Journal of Engineering Science and Technology Review 18 (1) (2025) 157-163

Lecture Note

JOURNAL OF
Engineering Science and Technology Review

www.jestr.org

Simulating Aquatic Ecosystems as a Valuable Biotechnology Tool for Comprehending and Controlling Hazardous Chemical Substances

Nikolaos Stasinopoulos, Michail Chalaris* and Anastasia Tezari

School of Chemistry, Faculty of Sciences, Democritus University of Thrace, St. Lucas 65 404 Kavala, Greece.

Received 4 January 2024; Accepted 10 December 2024

Abstract

Aquatic ecosystems stand as pivotal elements within our environment, hosting a myriad of life forms and providing essential services. These ecosystems are increasingly threatened by hazardous chemical substances, posing significant risks to both environmental and human health. To address these challenges, biotechnological tools, particularly ecological simulation models, have become essential. These models enhance our understanding of the behavior and impact of harmful chemicals in aquatic environments. By integrating quantitative structure-activity relationship (QSAR) models, predictive simulations, and environmental risk assessments, biotechnology offers innovative strategies for mitigating chemical hazards in these ecosystems. This approach not only deepens our comprehension but also aids in developing effective management practices to protect aquatic life and human communities.

Keywords: Aquatic Ecosystems, Ecological Simulation Models, QSAR Models, Chemical Hazards, Biotechnology Tools.

1. Introduction

Aquatic ecosystem simulations are essential in biotechnology for understanding and managing the behavior and dispersion of hazardous chemical substances in water bodies. These models predict the fate and transport of such chemicals by incorporating detailed biological and biochemical properties, alongside varying environmental conditions. This predictive capability is crucial for assessing potential biological and environmental impacts, including effects on aquatic species, habitats, ecosystems, and the risks of bioaccumulation and ecological disruptions.

By providing insights into chemical dispersion and reactions, simulation tools are vital for developing effective mitigation strategies. They enable researchers and regulators to identify intervention points, such as implementing containment measures, exploring water treatment options, or designing ecological restoration plans. Moreover, these models support regulatory compliance by helping organizations adhere to environmental regulations and demonstrate responsible management of hazardous substances.

Integrating real-time monitoring data into ecosystem models enhances their function as early warning systems. Upon detecting dangerous substances, simulations can forecast their likely spread and impact, facilitating timely and strategic responses. In events like chemical spills, simulations assist in optimizing cleanup efforts by determining the most effective methods for removing or neutralizing harmful substances, thereby minimizing long-term ecological damage [1].

Simulations also inform the design of bioremediation projects by predicting the growth and activity of specific microbial communities under different conditions, which is essential for the effective use of microorganisms in degrading certain hazardous chemicals. In research and development, simulations offer a controlled environment to study the behavior of dangerous substances, aiding in the creation of new biotechnological solutions to mitigate their effects. Additionally, simulations serve educational purposes, raising awareness among professionals, decision-makers, and the public about the potential risks associated with hazardous chemicals in aquatic ecosystems [2].

In summary, aquatic ecosystem simulations are integral to comprehensive risk assessments, enabling informed decision-making and effective risk management concerning hazardous chemicals in water bodies. They play a crucial role in predicting chemical behavior, assessing environmental impacts, guiding mitigation strategies, ensuring regulatory compliance, and facilitating education and awareness.

2. Biological aspects of modeling aquatic ecosystems

Understanding the interactions between hazardous chemical substances and aquatic ecosystems is crucial for assessing environmental risks and implementing effective management strategies. Key biological aspects to consider in this context include:

Bioaccumulation and Biomagnification: Hazardous chemicals can accumulate in aquatic organisms over time, leading to higher concentrations than those found in the surrounding environment. This process, known as bioaccumulation, can result in biomagnification, where chemical concentrations increase at each trophic level of the food web, potentially causing adverse effects on predators, including humans.

Species Sensitivity and Tolerance: Different species exhibit varying sensitivities to chemical pollutants. Some may develop tolerance through adaptive mechanisms, while others

*E-mail address: mchalaris@chem.duth.gr
ISSN: 1791-2377
doi:10.25103/jestr.181.17

remain highly susceptible. Assessing species-specific responses is essential for accurate ecological risk assessments.

Community and Ecosystem-Level Effects: Chemical pollutants can alter community structures by affecting species composition and interactions. These changes can lead to shifts in ecosystem functions, such as nutrient cycling and energy flow, potentially causing long-term ecological imbalances.

