical energy consumption for aeration (by approximately 60%), decreased excess sludge production (by about 90%), elimination of the organic carbon requirement, and substantial reduction in  $\text{CO}_2$  emissions into the atmosphere (by over 90%) [Al-Hazmi et al., 2021]. Another recently discovered process found in the



**Figure 2.** The nitrite ( $\text{NO}_2^-$ ) shunt and anammox as well as comammox processes in relation to the conventional nitrification/denitrification

nitrogen cycle is known as Comammox, which stands for Complete Ammonia Oxidation. The main idea behind the process is the conversion of ammonia to  $\text{NO}_3^-$  (traditionally carried out in two stages) by a single group of microorganisms referred to as complete ammonia-oxidizing bacteria (CAOB). In 2015, microorganisms of the genus *Nitrospira* were found to have the capacity for such conversion, and shortly thereafter a species of *Nitrospira inopinata* was isolated in pure culture. It is anticipated that complete nitrifiers could prove very useful in engineering systems, such as wastewater treatment plants, creating new opportunities for nitrogen removal from wastewater [Maddela et al., 2022]. The occurrence of *Nitrospira inopinata* has been confirmed in activated sludge reactors, moving-bed biofilm reactors, hybrid biofilms or side stream wastewater [Lu et al., 2020]. In artificial systems, comammox bacteria coexist together with other microorganisms. Wu et al. [2019] studied the possibility of removing ammonia nitrogen from sludge digester liquor as a result of the simultaneous partial-nitrification, anammox and comammox processes obtained in an SBR reactor. The solution turned out to be not only technologically effective (more than 98% removal efficacy) but also economically efficient. Another aspect of the issue was pointed out in a study conducted by Kits et. al [2019]. It was shown that during nitrification, complete nitrifiers can produce less  $\text{N}_2\text{O}$  (which is a greenhouse gas) compared to ammonia-oxidizing bacteria (AOB) responsible for nitrification. Comammox is also beginning to be reflected in modeling studies. Mehrani et al. [2022b] using data from the nitrification process in SBRs expanded the ASM1 model matrix to include, among other things, two-step nitrification (based on Mantis2) and also the comammox, which enabled a better representation of the processes taking place.

Increasingly, mathematical computer-based models are being utilized for wastewater treatment processes to predict various technological options, facilitating the identification of optimal solutions such as the aforementioned  $\text{NO}_2^-$  shunt method and reductions in aeration costs. Aeration constitutes the most energy-intensive process in wastewater treatment plants [Gu et al., 2023], often exceeding 50% of total energy consumption [Drewnowski et al., 2019]. Most current aeration systems rely on measuring oxygen concentrations in the nitrification tank for control. While this approach effectively maintains a consistent oxygen

concentration for adequate wastewater treatment, it tends to be inefficient in terms of energy, especially when influent pollutant loads fluctuate significantly. This situation calls for the adoption of more advanced aeration control processes based on online measurements of nitrogen compounds [Åmand et al., 2013]. This has become feasible with the development of more reliable ammonia ( $\text{NH}_4^+$ ) and nitrite/nitrate ( $\text{NO}_x$ ) probes [Åmand et al., 2013]. In the Ammonia-Based Aeration Control (ABAC) system, the regulation of oxygen concentration is rooted in  $\text{NH}_4^+$  concentration measurements. ABAC offers two control methods based on the location of  $\text{NH}_4^+$  concentration measurement: feedback control, when measured at the nitrification tank outlet, and feedforward control, at the inlet of the nitrification tank. ABAC-based regulation results in significant energy savings (approximately 10-20%) and improved denitrification with reduced consumption of alkalinity and organic carbon. While feedforward control is more complex, it still ensures compliance with wastewater quality standards with lower energy consumption. The Ammonia vs. Nitrate/Nitrite Control (AVN) system was initially developed for treatments involving shortened nitrification to eliminate the second nitrification step (oxidation of  $\text{NO}_2^-$  to  $\text{NO}_3^-$ ) [Al-Omari et al., 2015]. Additionally, the application of AVN controls may enhance nitrogen removal efficiency in conventional nitrification-denitrification processes [Regmi et al., 2022]. Adjustment of the  $\text{NO}_3^-$  load for denitrification is achieved by configuring specific concentrations and  $\text{NH}_4^+$  to  $\text{NO}_x$  ratios at the outlet [Mehrani et al., 2022b].

