The Endless Possibilities of Modelling of Toxic Chemical Warfare Agents and Possible Impacts of Their Release in Water Sensitive Areas

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Abstract: - Nerve agents are chemical compounds that constitute chemical weapons with many effects on human health as well as the environment. In this work, an analysis of the properties of several nerve agents and their dispersion in aquatic ecosystems is proposed, by exploring the possibilities of state-of-the-art computational methods, such as molecular dynamic simulations, quantitative structure-activity relationship models such and other simple computational models for the simulation of a water ecosystem.

Key-Words: - water terrorism, nerve agents, Molecular Dynamics simulations, risk assessment, aquatic ecosystems, QSAR Models.

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1 Introduction

The understanding of nerve agents may be quite critical, as they constitute chemical weapons and part of the weapons of mass destruction with multiple effects on human health and the environment. This work explores an original and unique idea, by equally combining theoretical aspects, molecular simulation techniques, and concepts for the first time, with practical applications for safety on a large scale, proposing a complete analysis and study will be carried out for a set of liquid nerve agents, identifying their structure and properties, by using classical molecular simulations in combination with machine learning. Additionally, the well-known Quantitative and qualitative structure–activity relationships (QSARs) could be an excellent tool to understand the chemical behavior of these substances.

As a final step, the modelling of the effects of their release in water sensitive areas is proposed. Simple models could be used to simulate the ecosystems of water sensitive areas and demonstrate the possible consequences of a release, [1].

The impact of molecular dynamics (MD) simulations in molecular modeling, particularly in the realm of substance research, has witnessed a substantial expansion in recent years. Molecular simulations serve as highly valuable tools for gaining profound insights into the physicochemical properties of nerve agents, ultimately facilitating the development of innovative methods for their early detection, protection, and decontamination.

These simulations meticulously capture the behavior of nerve agents at the atomic level, providing a remarkably detailed temporal resolution. They have demonstrated their worth in unraveling the functional mechanisms of nerve agents and aiding in the resolution of complex chemical challenges. These simulations leverage the techniques of theoretical chemistry, integrated into efficient computer programs, to calculate the structures, interactions, and properties of molecules.

The potency of these simulations lies in several aspects. Firstly, they meticulously record the position and motion of every atom at each point in time, a feat challenging to achieve through any experimental technique. Secondly, the simulation

conditions are precisely defined, allowing for precise control over numerous structural and dynamic properties. By comparing simulations conducted under varying conditions, one can discern the effects of a wide array of molecular perturbations.

Quantitative and qualitative structure-activity relationships, commonly known as QSARs, represent a modeling approach which serves both as a fundamental framework and a toolkit for over a century. QSARs can be applied across various domains within the natural sciences, as a means to acquire insights and generate new knowledge by establishing connections between molecular or material structures and chemistry-related phenomena. QSAR has its foundational origins rooted in physical organic chemistry, contributing significantly to our understanding of chemical reactivity. The enduring relevance of QSAR is further exemplified by its achievements in the systematic examination of the adverse outcomes caused by chemical substances. The multifaceted roles of QSAR as a scientific methodology have distinguished it as a unique approach for the acquisition of novel insights.

Finally, anomalous relaxation, nonlinear transport phenomena, and field-induced effects in composite and biological materials, as well as in materials undergoing internal physical and chemical reactions and phase transitions, have garnered significant attention from researchers and medical professionals. These phenomena are ubiquitous in nature and find active application in advanced industrial and biomedical technologies, [2].

2 Nerve Agents

2.1 Effects of Nerve Agents

Chemical weapons usage dates back to antiquity, however, they became weapons of mass destruction during World War I. Modern chemical weapons include lethal nerve agents. In general, chemical weapons are categorized according to their physical state when being delivered (i.e., solid, liquid, gas) and their physical characteristics (such as their persistence, their mode of action on the human body, and their level of lethality), [3].

The level of lethality varies a lot, with chemical agents, like tear gas, acting only as irritants or incapacitants being unable to cause death unless they are used in a very large quantity, while others being highly lethal. Nerve agents are typical examples. They are classified as highly poisonous chemical agents that disrupt the normal function of the human nervous system. These substances may be absorbed in the human body through inhalation or through the skin and they may be used in chemical warfare. With only a few drops absorbed through the skin, substances like Sarin, Soman, Novichok, Tabun, and VX can paralyze almost instantly and kill in a few minutes. They are usually known by their chemical name and a two-letter military designation, for example cyclosarin (GF), tabun (GA), sarin (GB), dimethyl methylphosphonate (DMMP), diisopropyl methylphosphonate (DIMP), soman (GD), N, N-diethyl 2(methyl-(2-methylpropoxy)phosphoryl)sulfanylethanamide (VR) and 22-(diisopropylamino)ethyl-O-ethyl methylphosphonothioate (VX).