Incorporating these biological aspects into models enhances the accuracy of predictions regarding the fate and impact of hazardous chemicals in aquatic ecosystems, thereby informing more effective environmental management and conservation efforts. To begin with, the toxicity of chemicals, which is usually dose-dependent, is taken into account by biological models. The most critical factors for the models are the concentration of the substance and its bioavailability. As levels of sensitivity to toxicants vary from organism to organism, models often include multiple species to represent this diversity. As it is possible for dangerous chemicals to enter the tissues of aquatic foods. The models analyze the biomagnification and bioaccumulation of these substances as they move up the food chain, potentially reaching higher trophic levels. The biology of each organism, including its feeding habits and metabolic processes, determines how chemicals are transported through the ecosystem.

Predator-prey interactions, their competition and other ecological relationships can be captured by various ecological models. These interactions affect the distribution and abundance of species in the ecosystem and can be disrupted by a potential influx of hazardous substances into the ecosystem and lead to cascading effects within. Various life history traits of organisms, such as reproduction rates, growth rates, and mortality rates, may be incorporated into biological models. From these characteristics we have a picture of how populations respond to various changes in the environment as well as to exposure to chemical substances. The resilience of aquatic ecosystems from chemical disturbances has different levels. The resilience of ecosystems varies due to the presence of comparable species or ecological processes that contribute to mitigating the effects of hazardous chemicals. The models are possible to help in the recovery of the ecosystem after chemical analyses [3].

An essential factor influencing water ecosystems is the behavior and dynamics of microbial communities, which determine the transformation and fate of chemical substances. Through modeling, researchers can analyze the structure and activity of these microorganisms, gaining insights into their role in degrading and breaking down harmful chemicals. Aquatic organisms within ecosystems display specific habitat preferences, which models must account for when predicting species distribution and population changes in environments containing hazardous substances.

Moreover, these models often include evolutionary processes to anticipate population responses under chemical stress. Over time, certain species can adapt to chemical exposure through genetic modifications, enhancing their survival. In addition, when ecosystems supply drinking water or food resources, models can integrate human biological interactions to assess the potential health risks posed by consuming contaminated water or aquatic organisms. This approach improves understanding of how exposure to hazardous substances may impact human health [4].

3. Ecological Simulation Models

In environmental science, understanding the complex dynamics within aquatic ecosystems remains a significant challenge. These ecosystems are highly intricate, influenced by biological processes and environmental variables. However, one of the most profound disturbances comes from the introduction of hazardous chemical substances. To address this issue effectively and devise sustainable management solutions, ecological simulation models have become an invaluable resource [5].

These models simulate how hazardous chemicals move and behave within aquatic environments, accounting for bioaccumulation and biomagnification. Such predictions are vital because contaminants can build up within aquatic species and eventually enter human food systems when people consume polluted water or aquatic organisms. By integrating human exposure pathways into these models, researchers can evaluate health risks tied to chemical contamination. For instance, Quantitative Structure-Activity Relationship (QSAR) models can estimate the toxicity of chemical compounds and their potential concentrations in pathways relevant to human health. This provides a broader perspective, highlighting the importance of predictive modeling as an early warning tool for mitigating health risks linked to water pollution.

QSAR models serve as tools to predict chemical behavior—such as toxicity and environmental persistence—based on a substance's molecular structure. By leveraging mathematical relationships, QSAR methods correlate the physical and chemical properties of a compound with its biological activity, enabling scientists to assess toxicity and environmental impact without extensive laboratory testing. When combined with ecological simulations, these models offer three key benefits:

i. Predicting Chemical Behavior: QSAR models anticipate how chemicals will behave across various environmental compartments, such as water, soil, and sediments. Meanwhile, ecological simulations evaluate the consequences of these chemicals on ecosystems and species.
ii. Analyzing Toxicity: Using QSAR data, simulations can estimate the effects of toxic substances on individual species and predict the cascading impacts on populations and ecosystems.
iii. Supporting Risk Assessment: These tools provide a robust framework for assessing environmental risks associated with hazardous chemicals and proposing measures to mitigate such risks.

3.1. Human

At their core, ecological simulation models function as computational frameworks that replicate interactions between species, chemicals, and environmental factors within aquatic systems. These models allow scientists to uncover hidden relationships and observe how hazardous chemicals influence both ecosystems and human health.

