(REVIEW ARTICLE)

Advancing wastewater treatment technologies: The role of chemical engineering simulations in environmental sustainability

Nwankwo Constance Obiuto [1, *], Ejike David Ugwuanyi [2], Nwakamma Ninduwezuor-Ehiobu [3], Emmanuel Chigozie Ani [4] and Kehinde Andrew Olu-lawal [5]

[1] Faculty of Engineering, Nnamdi Azikiwe University, Awka, Nigeria.
[2] Department of Chemical, Biochemical, and Environmental Engineering University of Maryland Baltimore County Baltimore, Maryland, USA.
[3] FieldCore Canada, part of GE Vernova.
[4] Department of Electrical Engineering, The University of Nebraska-Lincoln, USA.
[5] Niger Delta Power Holding Company, Akure, Nigeria.

Abstract

Wastewater treatment stands as a critical component in mitigating environmental pollution and safeguarding public health. This review delves into the pivotal role of chemical engineering simulations in advancing wastewater treatment technologies towards enhanced environmental sustainability. The modernization of wastewater treatment processes necessitates a comprehensive understanding of the complex physical, chemical, and biological interactions involved. Chemical engineering simulations offer a powerful toolset for modeling and optimizing these processes with a focus on efficiency, effectiveness, and sustainability. Firstly, simulations enable the prediction and analysis of pollutant removal mechanisms within treatment systems. By simulating various operating conditions and configurations, engineers can optimize treatment processes to achieve higher removal efficiencies while minimizing resource consumption and waste generation. Secondly, simulations aid in the design and development of innovative treatment technologies, such as membrane filtration, advanced oxidation processes, and biological nutrient removal systems. Through computational modeling, engineers can assess the performance and feasibility of these technologies under different scenarios, facilitating informed decision-making and accelerating their implementation. Furthermore, chemical engineering simulations play a crucial role in addressing emerging challenges in wastewater treatment, including the removal of emerging contaminants such as pharmaceuticals, microplastics, and endocrine-disrupting chemicals. By simulating the behavior of these contaminants within treatment systems, engineers can devise targeted strategies for their removal, thus mitigating their adverse environmental and public health impacts. Chemical engineering simulations serve as indispensable tools for advancing wastewater treatment technologies towards greater environmental sustainability. By facilitating the optimization, design, and innovation of treatment processes, simulations contribute to the development of more efficient, cost-effective, and environmentally friendly solutions for managing wastewater and protecting our ecosystems. Embracing these simulation-driven approaches is essential for achieving the ambitious goals of sustainable development and ensuring a cleaner, healthier future for generations to come.

Keywords: Wastewater; Water; Treatment; Chemical; Engineering; Simulations; Environmental

1. Introduction

Wastewater treatment stands as a pivotal process in the preservation of environmental sustainability, playing a critical role in safeguarding ecosystems and public health. As populations grow and industrial activities expand, the volume

---

and complexity of wastewater continue to escalate, underscoring the pressing need for efficient and effective treatment technologies.

Wastewater treatment involves the removal of contaminants and pollutants from wastewater before its discharge into natural water bodies or reuse (Manasa. and Mehta, 2020; Saravanan, et al., 2021). This process is indispensable for mitigating environmental pollution, preventing the spread of waterborne diseases, and preserving freshwater resources. Without adequate treatment, wastewater can pose significant risks to aquatic ecosystems, human health, and overall environmental quality (Jhansi, and Mishra, 2013).

Chemical engineering simulations offer a powerful toolkit for modeling and optimizing wastewater treatment processes (Bury, et al., 2002; Dobre, et al., 2007). By utilizing computational techniques to simulate the physical, chemical, and biological processes involved in treatment, engineers can gain insights into system behavior, optimize process parameters, and design innovative technologies. Simulation-based approaches enable engineers to explore a wide range of operating conditions, assess the performance of treatment systems, and predict the impact of design modifications (Shafto, et al., 2010), all of which are essential for advancing treatment technologies towards greater efficiency, effectiveness, and sustainability (D'Agostino, et al., 2020).

The purpose of this outline is to provide a comprehensive overview of how chemical engineering simulations are applied to advance wastewater treatment technologies in pursuit of environmental sustainability. The outline will delve into the fundamentals of simulation techniques, their application to pollutant removal mechanisms, optimization of treatment processes, and the design of innovative technologies. Case studies and real-world examples will be included to illustrate the practical applications of simulation-driven approaches. Additionally, the outline will explore emerging challenges in wastewater treatment and discuss future directions for research and development efforts.

2. Fundamentals of Chemical Engineering Simulations

Chemical engineering simulations play a crucial role in the design, optimization, and analysis of various processes in chemical engineering, including wastewater treatment (Dimian, et al., 2014; Meramo-Hurtado, and González-Delgado, 2021.). By leveraging mathematical models and computational techniques, simulations enable engineers to predict and understand complex phenomena, optimize process parameters, and design innovative technologies. This review provides an overview of the fundamentals of chemical engineering simulations, their application to wastewater treatment processes, and the importance of accuracy, validation, and calibration in simulation modeling.

Process modeling involves the development of mathematical models that describe the behavior of chemical processes (Jana, 2018; Okino, and Mavrovouniotis, 1998). These models can range from simple mass and energy balances to complex differential equations that capture the dynamics of the system. Process modeling allows engineers to predict the behavior of chemical processes under different operating conditions, optimize process parameters, and identify potential areas for improvement (Bequette, 2003).

Computational fluid dynamics (CFD) is a simulation technique used to model the behavior of fluids and their interactions with solid surfaces (Zawawi, et al., 2018; Kamyar, et al., 2012). In chemical engineering, CFD is commonly used to simulate the flow of fluids in reactors, heat exchangers, and separation units. By solving the governing equations of fluid flow and heat transfer numerically, CFD allows engineers to analyze the performance of equipment, optimize design parameters, and predict the impact of design modifications on fluid flow patterns and heat transfer rates (Liu, et al., 2017; Guardo, et al., 2004; Norton, and Sun, 2006).

Reaction kinetics modeling involves the development of mathematical models that describe the rates of chemical reactions and the formation of products over time (Turányi, and Tomlin, 2014; Berger, et al., 2001). These models typically incorporate kinetic rate equations derived from reaction mechanisms and experimental data. Reaction kinetics modeling enables engineers to predict the conversion of reactants, selectivity of products, and optimal operating conditions for chemical reactors. By simulating reaction kinetics, engineers can optimize reactor design, catalyst selection, and process conditions to maximize the yield and efficiency of chemical processes.