Electronic nose systems, due to the gas sensors employed in them, are used to analyze and classify gas mixtures and, in particular, distinguish between components present in a given mixture [Piłat-Rożek et al., 2023]. Multivariate data from the sensors also allow prediction of parameters related to wastewater quality such as COD, ammonia nitrogen (AN), TN and TP [Wang et al., 2023] or other environmental parameters associated with air and odor pollution [Guz et al., 2015]. Monitoring of wastewater treatment plants is one of the future applications of e-noses as they can be used to classify samples from different stages of treatment [Piłat-Rożek et al., 2023] and identify sources or assess concentration of the odors [Giuliani et al., 2012]. Since gas sensor arrays enable the differentiation of contaminants, electronic noses can be employed to detect

unusual situations in wastewater treatment plants that may lead to failures [Bourgeois et al., 2003]. These anomalies can be distinguished from the normal operation of wastewater treatment plants using supervised learning algorithms. Described system can also be applied in fast and cheap estimation of treated wastewater and used for managing and control processes occurring in WWTP devices [Guz et al., 2015; Łagód et al., 2022].

The ongoing developments in mathematical modeling and its application in wastewater treatment have led to groundbreaking advancements. Emerging methodologies like the  $\text{NO}_2^-$  shunt and the utilization of advanced control systems have the potential to revolutionize wastewater treatment processes, making them more efficient, cost-effective, and environmentally friendly. These innovations mark a significant step toward achieving sustainability in wastewater treatment, addressing both economic and environmental concerns. As research continues to push the boundaries of what is possible in this field, the future of wastewater treatment holds promise for more efficient and sustainable practices.

## BALANCING ECONOMIC AND ECOLOGICAL ASPECTS: A MULTI-CRITERIA APPROACH TO OPTIMIZE WASTEWATER TREATMENT PLANT OPERATIONS