For example, chemical warfare agents (CWAs) represent particularly dangerous substances with the potential to devastate aquatic ecosystems and pose significant risks to human populations. Traditional methods often struggle to capture the intricacies of how CWAs interact with organisms and environmental variables. In contrast, ecological simulation models provide a virtual platform to analyze these interactions under controlled yet realistic conditions.

3.2. Predicting the Unpredictable

One of the greatest strengths of ecological simulations is their predictive capability. By modeling the behavior and spread of hazardous substances like CWAs, scientists can anticipate how these chemicals might disperse, transform, or accumulate within aquatic systems.

This foresight is more than theoretical; it has practical implications for proactive decision-making and risk management. Understanding the behavior of hazardous substances allows policymakers and environmental managers to implement containment strategies, design effective treatment solutions, and mitigate potential threats to ecosystems and human health.

3.3. Unveiling Environmental Impacts

Beyond prediction, ecological simulations provide critical insights into the environmental impacts of chemical releases. These models can illustrate how pollutants ripple through aquatic systems, affecting species diversity, habitats, and overall ecosystem stability [6].

Key phenomena, such as bioaccumulation and the disruption of ecological processes, are also addressed. For instance, simulations can demonstrate how contaminants accumulate within specific species, reaching concentrations that pose significant ecological risks. These insights are fundamental to creating targeted management and conservation strategies that safeguard aquatic ecosystems.

3.4. Navigating the Regulatory Landscape

In an era of stringent environmental regulations, ecological simulations assist organizations in meeting compliance standards. By modeling the interactions between hazardous substances and aquatic systems, organizations can demonstrate a proactive approach to environmental stewardship. This includes ensuring regulatory requirements are met and showcasing effective measures for minimizing environmental harm.

In exploring the applications of ecological simulation models, we uncover their potential to bridge knowledge gaps and provide actionable insights. These tools empower researchers, policymakers, and environmental managers to study the interplay between hazardous chemicals and aquatic environments. Ultimately, they equip us with the data needed to protect ecosystem health and safeguard communities reliant on clean water and sustainable food systems.

4. Risk Assessment

Hazardous chemical substances pose a serious threat to the stability of aquatic ecosystems, leading to profound environmental and ecological disruptions. To address these concerns, simulations of aquatic ecosystems have emerged as indispensable tools in contemporary risk assessment frameworks [7]. These models effectively translate the intricate interactions between pollutants, aquatic organisms, and environmental factors into quantifiable outcomes. By analyzing risks that are otherwise challenging to measure, these simulations enable the evaluation of chemical contaminants' potential effects and provide projections of their long-term consequences.

The predictive capabilities of these tools are particularly valuable for improving decision-making and implementing effective risk management strategies. Aquatic ecosystem models offer critical insights to a range of stakeholders, including scientists, policymakers, and environmental managers. With evidence rooted in data, authorities can develop preventative measures, minimize environmental harm, and enhance the resilience of aquatic systems. Additionally, these simulations facilitate a deeper understanding of vulnerabilities, enabling decision-makers to balance human activities with the preservation of ecosystems and the well-being of dependent communities.

In essence, aquatic ecosystem simulations serve as a vital link between uncertainty and informed action. By delivering a scientifically robust foundation for risk evaluation and intervention planning, these tools play a key role in safeguarding water resources and promoting ecological sustainability over the long term.

5. Monitoring and Early Warning

In today’s interconnected and fast-paced world, addressing emerging threats to aquatic ecosystems requires both speed and accuracy. The integration of real-time monitoring data with ecosystem models offers a powerful foundation for developing effective early warning systems [7]. This synergy between advanced technology and ecological knowledge facilitates a constant stream of real-time insights, enabling continuous monitoring of aquatic environments. By incorporating live data on hazardous substances' presence and behavior, ecosystem models can process and interpret this information into actionable predictions.

These predictive simulations are instrumental in identifying the pathways, distribution, and potential impacts of pollutants. By offering critical foresight, they enable authorities to anticipate environmental risks before they escalate. Functioning as a proactive early warning mechanism, this system empowers decision-makers to act strategically—allocating resources precisely where they are needed to minimize damage.

Such capabilities are vital for preventing environmental crises and protecting the health of water systems. By detecting risks at their onset, these tools ensure swift and effective responses, thereby averting long-term harm to aquatic ecosystems and the communities reliant on them. Ultimately, integrating monitoring technologies with predictive models strengthens our ability to safeguard water resources amid growing environmental challenges.