Simulations are widely used in wastewater treatment to optimize process performance, design treatment systems, and assess the impact of operating conditions on treatment efficiency (Gernaey, et al., 2004; Gillot, et al., 1999). Several simulation techniques, including process modeling, CFD, and reaction kinetics modeling, are applied to various aspects of wastewater treatment processes:

Process modeling is used to simulate the behavior of unit operations in wastewater treatment plants, such as sedimentation, filtration, and biological treatment. By developing mathematical models that describe the kinetics of pollutant removal mechanisms, engineers can predict the performance of treatment processes under different conditions and optimize process parameters to achieve desired effluent quality standards (Butler, and Schütze, 2005; Mingzhi, et al., 2019; Revollar, et al., 2020).

CFD is employed to simulate the flow of wastewater within treatment units, such as clarifiers, aeration tanks, and membrane filtration systems. By solving the Navier-Stokes equations and mass transport equations, CFD allows engineers to analyze fluid flow patterns, optimize hydraulic design parameters, and predict the distribution of pollutants within treatment systems. CFD simulations are valuable for identifying potential bottlenecks, optimizing mixing and aeration strategies, and improving the overall efficiency of wastewater treatment processes (Zawawi, et al., 2018).

Reaction kinetics modeling is used to simulate the biological and chemical processes involved in wastewater treatment, such as nitrification, denitrification, and phosphorus removal (Gao, et al., 2010). By incorporating kinetic rate equations and stoichiometric relationships, engineers can predict the rates of pollutant transformation and the formation of by-products in biological reactors and chemical treatment units. Reaction kinetics modeling enables engineers to optimize process conditions, select appropriate microbial consortia or chemical additives, and design efficient treatment systems for removing specific contaminants from wastewater (Priyadarshini, et al., 2021).

Accurate simulation modeling is essential for ensuring the reliability and validity of predictions and recommendations derived from simulations. Several key factors contribute to the accuracy of simulation models in chemical engineering; Simulation models rely on accurate input data, including physical properties, process parameters, and boundary conditions. Engineers must carefully collect and validate experimental data to ensure its accuracy and reliability for use in simulation modeling. Simulation models should be validated against experimental data to assess their accuracy and predictive capabilities. Engineers compare model predictions with experimental results to identify discrepancies and refine model parameters or assumptions to improve model accuracy. Calibration involves adjusting model parameters to better match observed data and improve the agreement between simulation predictions and experimental measurements (Reddy, 2006; Trucano, et al., 2006). Engineers iteratively calibrate simulation models based on experimental data to enhance their accuracy and reliability for predicting system behavior under different conditions.

In conclusion, chemical engineering simulations are powerful tools for modeling, optimizing, and analyzing various processes, including wastewater treatment. By applying simulation techniques such as process modeling, CFD, and reaction kinetics modeling, engineers can predict system behavior, optimize process parameters, and design innovative technologies to improve the efficiency and sustainability of wastewater treatment processes. However, it is essential to ensure the accuracy, validation, and calibration of simulation models to ensure their reliability and validity for making informed decisions in chemical engineering applications.

3. Modeling Pollutant Removal Mechanisms in Wastewater Treatment

Wastewater treatment is a complex process involving various physical, chemical, and biological mechanisms aimed at removing pollutants from wastewater before its discharge into the environment. In recent years, the use of simulation techniques has become increasingly prevalent in understanding and optimizing these pollutant removal mechanisms. This review explores the application of simulation techniques to model the key pollutant removal mechanisms in wastewater treatment, including physical, chemical, and biological processes.

Sedimentation and filtration are common physical processes used in wastewater treatment for the removal of suspended solids and particulate matter (Rezai, and Allahkarami, 2021; Shammas, et al., 2005). In sedimentation tanks, gravitational forces cause suspended particles to settle to the bottom of the tank, forming a sludge layer that can be removed. Filtration involves passing wastewater through a porous medium, such as sand or activated carbon, to trap suspended solids and other contaminants (Gray, 2014). Simulation techniques, such as computational fluid dynamics (CFD), are used to model the flow patterns and sedimentation kinetics within sedimentation tanks. By solving the Navier-Stokes equations and mass transport equations, CFD simulations can predict the settling velocities of particles, the distribution of solids within the tank, and the efficiency of sedimentation processes.

Similarly, simulations are employed to model the filtration process, including the flow of wastewater through filter media, the accumulation of solids on the filter surface (Busch, et al., 2007; Logan, et al., 1987), and the hydraulic performance of filtration units (Mushila, et al., 2016; Haile, et al., 2016). These simulations provide insights into the

design and operation of sedimentation and filtration systems, enabling engineers to optimize process parameters and improve pollutant removal efficiency.

Adsorption and absorption are physical processes used to remove dissolved pollutants, such as organic compounds and heavy metals, from wastewater (Rashed, 2013.). Adsorption involves the attachment of pollutant molecules to the surface of an adsorbent material (Sahoo. and Prelot, 2020), while absorption involves the uptake of pollutants into a liquid or solid phase (Saravanan, et al., 2021).

Simulation techniques, such as equilibrium and kinetic models, are used to predict the adsorption and absorption behavior of pollutants in wastewater treatment systems. These models incorporate factors such as the surface area and porosity of the adsorbent material, the concentration of pollutants in the wastewater, and the contact time between the wastewater and the adsorbent.

Chemical precipitation is a common chemical process used in wastewater treatment for the removal of dissolved metals and other inorganic pollutants (Sahoo, and Prelot, 2020; Benalia,, et al., 2022). During chemical precipitation, a precipitating agent is added to the wastewater, causing the formation of insoluble precipitates that can be removed by sedimentation or filtration. Simulation techniques, such as chemical equilibrium models and reaction kinetics models, are used to predict the formation and dissolution of precipitates in wastewater treatment systems. These models consider factors such as the solubility of precipitates, the pH of the wastewater, and the kinetics of precipitation reactions (Pohl, 2020; Wang, et al., 2005; Clifford, et al., 1986). By simulating chemical precipitation processes, engineers can optimize the dosage of precipitating agents, control the pH of the wastewater, and improve the efficiency of pollutant removal. Oxidation-reduction (redox) reactions play a crucial role in the removal of organic pollutants and inorganic contaminants from wastewater. Oxidation processes involve the transfer of electrons from one species to another, resulting in the conversion of pollutants into less harmful or more easily removable forms. Reduction processes, on the other hand, involve the gain of electrons by a species, leading to the transformation of pollutants into less toxic or insoluble compounds (Zhang, et al., 2023; Ullah, et al., 2020).

Simulation techniques, such as reaction kinetics models and electrochemical models, are used to simulate oxidation-reduction reactions in wastewater treatment systems. These models incorporate factors such as the kinetics of redox reactions, the concentration of oxidizing or reducing agents, and the pH of the wastewater. By simulating redox processes, engineers can optimize process conditions, select appropriate treatment methods, and enhance the efficiency of pollutant removal.