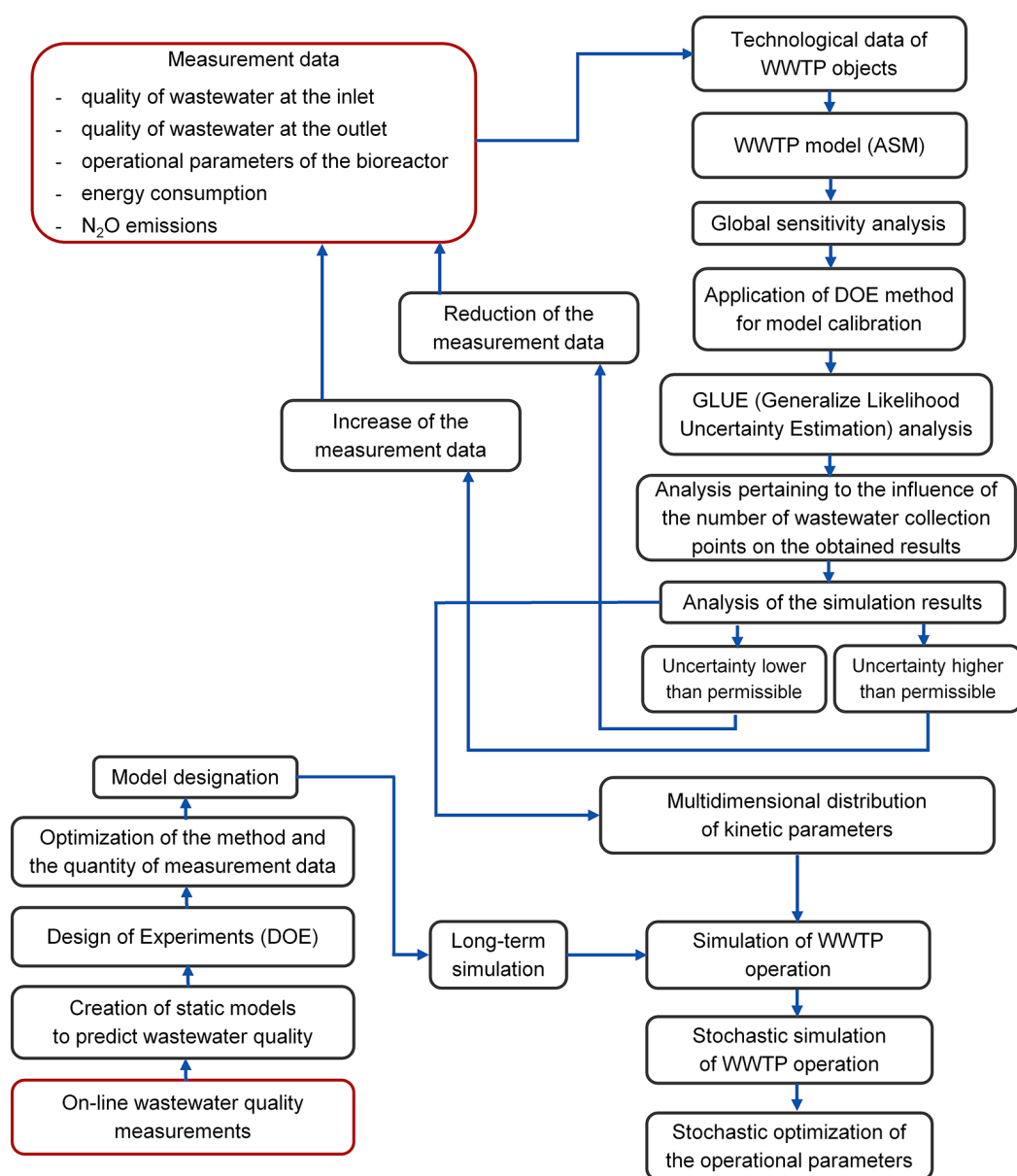
The future of control systems in WWTPs is moving towards what is commonly referred to as “smart process control systems”. These systems will primarily feature a simulation model implemented within computer software, complete with suitable algorithms for controlling biochemical processes. The success of these systems relies on real-time measurements taken at selected points within a bioreactor. Unfortunately, this approach, which falls under the country’s priorities, does not adequately address environmental concerns related to greenhouse gas emissions reduction. WWTPs have been identified as contributors to greenhouse gas emissions [Daelman et al., 2013; Zaborowska et al., 2019; Szeląg et al., 2023], especially during biological nitrogen removal processes [Sabba et al., 2018]. Furthermore, critical aspects such as optimizing the selection of sample collection points within the WWTP, acquiring measurement data for model calibration, and

considering the interactions between calibrated kinetic parameters have often been overlooked [Andraka et al., 2018]. The uncertainties associated with identified WWTP model parameters are not factored in during system construction, which can affect settings and simulation outcomes [Szeląg et al., 2022]. The procedures devised for calibrating and optimizing model parameters often involve iteratively adjusting parameter values until a strong correlation between calculated results and measurements is achieved [Mąkinia and Zaborowska, 2020]. However, this correlation does not always guarantee satisfactory results. Despite the significant influence of wastewater quality at the inlet on the chosen optimization strategies, there have been no efforts to establish a methodology for optimizing wastewater quality prediction, accounting for the duration of the conducted studies. Consequently, the development and implementation of these systems require multi-year and costly investigations, limiting their practicality [Barbusiński et al., 2020; Szeląg et al., 2020]. In Figure 3, these aforementioned limitations are addressed and a methodology for designing an integrated system to optimize WWTP operations is presented [Drewnowski and Szeląg, 2020].