6. Designing Bioremediation Strategies

Nature provides an effective remedy for addressing hazardous chemicals through bioremediation, a natural process that utilizes the capabilities of microorganisms to degrade and neutralize pollutants. These microorganisms, though microscopic and often overlooked, play a critical role in restoring ecological equilibrium. Their efficiency, however, depends on several factors, such as environmental conditions, pollutant levels, and the diversity and composition of microbial communities [8, 9].

In this context, simulations have become invaluable tools for designing and optimizing bioremediation approaches. By employing computational techniques, these models can predict the growth, activity, and behavior of specific microbial communities under different environmental scenarios. This enables scientists to better understand the intricate interactions between microorganisms and contaminants, facilitating the development of tailored bioremediation strategies suited to various ecosystems.

The predictive capabilities of simulations ensure that bioremediation efforts are not only scientifically robust but also efficient in terms of time and resources. Acting as tools for ecological restoration, these simulations provide a structured framework to forecast outcomes and fine-tune interventions. By leveraging microbial processes effectively, this approach addresses pollution challenges while fostering long-term resilience and health within the environment.

7. Optimizing Cleanup Efforts

Chemical spills in aquatic ecosystems present urgent challenges that demand swift and precise action. These unexpected incidents disrupt the delicate ecological balance, requiring coordinated responses to minimize both their immediate effects and long-term consequences. In such scenarios, simulations emerge as critical tools, providing predictive insights to guide and enhance cleanup operations [7]. Using computational models, simulations evaluate optimal methods for removing or neutralizing hazardous substances. These models consider various factors, including the nature of the spill, prevailing environmental conditions, and the behavior of contaminants within the ecosystem. By identifying the most effective response strategies, simulations help to limit ecological damage while ensuring that interventions are both timely and resource-efficient.

This predictive capability not only addresses the immediate threats posed by chemical spills but also contributes to the long-term health and resilience of aquatic ecosystems. Acting as strategic allies in environmental recovery, simulations empower decision-makers to implement effective measures that protect vital water resources and the diverse species they support.

8. Research and Development

In research and development, simulations serve as both analytical instruments and creative platforms, empowering scientists to explore the behavior of hazardous substances within controlled virtual environments. This method supports the creation of innovative biotechnological approaches to manage and reduce the impact of these pollutants. By acting as a virtual laboratory, simulations enable a detailed analysis of the intricate interactions between contaminants and biological systems, providing essential insights for designing effective remediation strategies.

This approach not only deepens our understanding of complex environmental issues but also accelerates the formulation of targeted solutions aimed at protecting and restoring aquatic ecosystems. Through simulations, researchers can test and refine interventions efficiently, paving the way for sustainable management of pollution challenges.

9. Education and Training

The value of simulations extends well beyond the confines of laboratories, serving as essential tools for education and professional training. By converting complex ecological processes into clear, accessible models, simulations help raise awareness about the risks posed by hazardous chemicals in aquatic ecosystems. This educational function is vital, as it equips professionals, decision-makers, and the broader public with the knowledge necessary to understand and address potential environmental threats effectively.

Simulations act as interactive platforms for developing skills and sharing knowledge. They enable stakeholders to visualize the immediate and long-term consequences of contamination, explore viable mitigation techniques, and assess the broader impacts on ecosystems. Through this process, simulations foster a sense of readiness and vigilance, empowering policymakers, scientists, and community members to take proactive steps toward protecting water systems.

In essence, simulations stand as pillars of both understanding and management. They offer the critical insights needed to drive informed decisions and implement timely interventions. By leveraging their transformative capabilities, simulations become integral to the collective effort to preserve aquatic ecosystems and ensure their essential role in supporting life on Earth.

10. Biology in Aquatic Ecosystem Modeling for Dangerous Chemical Substances

Modeling the behavior of hazardous chemicals in aquatic ecosystems relies on a profound understanding of the biological processes that govern these intricate environments. This chapter explores the fundamental biological aspects that are essential for building ecological simulations and predicting their outcomes [10].

10.1. Navigating Toxicity and Bioavailability

In aquatic systems, the toxicity of chemicals depends on their dose and bioavailability—how much of the substance can be absorbed by organisms and cause harm. Different species within aquatic ecosystems exhibit varying levels of sensitivity to pollutants, reflecting the system's biological diversity. Models must, therefore, account for these variations and incorporate a wide range of species to accurately represent the ecosystem's complexity [11].