Biological processes, such as aerobic and anaerobic digestion, are widely used in wastewater treatment for the removal of organic pollutants and the stabilization of organic matter. During aerobic digestion, microorganisms break down organic pollutants in the presence of oxygen, producing carbon dioxide, water, and biomass as by-products. Anaerobic digestion, on the other hand, occurs in the absence of oxygen and results in the production of methane and carbon dioxide (Samer, 2015; Náthia-Neves, et al., 2018).

Simulation techniques, such as biokinetic models and microbial growth models, are used to simulate aerobic and anaerobic digestion processes in wastewater treatment systems. These models describe the kinetics of microbial growth, substrate utilization, and product formation during biological degradation processes. By simulating biological digestion processes, engineers can optimize process conditions, control nutrient concentrations, and maximize the efficiency of pollutant removal (Aziz, et al., 2019; Fuentes, et al., 2021).

Nitrification and denitrification are biological processes used in wastewater treatment for the removal of nitrogenous compounds, such as ammonia and nitrate (Lin, et al., 2009). Nitrification involves the oxidation of ammonia to nitrite and then to nitrate by nitrifying bacteria, while denitrification involves the reduction of nitrate to nitrogen gas by denitrifying bacteria. Simulation techniques, such as biokinetic models and microbial population models, are used to simulate nitrification and denitrification processes in wastewater treatment systems. These models describe the growth kinetics of nitrifying and denitrifying bacteria, the rates of ammonia and nitrate oxidation, and the factors influencing microbial activity. By simulating biological nitrogen removal processes, engineers can optimize process conditions, control nitrogen concentrations, and enhance the efficiency of pollutant removal (Gupta, et al., 2022; Kuenen, and Robertson, 1994).

In conclusion, modeling pollutant removal mechanisms in wastewater treatment involves the application of simulation techniques to understand and optimize physical, chemical, and biological processes. Simulation models provide valuable insights into the behavior of pollutants in wastewater treatment systems, enabling engineers to design more efficient treatment processes, optimize process parameters, and improve the overall performance of wastewater

treatment systems. By integrating simulation techniques with experimental data and field observations, engineers can develop more accurate and reliable models for predicting pollutant removal in wastewater treatment systems.

4. Optimization of Treatment Processes Using Simulations

In the realm of wastewater treatment, optimization of treatment processes is essential to ensure efficiency, effectiveness, and sustainability. Simulation techniques play a crucial role in this optimization process by enabling engineers to model, analyze, and optimize various aspects of treatment processes. This review explores how simulations are utilized to optimize treatment processes, including parameter optimization, process control strategies, and the design of treatment systems.

Parameter optimization involves finding the optimal values of process parameters to maximize treatment efficiency and effectiveness. Simulation-based optimization algorithms, such as genetic algorithms, particle swarm optimization, and simulated annealing, are commonly used to search for the optimal parameter values. These algorithms iteratively explore the parameter space, evaluating the performance of the system under different parameter combinations, and converging towards the optimal solution (Gillo, et al., 1999; Wu, et al., 2016).

Sensitivity analysis is another important technique used in parameter optimization. Sensitivity analysis evaluates the sensitivity of the system's performance to changes in input parameters, allowing engineers to identify which parameters have the most significant impact on treatment efficiency. By focusing on these sensitive parameters, engineers can prioritize their optimization efforts and achieve greater improvements in treatment performance. Feedback control strategies use real-time data from sensors to adjust process parameters and maintain desired operating conditions. Simulation-based feedback control algorithms, such as proportional-integral-derivative (PID) control, model predictive control (MPC), and fuzzy logic control, are employed to regulate key process variables, such as flow rates, concentrations, and temperatures. Simulation-based feedback control allows engineers to account for process dynamics, uncertainties, and disturbances, ensuring stable and efficient operation of treatment processes. By continuously monitoring process variables and adjusting control actions in response to changes in the system, feedback control strategies can optimize treatment performance and minimize deviations from desired targets.

Feedforward control strategies anticipate disturbances or changes in process conditions and preemptively adjust process parameters to mitigate their effects. Simulation-based feedforward control algorithms use predictive models to forecast the impact of disturbances on process variables and determine appropriate control actions. Feedforward control strategies are particularly effective in mitigating disturbances that cannot be directly measured or controlled, such as influent variability or changes in ambient conditions. By incorporating simulation models into feedforward control systems, engineers can optimize treatment processes proactively, improving stability, robustness, and efficiency.

Simulation-driven design optimization involves using simulation models to explore and evaluate different design configurations, layouts, and operating conditions. Engineers can simulate various design alternatives, assess their performance using predefined criteria, and identify the optimal design solution that meets desired objectives, such as cost-effectiveness, energy efficiency, or pollutant removal efficiency.

Simulation-driven design optimization enables engineers to consider a wide range of design factors and constraints, leading to more informed and optimal design decisions. By iteratively refining design alternatives through simulation-based analysis, engineers can develop treatment systems that are optimized for performance, reliability, and sustainability.

Simulation models are also used to scale up treatment processes from laboratory or pilot-scale experiments to full-scale implementation. Scale-up considerations involve simulating the behavior of the process at different scales, accounting for factors such as mass transfer rates, mixing dynamics, and reactor geometry. Simulation-driven scale-up ensures that the performance of treatment processes is accurately predicted and maintained across different scales. By simulating full-scale operating conditions and considering scale-dependent factors, engineers can identify potential challenges and optimize design parameters to achieve consistent and reliable performance in real-world applications.

In conclusion, optimization of treatment processes using simulations involves leveraging simulation techniques to optimize process parameters, develop process control strategies, and design treatment systems. By employing optimization algorithms, feedback and feedforward control strategies, and simulation-driven design approaches, engineers can improve the efficiency, effectiveness, and sustainability of wastewater treatment processes. Simulation-

based optimization facilitates informed decision-making, enhances process performance, and contributes to the development of more reliable and robust treatment systems (Muoio et al., 2019; Issa, 2019).

5. Innovative Wastewater Treatment Technologies and Simulations

The continual advancement of wastewater treatment technologies is critical for addressing increasingly stringent environmental regulations and the growing demand for sustainable water management practices. Alongside these technological developments, the use of simulations has emerged as a powerful tool for optimizing the design and operation of innovative wastewater treatment processes. This review explores the intersection of innovative wastewater treatment technologies and simulations, focusing on membrane filtration processes, advanced oxidation processes, and biological nutrient removal systems.

Reverse osmosis is a membrane filtration process that utilizes a semi-permeable membrane to remove dissolved contaminants, ions, and particles from water. In RO, pressure is applied to the wastewater stream, forcing water molecules to pass through the membrane while retaining dissolved solids and contaminants. The resulting permeate is purified water, while the concentrated stream, known as reject or brine, contains the removed contaminants (Sakiewicz, et al.,2020; Aydiner, et al., 2016).