Nerve agents are responsible for severe damages to the human central nervous system, as they disrupt the normal function of the enzyme acetylcholinesterase (AChE). Our body uses acetylcholine for cell communication, by sending an electrical impulse. AChE prevents the acetylcholine molecules from building up on the receptors. For this reason, it is crucial to know the precise properties of these substances and how to tackle them, [4].

Therefore, when AChE is inhibited, acetylcholine accumulates on neural and neuromuscular junctions, stimulating excessively, causing a cholinergic syndrome, which involves central, nicotinic, and muscarinic effects, such as miosis, sweating, nausea, diarrhea, increased salivation, and airway secretions, central respiratory depression, respiratory failure, rhinorrhea, bronchoconstriction, ataxia, altered mental status, involuntary urination and defecation, bradycardia or tachycardia, convulsion, fasciculations, hyperthermia, lethargy, and coma. The recognition of the toxidrome in its early stages is crucial for administering an antidote, such as atropine, diazepam, and pyridostigmine. In addition, besides the acute effects caused by poisoning with nerve agents, many studies have made clear that survivors of intermediate or high-level exposure may experience many neurological and neuropsychological symptoms, [5].

2.2 Chronology of Nerve Agents' Usage

Nerve agents were first invented in the 1930s by accident, as German scientists were trying to find alternative solutions to replace nicotine as

insecticide. They discovered two organic compounds, later known as tabun and sarin, that contained phosphorus and were very efficient in killing insect pests. However, they were found to be very toxic for commercial use. Wehrmacht characterized these two substances as chemical weapons and tried to manufacture them on a big scale. When the 3rd Reich collapsed, sarin was acquired by the Soviet Union. Later on, in the 1950s, another substance, known as VX, was manufactured in the UK. Again, it was very toxic to be used in the agricultural sector, and it was forwarded to the Porton Down Chemical Weapons Research Centre of UK, and then to the US government. Throughout the years, many other nerve agents have been produced, but not many things are known about them. Furthermore, till the 1980s, it is believed that nerve agents were not used in warfare. Sarin was used by the forces of Saddam Hussein during the Iran-Iraq war. Specifically in 1988, approximately 5000 Kurdish citizens were killed in Halabja. On 5 March 2018, the former Russian spy Sergei Skripal alongside his daughter, was found unconscious in a park and they were hospitalized in a critical condition in Salisbury, UK, following exposure to an unknown nerve agent. The most probable substance responsible for this event is the nerve agent Novichok, [6].

Even three decades after signing the Chemical Weapons Convention, chemical warfare agents (CWAs) remain a threat. The development of novel methods for the detection of CWAs, protection from CWAs, and CWA decontamination motivates research on their physicochemical properties. Several attempts have been made to identify the structure and the properties of nerve agents' compounds, [7]. However, this is not an easy task, and so far, only sarin has been adequately described, which is due to several reasons. After the signing of the Chemical Weapons Convention in 1997, substances like nerve agents have been prohibited to use and produce due to their extreme toxicity. Specifically, on April 29, 1997, the Chemical Weapons Convention (CWC) entered into force. Initially, it was approved by the United Nations Conference in 1992. The goal was, and still is, the total disarmament of chemical weapons. According to the treaty, the country that signed must destroy all chemical weapons it may have on the ground but also on the territory of other countries, as well as their production facilities. For the specific convention, as chemical weapons are considered specific toxic chemicals and any chemical reagent involved in any stage of their production as well as ammunition and devices, specially designed to cause death or other harm. As of 2013, the only countries that had neither signed nor joined the CWC were Angola, Egypt, North Korea, and South Sudan, [8].

2.3 Necessity of Modelling Nerve Agents' Properties

For this reason, there is not much data available, as all experimental studies must use less toxic simulant compounds, and only in silico experiments, such as molecular simulations, since there is no way to actually test these substances on human beings and/or animals, due to bioethics. Therefore, the modelling of the resting nerve agents is a necessity in order to deepen our knowledge regarding their properties and their effects on human health and the ecosystems.