10.2. Unpacking Biomagnification and Bioaccumulation

Once hazardous substances enter an aquatic environment, they can accumulate in organisms and move up the food chain. This process, known as bioaccumulation and biomagnification, depends on the biology of the organisms involved. Factors like feeding behaviors, metabolic rates, and ecological roles play critical roles in determining how contaminants transfer and intensify across trophic levels. Models help simulate these pathways, providing insights into the distribution of chemicals within ecosystems [12].

10.3. Species Interactions: A Dance of Life and Survival

Aquatic ecosystems are shaped by complex interactions, including predator-prey relationships, resource competition, and other ecological dynamics. These relationships determine species distribution and population stability. However, the introduction of hazardous chemicals can disrupt these interactions, triggering cascading effects throughout the ecosystem. Models analyze these disruptions to assess potential impacts and identify strategies to mitigate ecological imbalance.

10.4. Life History Traits: The Blueprint of Survival

Life history traits—such as reproduction rates, growth patterns, and mortality—are key biological factors that influence how populations respond to chemical stressors.

These traits act as the engine for adaptation, determining the resilience or vulnerability of species. Incorporating life history traits into models allows for accurate predictions of population dynamics under changing environmental conditions.

10.5. Ecological Resilience: Bouncing Back from Adversity

Aquatic ecosystems are dynamic and possess varying degrees of resilience when exposed to chemical contamination. Simulations evaluate an ecosystem's capacity for recovery by analyzing its biological and structural components. Understanding resilience helps predict long-term ecosystem health and informs management strategies aimed at restoration..

10.6. Microbial Communities: Nature's Cleanup Crew

Microbial communities play a vital role in breaking down and neutralizing hazardous chemicals within aquatic environments. These microscopic organisms act as nature's cleanup crew, facilitating bioremediation. Models analyze microbial activity and community composition, highlighting their role in detoxifying pollutants and maintaining ecosystem balance.

10.7. Habitat Preferences: Nature's Niche

Each aquatic species occupies a specific niche, with distinct habitat preferences that influence their distribution and survival. Models consider these preferences when assessing the impact of hazardous chemicals, as they determine which species are most vulnerable and how contaminants spread within the ecosystem. Understanding these niches provides essential insights into the structure and functioning of aquatic systems.

10.8. Adaptation and Evolution: Nature's Response to Change

Over time, aquatic species may undergo genetic adaptations to cope with chemical stressors. These evolutionary processes allow populations to survive and persist in contaminated environments. Ecological models incorporate these adaptive responses to predict how species might evolve under prolonged exposure to hazardous substances, offering a long-term perspective on ecosystem stability.

10.9. Human Health Considerations: A Holistic Perspective

Aquatic ecosystems often provide essential resources, such as drinking water and food. As a result, human health is closely linked to the biology of these systems. Models extend their analyses to include the risks posed by chemical contaminants to human populations through the consumption of polluted water or aquatic organisms. This broader perspective ensures that ecosystem management strategies prioritize public health and safety.

10.10 Broader Ecological Impact

The consequences of chemical contamination in aquatic systems extend beyond water bodies, affecting adjacent terrestrial ecosystems. Contaminants like heavy metals, pesticides, and industrial pollutants can accumulate in aquatic organisms, which serve as food sources for terrestrial wildlife. This bioaccumulation can lead to toxic effects in birds, mammals, and other species that rely on aquatic prey. Additionally, contaminated water can migrate via runoff or groundwater flow, introducing pollutants into soils and disrupting plant health, soil microbial communities, and terrestrial ecosystem functions. These interconnections underscore the need to address chemical contamination as a broader environmental concern that spans aquatic and terrestrial boundaries.

In summary, understanding the biological foundations of aquatic ecosystems is essential for building accurate and reliable models to address hazardous chemical contamination. These models integrate knowledge of species biology, ecological interactions, and adaptive processes to provide a comprehensive understanding of how contaminants influence ecosystem health. By bridging aquatic and terrestrial systems, they offer holistic insights to guide sustainable environmental management and protection strategies.

11. Examples

AQUATOX is a simulation model specifically designed to represent aquatic ecosystems. It forecasts the behavior and fate of pollutants, including nutrients and organic chemicals, while assessing their impacts on various ecosystem components, such as fish, invertebrates, and aquatic plants. As a versatile tool, AQUATOX is particularly useful for ecologists, biologists, water quality experts, and professionals conducting ecological risk assessments for aquatic environments. While it integrates principles from traditional ecosystem and chemodynamic models, AQUATOX was purposefully developed as a practical and user-friendly model tailored to meet the needs of environmental analysts from the outset [13].