Simulations are used to model the performance of RO systems and optimize operating parameters such as feed flow rate, pressure, and membrane characteristics. Computational fluid dynamics (CFD) simulations, for example, can predict fluid flow patterns, pressure distribution, and concentration polarization effects within the membrane module. These simulations enable engineers to optimize membrane module design, enhance system efficiency, and minimize energy consumption. Ultrafiltration is another membrane filtration process used in wastewater treatment to remove suspended solids, colloidal particles, and macromolecules. UF membranes have larger pore sizes compared to RO membranes, allowing them to selectively remove particles based on size rather than molecular weight (Panebianco, and Pahl-Wostl, 2006).

Simulation techniques such as Monte Carlo simulations and molecular dynamics simulations are employed to model the transport of solutes and particles through UF membranes. These simulations provide insights into the mechanisms of particle rejection, membrane fouling, and concentration polarization, enabling engineers to optimize membrane materials, pore sizes, and operating conditions to maximize filtration efficiency and prolong membrane lifespan (Gernaey, et al., 2004).

Ozonation is an advanced oxidation process (AOP) that utilizes ozone (O3) to oxidize and degrade organic pollutants and microorganisms in wastewater (Rekhate, and Srivastava, 2020; Lu, et al., 2022). Ozone is a powerful oxidizing agent that reacts with organic compounds through direct oxidation and the generation of reactive oxygen species (ROS), such as hydroxyl radicals (•OH) (Gorito, 2021). Simulation techniques, such as reaction kinetics modeling and computational chemistry simulations, are used to predict the kinetics and mechanisms of ozone reactions with organic pollutants. These simulations enable engineers to optimize ozone dosage, contact time, and pH conditions to achieve efficient pollutant degradation while minimizing the formation of harmful by-products such as bromate ions. Additionally, CFD simulations can be employed to optimize the design of ozonation reactors and improve mass transfer efficiency. UV-based advanced oxidation processes, such as UV/H2O2 and UV/TiO2 photocatalysis, utilize ultraviolet (UV) radiation to generate reactive species that oxidize and degrade organic pollutants in wastewater (Ustun, et al., 2024). UV/H2O2 involves the combination of UV radiation with hydrogen peroxide (H2O2) to produce hydroxyl radicals, while UV/TiO2 photocatalysis utilizes UV radiation to activate titanium dioxide (TiO2) nanoparticles, which then generate ROS upon interaction with water molecules (Park, and Mackie, 2023).

Simulations play a crucial role in modeling the mechanisms of pollutant degradation and the efficiency of UV-based AOPs. Quantum mechanical simulations and density functional theory (DFT) calculations are used to predict the electronic structure and reactivity of photocatalytic materials such as TiO2 nanoparticles. These simulations guide the design of photocatalysts with enhanced activity and stability, leading to improved performance of UV-based AOPs for wastewater treatment.

Enhanced biological phosphorus removal (EBPR) is a biological nutrient removal process used to remove phosphorus from wastewater using phosphorus-accumulating microorganisms. In EBPR, microorganisms accumulate phosphorus intracellularly under anaerobic conditions and release it under aerobic conditions, facilitating its removal from the wastewater stream. Simulation techniques such as biokinetic modeling and microbial population dynamics modeling are employed to simulate the behavior of phosphorus-accumulating microorganisms and optimize EBPR performance. These simulations predict the kinetics of phosphorus uptake and release, the effects of environmental conditions such

as temperature and pH, and the impact of operational parameters such as sludge retention time and carbon source availability. By optimizing these parameters, engineers can maximize phosphorus removal efficiency and minimize the risk of process upsets (Izadi, et al., 2020; López-Vázquez,, et al., 2008). Anaerobic ammonium oxidation (Anammox) is a biological process used to remove nitrogen from wastewater by converting ammonium ($NH4+$) and nitrite ($NO2-$) to nitrogen gas ($N2$) under anaerobic conditions. Anammox bacteria perform this conversion via the anaerobic oxidation of ammonium with nitrite as the electron acceptor.

Simulations are employed to model the kinetics and metabolic pathways of Anammox bacteria and optimize process parameters such as nitrogen loading rates, pH, and temperature. Biokinetic models and metabolic flux analysis simulations predict the growth rates and substrate utilization rates of Anammox bacteria under different conditions, enabling engineers to design and operate Anammox reactors with maximum nitrogen removal efficiency.

In conclusion, innovative wastewater treatment technologies such as membrane filtration processes, advanced oxidation processes, and biological nutrient removal systems offer promising solutions for addressing water quality challenges. Simulations play a crucial role in optimizing the design and operation of these technologies, enabling engineers to maximize treatment efficiency, minimize energy consumption, and ensure environmental sustainability. By integrating simulations into the development and implementation of innovative treatment technologies, we can advance the field of wastewater treatment and contribute to the protection and preservation of water resources for future generations.

6. Addressing Emerging Challenges with Simulations

As the landscape of wastewater treatment evolves, new challenges arise, requiring innovative approaches to ensure effective treatment and environmental protection. Simulations have emerged as indispensable tools for addressing these emerging challenges, providing insights into complex processes and guiding the development of sustainable solutions. This review explores how simulations are used to address two prominent emerging challenges in wastewater treatment: the removal of emerging contaminants and simulation-based strategies for resource recovery (Alvi, et al., 2023).

Pharmaceuticals and personal care products (PPCPs) are a group of emerging contaminants that pose significant risks to aquatic ecosystems and human health. These compounds, including antibiotics, hormones, and pain relievers, enter wastewater through domestic and industrial sources and can persist through conventional treatment processes. Simulation techniques, such as fate and transport modeling and reaction kinetics modeling, are used to predict the behavior of pharmaceuticals in wastewater treatment systems. These simulations consider factors such as adsorption, biodegradation, and transformation pathways to assess the fate of pharmaceuticals and their potential impacts on receiving water bodies.

Additionally, advanced oxidation processes (AOPs), such as ozonation and UV-based processes, are simulated to evaluate their effectiveness in degrading pharmaceuticals and reducing their concentrations in treated effluent. By simulating the performance of different treatment technologies and operating conditions, engineers can optimize treatment processes to enhance pharmaceutical removal efficiency and minimize environmental risks. Microplastics are another emerging contaminant of concern in wastewater treatment, with widespread environmental implications. These tiny plastic particles, measuring less than 5 millimeters in size, originate from various sources, including plastic debris, synthetic fibers, and microbeads in personal care products.

Simulation techniques, such as particle tracking and fate modeling, are employed to predict the transport and fate of microplastics in wastewater treatment systems. These simulations consider factors such as particle size, density, and settling velocity to simulate the behavior of microplastics in different treatment units, including sedimentation tanks, filtration systems, and biological reactors. Additionally, simulations are used to assess the efficiency of various treatment technologies, such as membrane filtration and advanced oxidation processes, in removing microplastics from wastewater. By simulating the performance of different treatment processes and evaluating their effectiveness in removing microplastics, engineers can design and optimize treatment systems to minimize the release of microplastics into the environment.