Multiscale simulation and homogenization techniques, particularly for materials like the substances we study, have emerged as the primary computational technologies and engineering tools in the field of material modeling and design. Nevertheless, concurrent multiscale simulations demand substantial computational resources due to the exponential increase in CPU time as spatial and temporal scales expand. With only a few exceptions, both hierarchical and concurrent multiscale modeling methods have not found widespread adoption in the industrial sector, primarily due to their computational expenses.

Recent advancements in artificial intelligence technology, coupled with rapid growth in computational resources and data availability, have spurred the widespread integration of machine learning-based methodologies. These methods aim to enhance the computational efficiency and accuracy of multiscale simulations and their various applications. While the anticipation of a revolutionary impact from artificial intelligence and machine learning in computational materials and mechanics is high, machine learning-based multiscale modeling and simulation are still in their early stages. This work presents several perspectives on innovative techniques, such as machine learning-based multiscale modeling and simulation of materials, as well as their applications in defect mechanics modeling and material design. These approaches hold the potential to eventually replace conventional multiscale modeling methods, [9].

Regulatory chemical risk assessment has traditionally focused on typical hazardous chemicals

rather than chemical weapons. Predictive models are indispensable for estimating chemical toxicity, both for scientific research and regulatory purposes. However, conventional models face significant challenges in the case of nerve agents, primarily due to the lack of information about their specific modes of toxic action. Therefore, alternative models that rely on different types of information, rather than modes of action, must be developed. The objective of this study is to explore the current state-of-the-art in predictive models based on quantitative structure–activity relationship techniques for assessing the toxicity of substances. Additionally, it aims to identify future challenges that hinder more reliable risk assessment in the context of environmental risk assessment. These alternative models are essential not only to overcome the limitations of conventional models but also to enhance their overall performance, [10].

3 Molecular Dynamics

3.1 Molecular Dynamics Simulations

Molecular dynamics (MD) is a method of computer simulations for the analysis of the physical properties and movements of atoms and / or molecules, applied mostly in chemical physics, material science and biophysics. The representation of the model can be at various levels of details, with the atomistic representation leading to the best reproduction of the actual system.

Atoms and molecules interact for a specific time period, providing an insight into the system's dynamics and dynamic evolution. The trajectories of the selected atoms and molecules are calculated numerically by solving the Newtonian motion equations for a system of interacting particles. The forces developed between the interacting particles, as well as their potential energies, are usually calculated by using either interatomic potentials (mathematical functions used for the calculation of the potential energy of a system of atoms with given positions in space) or molecular mechanic force fields (computational methods used for the estimate of the forces between atoms within molecules and also between molecules). Force field equations may be complex, but the calculation remains quite simple, allowing the determination of several physical quantities, such as springs for bond length and angles, periodic functions for bond rotations, Lennard–Jones potentials, Coulomb's law for van der Waals and electrostatic interactions. Then, the classical Newton's equations of motion are used to calculate the position, the velocity, and the acceleration of the atoms or molecules.

Since molecular systems are very complex, involving typically a large number of particles interacting with each other, the determination of their properties analytically is almost impossible (Figure 1). MD methods are very useful for the determination of the properties of these complex chemical compounds, especially chemical warfare substances such as nerve agents, by circumventing this problem and using numerical methods. Force field equations can be parameterized in many different ways, and each equation cannot necessarily allow the representation of each molecule type. With the proper selection of parameters and algorithms, cumulative errors in numerical integrations can be eliminated to a great extent.

The complex and time-consuming calculations of MD simulations can be particularly suitable for the application of Machine Learning (ML) techniques, such as neural networks and deep learning architectures. Many of the challenges faced in MD simulations may be formulated as ML problems, addressing the potential energy surface, the free energy surface, the coarse graining, the kinetics, the sampling and the thermodynamics.

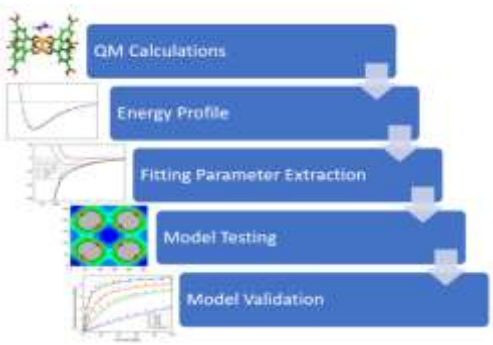

Fig. 1: Steps of MD simulation

To conclude about proposed Force Field (Potential Model) Development methods, structures proposed in the literature for each nerve agent if they are available may be used. At first all the molecular structures of the study agents will be created in a software along with the Steepest Descent Algorithm in order to determine the most stable molecular geometry in each case. Afterwards, extended charge equilibration (eQeq) technique will be employed on the rigid body structures to estimate in increased precision the atomic partial charges for each atom/atoms group (molecular sites).