AQUATOX and similar models can provide us with powerful tools to simulate the fate of pollutants and predict ecosystem responses, although they are subject to inherent limitations that we need to recognise when interpreting the results. The quality and resolution of input data, such as pollutant loads, environmental conditions and biological parameters, are factors on which the accuracy of these models depends primarily, but also parallel factors that can be difficult to obtain accurately. In addition, the complexity of real ecosystems, including spatial heterogeneity, synergistic effects between multiple stressors and adaptive species behaviour, can challenge model predictions. These models may not fully capture local-scale variability or long-term dynamics, although efforts are being made to validate them by comparing them to field data. This makes it necessary for ecological risk assessments to be supported by careful application and the use of complementary field studies.

AQUATOX Applications. AQUATOX can be used to address a wide variety of issues requiring a better understanding of the processes relating the chemical and physical environment to the biological community. Possible applications of AQUATOX include:

- Developing numeric nutrient targets based on desired biological endpoints.
- Evaluating which of several stressors is causing observed biological impairment.
- Predicting effects of pesticides and other toxic substances on aquatic life.
- Evaluating potential ecosystem responses to climate change.
- Determining effects of land use changes on aquatic life by using the linkage with BASINS.

- Estimating time to recovery of contaminated fish tissues to safe levels after reducing pollutant loads.

To highlight the practical applications of AQUATOX, several case studies demonstrate its effectiveness in predicting ecological impacts and guiding water system management strategies. For instance, AQUATOX has been successfully applied to evaluate nutrient loading and establish water quality objectives for rivers and reservoirs, including Onondaga Lake in New York and Coralville Reservoir in Iowa. By simulating nutrient dynamics, algal blooms, and dissolved oxygen levels, these projects provided critical insights that informed decisions to reduce nutrient pollution and enhance ecosystem health (US EPA).

Beyond nutrient management, AQUATOX has also been employed for ecological risk assessments. In one notable case, the model was used to predict the recovery of contaminated fish populations in Dalyan Lagoon, Turkey, following exposure to Dieldrin, a persistent organic pollutant. The simulations effectively tracked the dispersion of the contaminant and its biological effects, offering valuable guidance for mitigation efforts. This case underscored the model's ability to link chemical pollution with biological responses, supporting remediation strategies (US EPA).

For Onondaga Lake, simulations conducted with AQUATOX demonstrated a strong correlation between predicted dissolved oxygen levels and observed algal biomass data, leading to successful nutrient management plans. Similarly, in the Coralville Reservoir, the model accurately captured eutrophication trends, aligning closely with field observations. These results were instrumental in setting water quality goals and informing restoration initiatives (US EPA) [14].

In the case of Dalyan Lagoon, the model's predictions for Dieldrin dispersion and its ecological impacts matched post-remediation monitoring data with remarkable precision, showcasing its reliability for contamination assessments (US EPA). These examples collectively illustrate the versatility and robustness of AQUATOX in real-world scenarios, particularly in predicting pollutant behavior and ecological outcomes.

However, it is essential to recognize that the accuracy of AQUATOX simulations depends significantly on site-specific conditions and the quality of input data. To improve prediction reliability, continuous calibration and validation with localized data remain critical components of the modeling process [15].

12. Contribution to sustainability

The simulation and modeling of aquatic ecosystems in relation to hazardous chemical substances can significantly contribute to addressing global challenges and advancing the Sustainable Development Goals (SDGs), adopted by the United Nations in 2015. These goals, embraced by governments, industries, and organizations worldwide, aim for realization by 2030. Specifically, several SDGs are directly linked to the outcomes of this work:

i. SDG 3: Good Health and Well-Being
Exposure to hazardous chemical agents, such as nerve agents, through contaminated water poses severe health risks for communities living in affected areas. Ensuring good health and well-being becomes increasingly difficult when populations are exposed to these toxic substances. This research contributes to SDG 3 by improving our understanding of the behavior of hazardous chemicals in aquatic environments and offering innovative approaches to reduce chemical pollution, thereby mitigating its harmful impacts on human health [16].

ii. SDG 6: Clean Water and Sanitation
SDG 6 focuses on ensuring access to clean and safe drinking water while addressing water quality concerns. The contamination of water-sensitive areas by toxic chemical agents severely hampers efforts to meet this goal. This study provides strategies for mitigating water pollution caused by chemical warfare agents, thus supporting the availability of clean water and safeguarding public health.