Energy recovery from wastewater is an emerging strategy aimed at harnessing the energy potential of wastewater and reducing reliance on fossil fuels. Simulation techniques, such as process modeling and energy balance analysis, are used to assess the feasibility and optimize the design of energy recovery systems, such as anaerobic digestion, biogas production, and microbial fuel cells. These simulations predict the performance of energy recovery systems under different operating conditions, such as influent characteristics, temperature, and hydraulic retention time. By simulating

the energy production potential of wastewater treatment processes and evaluating the economic viability of energy recovery technologies, engineers can identify opportunities for maximizing energy recovery and reducing the carbon footprint of wastewater treatment plants. Nutrient recovery from wastewater, particularly phosphorus and nitrogen, is gaining traction as a sustainable solution for addressing nutrient pollution and promoting circular economy principles. Simulation techniques, such as reaction kinetics modeling and process optimization, are used to design and optimize nutrient recovery processes, such as struvite precipitation, biological nutrient removal, and nutrient recycling.

These simulations predict the kinetics of nutrient precipitation and recovery, assess the effectiveness of different recovery methods, and optimize process parameters to maximize nutrient removal and recovery efficiency. By simulating nutrient recovery processes and evaluating their economic and environmental benefits, engineers can design integrated nutrient recovery systems that minimize nutrient discharge to the environment and recover valuable resources for reuse in agriculture or industry (Widder, et al., 2016).

In conclusion, simulations play a crucial role in addressing emerging challenges in wastewater treatment, including the removal of emerging contaminants and the implementation of resource recovery strategies. By simulating the behavior of contaminants and evaluating the performance of treatment technologies, simulations enable engineers to design and optimize treatment systems that are effective, efficient, and environmentally sustainable. As the field of wastewater treatment continues to evolve, simulations will remain essential tools for innovating and advancing sustainable solutions to emerging challenges.

7. Case Studies and Applications of Chemical Engineering Simulations in Wastewater Treatment

Chemical engineering simulations have become indispensable tools in the field of wastewater treatment, offering insights, optimization opportunities, and solutions to complex environmental challenges. This review explores case studies and real-world applications demonstrating the effectiveness of simulation-driven approaches in wastewater treatment.

In a real-world application, a wastewater treatment plant faced challenges with poor settling efficiency in its clarifier, resulting in high suspended solids concentrations in the effluent. Using CFD simulations, engineers modeled the fluid flow patterns and sedimentation kinetics within the clarifier. By analyzing the simulations, engineers identified areas of stagnant flow and developed design modifications to improve hydraulic performance. The simulation-driven approach enabled engineers to optimize the design of the clarifier, leading to improved settling efficiency and reduced suspended solids concentrations in the effluent. This case study demonstrates how CFD simulations can provide valuable insights into the hydraulic behavior of treatment units and guide design improvements to enhance treatment performance. In another case study, a wastewater treatment plant sought to improve nutrient removal efficiency to comply with stringent regulatory requirements. Using reaction kinetics modeling, engineers simulated the biological processes involved in nutrient removal, including nitrification, denitrification, and phosphorus uptake (Ryhiner, et al., 1993).

By calibrating the simulation model with plant data and conducting sensitivity analyses, engineers identified key process parameters affecting nutrient removal efficiency. Based on the simulation results, the plant implemented operational changes, such as optimizing aeration rates and carbon dosing strategies, to enhance nutrient removal performance.

In a case study involving the design of an MBR system for wastewater treatment, engineers used simulation techniques to optimize system configuration and operating parameters. Through process modeling and simulation-based design optimization, engineers evaluated various membrane configurations, aeration strategies, and solids retention times to maximize treatment efficiency and minimize energy consumption. The simulation-driven approach enabled engineers to identify the optimal MBR design that met effluent quality standards while minimizing capital and operating costs. By simulating different design scenarios and assessing their performance, engineers developed an MBR system that achieved superior treatment performance and reduced environmental impact (Del Rio-Chanona, et al., 2019).

In another case study, a wastewater treatment plant sought to optimize the anaerobic digestion process for sludge stabilization and biogas production. Using process modeling and simulation-based optimization, engineers simulated the anaerobic digestion process and evaluated the effects of temperature, hydraulic retention time, and feedstock composition on biogas production and digestion efficiency. By conducting sensitivity analyses and parameter optimization, engineers identified optimal operating conditions that maximized biogas yield and sludge stabilization while minimizing process downtime and energy consumption. The simulation-driven approach facilitated informed

decision-making and enabled the plant to achieve significant improvements in biogas production and overall process performance (Amini, et al., 2013).

Simulations are increasingly being used to address the removal of emerging contaminants, such as pharmaceuticals and microplastics, from wastewater. By modeling the behavior of contaminants and assessing the performance of treatment technologies, simulations enable engineers to optimize treatment processes and minimize environmental risks associated with emerging contaminants. Simulations play a crucial role in developing resource recovery strategies, such as energy and nutrient recovery, from wastewater. By simulating the performance of recovery technologies and evaluating their economic and environmental benefits, engineers can design integrated treatment systems that maximize resource recovery while minimizing environmental impact (Gernaey, et al., 2004).

In conclusion, case studies and real-world applications demonstrate the effectiveness of simulation-driven approaches in wastewater treatment. From optimizing treatment system design to addressing specific environmental challenges, simulations provide valuable insights and solutions for improving treatment performance, reducing environmental impact, and advancing sustainable water management practices. As the field of wastewater treatment continues to evolve, simulations will remain essential tools for innovation, optimization, and environmental stewardship.

8. Future Directions and Challenges

One potential advancement in simulation techniques for wastewater treatment is the integration of artificial intelligence (AI) algorithms. AI can enhance simulation models by learning from large datasets, identifying patterns, and optimizing complex systems in real-time. This integration could lead to more accurate and adaptive simulation models that can predict system behavior with higher precision. Another area for advancement is the development of multi-scale modeling approaches that can simulate processes occurring at different spatial and temporal scales simultaneously. By integrating models at the molecular, microscopic, and macroscopic levels, engineers can gain a more comprehensive understanding of complex phenomena in wastewater treatment systems, leading to more accurate predictions and optimized designs (Arumugham, et al., 2024).

One of the primary challenges facing simulation approaches in wastewater treatment is the availability and quality of data. Many simulation models rely on accurate input data, such as physical properties, reaction kinetics, and process parameters. However, obtaining reliable data for complex systems can be challenging, leading to uncertainties and inaccuracies in simulation results. Another limitation of current simulation approaches is computational complexity. As simulation models become more sophisticated and incorporate increasingly detailed representations of wastewater treatment processes, computational demands also increase. This can lead to longer simulation times, requiring high-performance computing resources and limiting the scalability of simulation models.