In the adopted approach, the assessment of WWTP operation is based on parameters such as wastewater quality at the outlet, energy consumption, and greenhouse gas emissions. Simulation of these variables is performed using a mechanistic model, specifically ASM. To determine the amount of measurement data and the number of experiments needed for model calibration, the design of experiments (DOE) method is employed [Barbusiński et al., 2021]. This method takes into consideration the number of parameters (both kinetic and stoichiometric) to be calibrated. To optimize the selection of parameters for analysis, a global sensitivity analysis is conducted. This helps identify and exclude kinetic and stoichiometric parameters that have a negligible impact on simulation results. Following this multi-criteria approach and employing the DOE method, data are generated and optimized for use in a statistical model that predicts influent wastewater quality. This is a critical step as online wastewater quality measurements are often costly and can be a limiting factor in long-term WWTP optimizations [Borzooei et al., 2019; Newhart et al., 2019].

The adopted solution allows to find a balance between the amount of measurement data and the complexity of the statistical method used





**Figure 3.** Multi-criteria concept of an integrated system for optimization of WWTP operation

to predict wastewater quality. Machine learning methods, including neural networks and their various adaptations, are utilized to achieve this, reducing measurement time and equipment operating costs. The presented methodology also addresses uncertainty analysis using the GLUE method during model calibration [Mannina et al., 2010; Szeląg et al., 2022]. This uncertainty pertains to the interactions among identified parameters and their impact on simulation results. Furthermore, this approach enables the exploration and analysis of the influence of various simplifications of wastewater quality indicators, with decisions based on the credibility of the obtained results. When the uncertainty is within

permissible limits set by a technologist, simplified testing approaches can be considered. If not, additional tests are required. The analyses result in a model with the assumed accuracy, determined by multidimensional distributions of kinetic parameters using the GLUE method. Therefore, by applying the developed statistical models for predicting influent wastewater quality, the calibrated WWTP model can estimate wastewater quality, energy consumption, and greenhouse gas emissions using the GLUE method, considering the interactions among calibrated parameters. The obtained results can exhibit variability. To account for this variability, stoichiometric concepts are integrated into bioreactor settings

during WWTP optimization. These settings are designed to ensure that the desired technological outcomes are achieved at the lowest possible cost. This holistic and innovative approach promises to greatly transform WWTP operations, aligning them with sustainability goals and addressing the environmental challenges posed by greenhouse gas emissions.

## CONCLUSIONS

The comparison of different WWTP optimization systems confirms that there is a clear focus on improving wastewater quality and cutting energy use. Despite advanced computational methods, Poland and Central Europe still prefer simpler tools like spreadsheets and control software. Simulation, integrated software, and AI are underused in practical wastewater treatment, primarily serving research rather than operations. One significant obstacle to using computer models for WWTPs is the lack of comparative or operational data needed for model calibration, validation, sensitivity assessment, and qualitative analysis. Gathering this data is time-consuming and costly. Nevertheless, computer models are increasingly used to predict various technological approaches and identify optimal solutions. Recent studies show the adoption of technologies like  $\text{NO}_2^-$  shunt and anammox processes in WWTPs, especially for the treatment of wastewater with high nitrogen content.

Considering the growing complexity of  $\text{NO}_2^-$  shunt compared to traditional processes, mathematical models and computer simulations for WWTP control are expected to become more common. Thus, besides reviewing current WWTP control systems, this paper presents a multi-criteria approach to an integrated system for WWTP optimization. The application of simulation software and optimization procedures is likely to phase out simpler calculation software in medium and large WWTPs. These systems will involve complex integrated expert systems, real-time data collection and processing, and simultaneous optimization. In contrast, small WWTPs will adopt these changes more slowly, continuing to rely on conventional processes and traditional control software. Data processing will also remain offline due to the high cost of measurement devices, making investments in online systems unfeasible.

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