iii. SDG 9: Industry, Innovation, and Infrastructure
Building resilient infrastructure and fostering innovation are central to SDG 9. Incidents involving chemical warfare agents in water-sensitive regions require innovative disaster risk management strategies and infrastructure protection measures. The development of precise ecological models, as presented in this study, offers critical insights for disaster management and infrastructure resilience. These findings promote safety, preparedness, and sustainability in addressing hazardous chemical incidents

iv. SDG 11: Sustainable Cities and Communities
Urban areas situated near water-sensitive regions are particularly vulnerable to contamination by chemical warfare agents. Ensuring the sustainability and resilience of cities and communities requires addressing these risks effectively. This study highlights the importance of mitigating chemical pollution to protect urban populations and maintain the long-term sustainability of cities.

v. SDG 13: Climate Action
Chemical warfare agents can lead to environmental damage, impacting soil and water quality and contributing to climate-related challenges. Managing these incidents aligns with broader climate action goals, as effective mitigation strategies help prevent further environmental degradation and support efforts to combat climate change.

vi. SDG 14: Life Below Water
Aquatic ecosystems such as wetlands, rivers, and coastal zones are essential habitats for marine life. Contamination by hazardous chemicals poses a substantial threat to marine biodiversity and the health of aquatic environments, jeopardizing the objectives of SDG 14. By addressing chemical pollution, this study supports the preservation and sustainability of aquatic ecosystems.

vii. SDG 15: Life on Land
Terrestrial ecosystems are closely connected to aquatic environments, particularly in water-sensitive regions. Chemical contamination, including from warfare agents, can spread from water to land, affecting soil quality, biodiversity, and terrestrial ecosystems. This study underscores the importance of managing these pollutants to prevent disruptions to life on land and ensure the preservation of biodiversity.

In conclusion, the modeling and simulation of hazardous chemicals in aquatic ecosystems represent a multidisciplinary approach that supports progress toward multiple SDGs. By offering solutions for pollution mitigation, ecological preservation, and public health protection, this work provides actionable insights to advance sustainability goals and promote environmental resilience.

13. Conclusions and Discussion

Incorporating the biological components of aquatic ecosystems into models for hazardous chemical substances requires a multidisciplinary approach. This integration combines essential insights into the characteristics of aquatic organisms, their ecological interactions, and their responses to chemical stress. Such models provide a comprehensive perspective on the potential effects of dangerous substances on ecosystem health, functionality, and species dynamics. As a result, simulating aquatic ecosystems becomes a vital tool for biological and biotechnological research, enabling a deeper understanding of the environmental impacts of chemical pollutants. By leveraging these simulations effectively, informed decisions can be made, and proactive measures can be implemented to protect both aquatic ecosystems and human well-being [17].

Europe's rivers, lakes, oceans, and seas are critical both ecologically and economically. In the coming years, significant investments in water-related initiatives are expected. The European Green Deal prioritizes the protection of biodiversity and ecosystems, highlighting the need to reduce pollution across air, water, and land while advancing toward a circular economy. Central to this initiative is the creation of a toxic-free environment that not only preserves the environment but also enhances the health and quality of life of European citizens.

The chemical warfare agents examined in this study are particularly harmful to living organisms, posing severe risks to both aquatic ecosystems and human health. Within the context of the European Green Deal, the modeling of these hazardous chemicals is essential to achieving a toxic-free environment. Furthermore, the rapid and efficient detection, assessment, and mitigation of these agents are critical to safeguarding aquatic ecosystems and public health within limited timeframes.

Acknowledgement

This work is carried out as part of the "GROWTH" project, funded under the "ERASMUS-EDU-2022-CB-VET" initiative by the European Education and Culture Executive Agency (EACEA). It is implemented within the framework of the "Erasmus+" Program, Key Action 2, with the primary objective of "Strengthening resilience through targeted national and local scientific and practical training activities aimed at capacity building, risk awareness, and addressing the impacts of man-made disasters" (Project Code: 80884).

References

[1] L. Schuijt, F. Peng, S. Berg, M. Dingemans, and P. Brink, "(Eco)toxicological tests for assessing impacts of chemical stress to aquatic ecosystems: Facts, challenges, and future," *Sci. Total Environ.*, vol. 795, Nov. 2021, Art. no. 148776

[2] D. Aksnes, K. Ulvestad, B. Baliño, J. Berntsen, J. Egge, and E. Svendsen, "Ecological modelling in coastal waters: Towards predictive physical-chemical-biological simulation models," *Ophelia*, vol. 41, no. 1, pp. 5–36, Feb. 2012.