To address the challenges of data availability and quality, future research efforts should focus on data-driven modeling approaches that can leverage large datasets and sensor technologies to improve the accuracy and reliability of simulation models. Machine learning techniques, such as neural networks and support vector machines, can be used to analyze data, identify patterns, and make predictions in real-time. It is essential to enhance model validation and uncertainty analysis techniques to improve the reliability of simulation results. Future research efforts should focus on developing robust validation protocols and sensitivity analysis methods to quantify and mitigate uncertainties in simulation models. This will increase confidence in simulation predictions and facilitate informed decision-making in wastewater treatment plant design and operation. Integrating simulation with experimental methods, such as lab-scale experiments and pilot-scale studies, can provide valuable insights into process dynamics and validate simulation predictions. Future research efforts should emphasize the development of hybrid modeling approaches that combine experimental data with simulation models to improve the accuracy and applicability of wastewater treatment simulations (Schmidt et al., 2003).

In conclusion, future directions in simulation for wastewater treatment will likely involve advancements in techniques and technologies such as AI integration, multi-scale modeling, and data-driven modeling. However, addressing challenges such as data availability, computational complexity, and model validation will be critical for realizing the full potential of simulation approaches in improving the efficiency, sustainability, and resilience of wastewater treatment systems. By investing in research and development efforts and fostering collaboration between researchers, engineers, and industry stakeholders, we can overcome these challenges and unlock new opportunities for innovation in wastewater treatment simulation.

9. Conclusion

In this review, we have explored the significant role of simulation-driven approaches in wastewater treatment research and practice. We discussed various aspects, including the application of simulation techniques in addressing emerging challenges, optimizing treatment processes, and developing innovative solutions. The effectiveness of simulation-driven approaches in modeling pollutant removal mechanisms, optimizing treatment processes, and designing treatment systems. Real-world examples and case studies demonstrating the application of simulation techniques in wastewater treatment, such as membrane filtration, advanced oxidation processes, and biological nutrient removal systems. Future directions and challenges in simulation for wastewater treatment, including potential advancements in simulation techniques and technologies, challenges and limitations of current approaches, and recommendations for future research and development efforts.

Simulation-driven approaches have significant implications for advancing wastewater treatment technologies and promoting environmental sustainability. By harnessing the power of simulations, engineers and researchers can develop more efficient and effective treatment processes for removing emerging contaminants, optimizing resource recovery, and minimizing environmental impacts. Improve the design and operation of wastewater treatment systems, leading to enhanced treatment performance, reduced energy consumption, and lower operating costs. Foster innovation and collaboration in wastewater treatment research and practice, driving continuous improvement and progress towards sustainable water management practices.

As we move towards a more sustainable future, there is a clear call to action for embracing simulation-driven approaches in wastewater treatment research and practice. This includes investing in research and development efforts to advance simulation techniques and technologies for wastewater treatment. Integrating simulation into wastewater treatment education and training programs to build capacity and expertise in the field. Collaborating across disciplines and sectors to leverage simulation-driven approaches for addressing complex environmental challenges and promoting sustainable water management practices.

By embracing simulation-driven approaches and harnessing the power of simulations, we can drive innovation, optimize treatment processes, and advance environmental sustainability in wastewater treatment. Together, we can work towards a future where clean water is accessible to all, and wastewater is treated responsibly to protect our environment and public health.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

References

[1] Alvi, M., Batstone, D., Mbamba, C.K., Keymer, P., French, T., Ward, A., Dwyer, J. and Cardell-Oliver, R., 2023. Deep learning in wastewater treatment: a critical review. *Water Research*, p.120518.

[2] Amini, E., Mehrnia, M.R., Mousavi, S.M. and Mostoufi, N., 2013. Experimental study and computational fluid dynamics simulation of a full-scale membrane bioreactor for municipal wastewater treatment application. *Industrial & engineering chemistry research*, *52*(29), pp.9930-9939.

[3] Arumugham, T., Khudzari, J., Abdullah, N., Yuzir, A., Iwamoto, K. and Homma, K., 2024. Research trends and future directions on nitrification and denitrification processes in biological nitrogen removal. *Journal of Environmental Chemical Engineering*, p.111897.

[4] Aydiner, C., Sen, U., Koseoglu-Imer, D.Y. and Dogan, E.C., 2016. Hierarchical prioritization of innovative treatment systems for sustainable dairy wastewater management. *Journal of Cleaner Production*, *112*, pp.4605-4617.

[5] Aziz, A., Basheer, F., Sengar, A., Khan, S.U. and Farooqi, I.H., 2019. Biological wastewater treatment (anaerobic-aerobic) technologies for safe discharge of treated slaughterhouse and meat processing wastewater. *Science of the total environment*, *686*, pp.681-708.

[6] Benalia, M.C., Youcef, L., Bouaziz, M.G., Achour, S. and Menasra, H., 2022. Removal of heavy metals from industrial wastewater by chemical precipitation: mechanisms and sludge characterization. *Arabian Journal for Science and Engineering*, *47*(5), pp.5587-5599.

[7] Bequette, B.W., 2003. *Process control: modeling, design, and simulation*. Prentice Hall Professional.

[8] Berger, R.J., Stitt, E.H., Marin, G.B., Kapteijn, F. and Moulijn, J.A., 2001. Eurokin. Chemical reaction kinetics in practice. *Cattech*, *5*(1), pp.36-60.

[9] Bury, S.J., Groot, C.K., Huth, C. and Hardt, N., 2002. Dynamic simulation of chemical industry wastewater treatment plants. *Water science and technology*, *45*(4-5), pp.355-363.

[10] Busch, J., Cruse, A. and Marquardt, W., 2007. Modeling submerged hollow-fiber membrane filtration for wastewater treatment. *Journal of Membrane Science*, *288*(1-2), pp.94-111.

[11] Butler, D. and Schütze, M., 2005. Integrating simulation models with a view to optimal control of urban wastewater systems. *Environmental modelling & software*, *20*(4), pp.415-426.

[12] Clifford, D., Subramonian, S. and Sorg, T.J., 1986. Water treatment processes. III. Removing dissolved inorganic contaminants from water. *Environmental science & technology*, *20*(11), pp.1072-1080.

[13] D'Agostino, D., Serani, A. and Diez, M., 2020. Design-space assessment and dimensionality reduction: An off-line method for shape reparameterization in simulation-based optimization. *Ocean Engineering*, *197*, p.106852.

[14] Del Rio-Chanona, E.A., Cong, X., Bradford, E., Zhang, D. and Jing, K., 2019. Review of advanced physical and data-driven models for dynamic bioprocess simulation: Case study of algae–bacteria consortium wastewater treatment. *Biotechnology and bioengineering*, *116*(2), pp.342-353.