[3] M. Chalaris, A. Giannopoulos, G. Koufioti, N. Stasinopoulos, and A. Tezari, "Comparative study of the methods used for the risk analysis of emergency water pollution accidents," *Ocean J. Chem. Pet. Eng.*, vol. 1, no. 1, pp. 1–19, Dec. 2021.

[4] F. A. Quintero, S. J. Patel, F. Muñoz, and M. Sam Mannan, "Review of Existing QSAR/QSPR Models Developed for Properties Used in Hazardous Chemicals Classification System," *Ind. Eng. Chem. Res.*, vol. 51, no. 49, pp. 16101–16115, Dec. 2012, doi: 10.1021/ie301079r.

[5] P. Gramatica, E. Papa, and A. Sangion, "QSAR research unit on environmental chemistry and ecotoxicology," *Environ. Sci.: Processes Imp.*, vol. 20, no. 20, pp. 38–47, Dec. 2018.

[6] B. Rodriguez-Brito *et al.*, "Viral and microbial community dynamics in four aquatic environments," *The ISME J.*, vol. 4, no. 6, pp. 739–751, Jun. 2010, doi: 10.1038/ismej.2010.1.

[7] K. Khan, K. Roy, and E. Benfenati, "Ecotoxicological QSAR modeling of endocrine disruptor chemicals," *J. Hazard. Mater.*, vol. 369, pp. 707–718, May 2019.

[8] D. Bourne, K. Morrow, and N. Webster, "Insights into the coral microbiome: Underpinning the health and resilience of reef ecosystems," *Ann. Rev. Microbiol.*, vol. 70, pp. 317–340, Jun. 2016.

[9] R. M. Kliegman, *Nelson textbook of pediatrics*, 21st edition. Philadelphia, MO: Elsevier, 2019.

[10] M. Miyamoto, H. Tanaka, and T. Katagi, "Ecotoxicological Risk Assessment of Pesticides in Aquatic Ecosystems," 2008. [Online]. Available: https://api.semanticscholar.org/CorpusID:46609895

[11] S. Sharma, "Bioremediation: Features, strategies and applications," *Asian J. Pharm. Life Sci.*, vol. 2, no.2, pp. 202 – 213, Jan. 2012.

[12] M. Chalaris, "Water, terrorist attacks, industrial accidents, and modeling possible impacts of these incidents in coastal ecosystems with computational model," in *Proc. 6th Int. Electron. Conf. Water Sci. Soft Hard Interventions Adapt Mitigate Abiotic Biotic Coastal Change Climate Change Human Interventions*, *Environ. Sci. Proc.* vol. 3 Nov. 2021, pp. 1-4.

[13] R. Park, J. Clough, and M. Wellman, "AQUATOX: Modeling environmental fate and ecological effects in aquatic ecosystems," *Ecol. Modell.*, vol. 213, no. 1, pp. 1–15, Mar. 2008.

[14] R. Park and J. Clough, "Aquatox (Release 3.1) Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems Volume 2: Technical Documentation," National Service Center for Environmental Publications (NSCEP), Washington, D.C, EPA-820-R-14-007, Apr. 2014. [Online]. Available: https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P100IJOL.TXT

[15] A. Erturk, R. A. Ambrose, and B. Rashleigh, "Case study: Dieldrin attack in Dalyan Lagoon, assessment of the fates and effects of toxic agents on water resources," in *Assess. Fate Effec. Toxic Agen. Water Resour.*, I. E. Gonenc, V. G. Koutitonsky, B. Rashleigh, R. B. Ambrose, and J. P. Wolflin, Eds., Dordrecht: Springer Netherlands, 2007, pp. 329–386.

[16] M. Chalaris, N. Stasinopoulos, and A. Tezari, "Analysis of the legal framework on hazardous substances: A multilevel correlation between international, European and national perspective," *J. Eng. Sci. Technol. Rev.*, vol. 14, no. 6, pp. 169–175, Dec. 2021.

[17] J. Fleeger, K. Carman, and R. Nisbet, "Indirect effects of contaminants in aquatic ecosystems," *Sci. Total Environ.*, vol. 317, no 1-3, pp. 207–233, Dec. 2003.