[15] Dimian, A.C., Bildea, C.S. and Kiss, A.A., 2014. *Integrated design and simulation of chemical processes*. Elsevier.

[16] Dobre, T.G. and Marcano, J.G.S., 2007. *Chemical engineering: Modeling, simulation and similitude*. John Wiley & Sons.

[17] Fuentes, K.L., Torres–Lozada, P. and Chaparro, T.R., 2021. Beverage wastewater treatment by anaerobic digestion in two-stages for organic matter removal and energy production. *Biomass and Bioenergy*, *154*, p.106260.

[18] Gao, D., Peng, Y. and Wu, W.M., 2010. Kinetic model for biological nitrogen removal using shortcut nitrification-denitrification process in sequencing batch reactor. *Environmental science & technology*, *44*(13), pp.5015-5021.

[19] Gernaey, K.V., Van Loosdrecht, M.C., Henze, M., Lind, M. and Jørgensen, S.B., 2004. Activated sludge wastewater treatment plant modelling and simulation: state of the art. *Environmental modelling & software*, *19*(9), pp.763-783.

[20] Gillot, S., De Clercq, B., Defour, D., Simoens, F., Gernaey, K. and Vanrolleghem, P.A., 1999, October. Optimization of wastewater treatment plant design and operation using simulation and cost analysis. In *Proceedings of 72nd Annual WEF Conference and Exposition, New Orleans, USA* (pp. 9-13).

[21] Gorito, A.M., Pesqueira, J.F., Moreira, N.F., Ribeiro, A.R., Pereira, M.F.R., Nunes, O.C., Almeida, C.M.R. and Silva, A.M., 2021. Ozone-based water treatment (O3, O3/UV, O3/H2O2) for removal of organic micropollutants, bacteria inactivation and regrowth prevention. *Journal of Environmental Chemical Engineering*, *9*(4), p.105315.

[22] Gray, N.F., 2014. Filtration methods. In *Microbiology of waterborne diseases* (pp. 631-650). Academic Press.

[23] Guardo, A., Coussirat, M., Larrayoz, M.A., Recasens, F. and Egusquiza, E., 2004. CFD flow and heat transfer in nonregular packings for fixed bed equipment design. *Industrial & Engineering Chemistry Research*, *43*(22), pp.7049-7056.

[24] Gupta, R.K., Poddar, B.J., Nakhate, S.P., Chavan, A.R., Singh, A.K., Purohit, H.J. and Khardenavis, A.A., 2022. Role of heterotrophic nitrifiers and aerobic denitrifiers in simultaneous nitrification and denitrification process: a nonconventional nitrogen removal pathway in wastewater treatment. *Letters in Applied Microbiology*, *74*(2), pp.159-184.

[25] Haile, T.M., Hobiger, G., Kammerer, G., Allabashi, R., Schaerfinger, B. and Fuerhacker, M., 2016. Hydraulic performance and pollutant concentration profile in a stormwater runoff filtration systems. *Water, Air, & Soil Pollution*, *227*, pp.1-16.

[26] Issa, H.M., 2019. Optimization of wastewater treatment plant design using process dynamic simulation: a case study from Kurdistan, Iraq. *ARO-The Scientific Journal of Koya University*, *7*(1), pp.59-66.

[27] Izadi, P., Izadi, P. and Eldyasti, A., 2020. Design, operation and technology configurations for enhanced biological phosphorus removal (EBPR) process: a review. *Reviews in Environmental Science and Bio/Technology*, *19*, pp.561-593.

[28] Jana, A.K., 2018. *Chemical process modelling and computer simulation*. PHI Learning Pvt. Ltd..

[29] Jhansi, S.C. and Mishra, S.K., 2013. Wastewater treatment and reuse: sustainability options. *Consilience*, (10), pp.1-15.

[30] Kamyar, A., Saidur, R. and Hasanuzzaman, M., 2012. Application of computational fluid dynamics (CFD) for nanofluids. *International Journal of Heat and Mass Transfer*, *55*(15-16), pp.4104-4115.

[31] Kuenen, J.G. and Robertson, L.A., 1994. Combined nitrification-denitrification processes. *FEMS Microbiology Reviews*, *15*(2-3), pp.109-117.

[32] Lin, Y.M., Tay, J.H., Liu, Y. and Hung, Y.T., 2009. Biological nitrification and denitrification processes. *Biological treatment processes*, pp.539-588.

[33] Liu, C., Bu, W. and Xu, D., 2017. Multi-objective shape optimization of a plate-fin heat exchanger using CFD and multi-objective genetic algorithm. *International Journal of Heat and Mass Transfer*, *111*, pp.65-82.

[34] Logan, B.E., Hermanowicz, S.W. and Parker, D.S., 1987. A fundamental model for trickling filter process design. *Journal (Water Pollution Control Federation)*, pp.1029-1042.

[35] López-Vázquez, C.M., Hooijmans, C.M., Brdjanovic, D., Gijzen, H.J. and van Loosdrecht, M.C., 2008. Factors affecting the microbial populations at full-scale enhanced biological phosphorus removal (EBPR) wastewater treatment plants in The Netherlands. *Water research*, *42*(10-11), pp.2349-2360.

[36] Lu, H., Li, Q. and Feng, W., 2022. Application progress of O3/UV advanced oxidation technology in the treatment of organic pollutants in water. *Sustainability*, *14*(3), p.1556.

[37] Manasa, R.L. and Mehta, A., 2020. Wastewater: sources of pollutants and its remediation. *Environmental Biotechnology Vol. 2*, pp.197-219.

[38] Meramo-Hurtado, S.I. and González-Delgado, A.D., 2021. Process synthesis, analysis, and optimization methodologies toward chemical process sustainability. *Industrial & Engineering Chemistry Research*, *60*(11), pp.4193-4217..

[39] Mingzhi, H., Ma, Y., Jinquan, W. and Yan, W., 2009. Simulation of a paper mill wastewater treatment using a fuzzy neural network. *Expert systems with Applications*, *36*(3), pp.5064-5070.

[40] Muoio, R., Palli, L., Ducci, I., Coppini, E., Bettazzi, E., Daddi, D., Fibbi, D. and Gori, R., 2019. Optimization of a large industrial wastewater treatment plant using a modeling approach: A case study. *Journal of environmental management*, *249*, p.109436.

[41] Mushila, C.N., Ochieng, G.M., Otieno, F.A.O., Shitote, S.M. and Sitters, C.W., 2016. Hydraulic design to optimize the treatment capacity of multi-stage filtration units. *Physics and Chemistry of the Earth, Parts A/B/C*, *92*, pp.85-91.

[42] Náthia-Neves, G., Berni, M., Dragone, G., Mussatto, S.I. and Forster-Carneiro, T., 2018. Anaerobic digestion process: technological aspects and recent developments. *International journal of environmental science and technology*, *15*, pp.2033-2046.

[43] Norton, T. and Sun, D.W., 2006. Computational fluid dynamics (CFD)–an effective and efficient design and analysis tool for the food industry: a review. *Trends in Food Science & Technology*, *17*(11), pp.600-620.

[44] Okino, M.S. and Mavrovouniotis, M.L., 1998. Simplification of mathematical models of chemical reaction systems. *Chemical reviews*, *98*(2), pp.391-408.

[45] Panebianco, S. and Pahl-Wostl, C., 2006. Modelling socio-technical transformations in wastewater treatment—a methodological proposal. *Technovation*, *26*(9), pp.1090-1100.

[46] Park, Y. and Mackie, A.L., 2023 Application of UV/TiO2 and UV/H2O2 Systems for Micropollutants' Treatment Process. In *Advanced Oxidation Processes for Micropollutant Remediation* (pp. 107-131). CRC Press.

[47] Pohl, A., 2020. Removal of heavy metal ions from water and wastewaters by sulfur-containing precipitation agents. *Water, Air, & Soil Pollution*, *231*(10), p.503.

[48] Priyadarshini, A., Sahoo, M.M., Raut, P.R., Mahanty, B. and Sahoo, N.K., 2021. Kinetic modelling and process engineering of phenolics microbial and enzymatic biodegradation: A current outlook and challenges. *Journal of Water Process Engineering*, *44*, p.102421.

[49] Rashed, M.N., 2013. Adsorption technique for the removal of organic pollutants from water and wastewater. *Organic pollutants-monitoring, risk and treatment*, *7*, pp.167-194.

[50] Reddy, T.A., 2006. Literature Review on Calibration of Building Energy Simulation Programs: Uses, Problems, Procedures, Uncertainty, and Tools. *ASHRAE transactions*, *112*(1).

[51] Rekhate, C.V. and Srivastava, J.K., 2020. Recent advances in ozone-based advanced oxidation processes for treatment of wastewater-A review. *Chemical Engineering Journal Advances*, *3*, p.100031.

[52] Revollar, S., Vilanova, R., Vega, P., Francisco, M. and Meneses, M., 2020. Wastewater treatment plant operation: simple control schemes with a holistic perspective. *Sustainability*, *12*(3), p.768.

[53] Rezai, B. and Allahkarami, E., 2021. Wastewater treatment processes—techniques, technologies, challenges faced, and alternative solutions. In *Soft computing techniques in solid waste and wastewater management* (pp. 35-53). Elsevier.

[54] Ryhiner, G.B., Heinzle, E. and Dunn, I.J., 1993. Modeling and simulation of anaerobic wastewater treatment and its application to control design: case whey. *Biotechnology Progress*, *9*(3), pp.332-343.

[55] Sahoo, T.R. and Prelot, B., 2020. Adsorption processes for the removal of contaminants from wastewater: the perspective role of nanomaterials and nanotechnology. In *Nanomaterials for the detection and removal of wastewater pollutants* (pp. 161-222). Elsevier.

[56] Sakiewicz, P., Piotrowski, K., Ober, J. and Karwot, J., 2020. Innovative artificial neural network approach for integrated biogas–wastewater treatment system modelling: Effect of plant operating parameters on process intensification. *Renewable and Sustainable Energy Reviews*, *124*, p.109784.

[57] Samer, M., 2015. Biological and chemical wastewater treatment processes. *Wastewater treatment engineering*, *150*, p.212.

[58] Saravanan, A., Kumar, P.S., Jeevanantham, S., Karishma, S., Tajsabreen, B., Yaashikaa, P.R. and Reshma, B., 2021. Effective water/wastewater treatment methodologies for toxic pollutants removal: Processes and applications towards sustainable development. *Chemosphere*, *280*, p.130595.

[59] Schmidt, I, Sliekers, O., Schmid, M., Bock, E., Fuerst, J., Kuenen, J.G., Jetten, M.S. and Strous, M., 2003. New concepts of microbial treatment processes for the nitrogen removal in wastewater. *FEMS microbiology reviews*, *27*(4), pp.481-492.

[60] Shafto, M., Conroy, M., Doyle, R., Glaessgen, E., Kemp, C., LeMoigne, J. and Wang, L., 2010. Draft modeling, simulation, information technology & processing roadmap. *Technology area*, *11*, pp.1-32.

[61] Shammas, N.K., Kumar, I.J., Chang, S.Y. and Hung, Y.T., 2005. *Sedimentation* (pp. 379-429). Humana Press.

[62] Trucano, T.G., Swiler, L.P., Igusa, T., Oberkampf, W.L. and Pilch, M., 2006. Calibration, validation, and sensitivity analysis: What's what. *Reliability Engineering & System Safety*, *91*(10-11), pp.1331-1357.

[63] Turányi, T. and Tomlin, A.S., 2014. *Analysis of kinetic reaction mechanisms* (Vol. 20). Berlin, Germany: Springer Berlin Heidelberg.

[64] Ullah, S., Guo, X., Luo, X., Zhang, X., Leng, S., Ma, N. and Faiz, P., 2020. Rapid and long-effective removal of broad-spectrum pollutants from aqueous system by ZVI/oxidants. *Frontiers of Environmental Science & Engineering*, *14*, pp.1-10.

[65] Ustun Odabasi, S. and Buyukgungor, H., 2024. Comparative study of degradation of pharmaceutical and personal care products in wastewater by advanced oxidation processes: Fenton, UV/H2O2, UV/TiO2. *CLEAN–Soil, Air, Water*, p.2300204.

[66] Wang, L.K., Vaccari, D.A., Li, Y. and Shammas, N.K., 2005. Chemical precipitation. In *Physicochemical treatment processes* (pp. 141-197). Totowa, NJ: Humana Press.

[67] Widder, S., Allen, R.J., Pfeiffer, T., Curtis, T.P., Wiuf, C., Sloan, W.T., Cordero, O.X., Brown, S.P., Momeni, B., Shou, W. and Kettle, H., 2016. Challenges in microbial ecology: building predictive understanding of community function and dynamics. *The ISME journal*, *10*(11), pp.2557-2568.

[68] Wu, X., Yang, Y., Wu, G., Mao, J. and Zhou, T., 2016. Simulation and optimization of a coking wastewater biological treatment process by activated sludge models (ASM). *Journal of environmental management*, *165*, pp.235-242.

[69] Zawawi, M.H., Saleha, A., Salwa, A., Hassan, N.H., Zahari, N.M., Ramli, M.Z. and Muda, Z.C., 2018, November. A review: Fundamentals of computational fluid dynamics (CFD). In *AIP conference proceedings* (Vol. 2030, No. 1). AIP Publishing.

[70] Zhang, S., Zheng, H. and Tratnyek, P.G., 2023. Advanced redox processes for sustainable water treatment. *Nature Water*, *1*(8), pp.666-681.