Finally, parameters from already published literature will combine to obtain the full potential model, for a fully flexible structure, using, Lennard-Jones 12-6, Potential with long range Ewald corrections, flexible harmonic bond potential, flexible harmonic angle potential and flexible harmonic dihedral potential. Alternative we will use the ML techniques to produce the aforementioned parameters. Data from several sources were incorporated into the models.

In order to perform MD simulations, several software packages may be used, such as LAMMPS, BOSS and CHARMM, while to employ Machine Learning methods to develop accurate atomic and interatomic potentials for molecular simulations, the ACEMD software package by Acellera could be employed. Moreover, specific software packages with proprietary license need to be included in order to employ further complex calculations in this project, such as Spartan 20 by Wavefun.com, YASARA Structure, DESMOND by Schrodinger Inc., and SCIGRESS and AMS by FUJITSU Ltd.

3.2 QSAR Models

Structure-activity relationship (SAR) and quantitative structure-activity relationship (QSAR) models, collectively known as (Q)SARs, are mathematical models utilized for the prediction of the physicochemical, biological, and environmental fate properties of compounds based on their chemical structure. These models can be found in both free and commercial software applications. The workflow of such models consists of the selection of data sets and extraction of descriptors, the variable selection, the construction of models and the validation. As the scope of such models is the delivery of reliable information, the last step, i.e., the scientific validation, is very important. It goes without saying that there are limitations in the substance that can be treated by each model, [11]. SAR refers to the assumption that similar molecules have similar activities. The challenge that these models have to face is the treatment of small differences in molecular level, since each activity (e.g., reaction ability etc) might be affected by multiple differences. As a result, such activities have to be modelled using multiple variables (Figure 2).

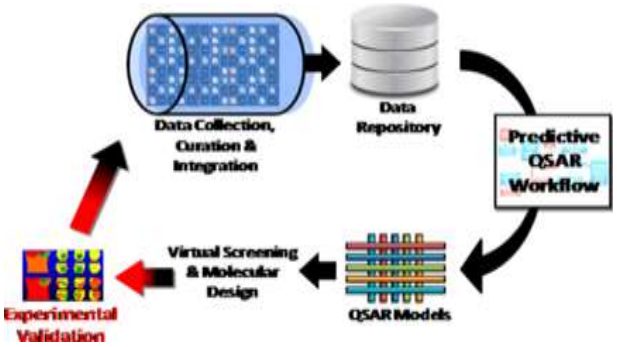

Fig. 2: An outline of QSAR Models

Another challenge, which concerns stronger trends too, is the fact that the hypotheses usually rely on a finite number of input data. Thus, one must be careful in order to avoid overfitting, i.e., to describe accurately the training data, but purely any new data, [12].

In a study like this, QSAR models could be used for the determination of the physiochemical, biological,
and toxic effects of several nerve agents.

An ecological model(s) will be developed, specifically for use in practical applications. Ecological modeling approaches are crucial for understanding the potential impact of toxic chemical warfare agents (CWAs) on water-sensitive areas for several reasons:

Risk Assessment: Ecological models help in assessing the risks associated with the release of chemical warfare agents (CWAs) into water-sensitive environments. They enable scientists and policymakers to quantify the potential ecological and human health impacts, helping in decision-making and risk management.

Complex Interactions: Water-sensitive regions frequently harbor diverse ecosystems characterized by intricate interactions among various species and environmental factors. Ecological models are capable of simulating these complex relationships, thereby offering insights into the potential disruption of these ecosystems by chemical warfare agents (CWAs).

Predictive Capability: These models possess the ability to forecast the dispersion and behavior of chemical warfare agents (CWAs) within aquatic environments. This information plays a pivotal role in response planning and the formulation of effective countermeasures to mitigate the contamination caused by CWAs.

Long-term Effects: Ecological models can effectively replicate the enduring consequences of exposure to chemical warfare agents (CWAs) on

aquatic ecosystems. Such modeling proves crucial in evaluating the persistence of contamination, recovery rates, and the likelihood of chronic ecological damage.

Protection of Biodiversity: Water-sensitive regions often house abundant biodiversity. Ecological models assist in assessing the potential harm that may be inflicted upon endangered or sensitive species and their habitats, thereby contributing to the preservation of these ecosystems.

Resource Allocation: In scenarios where resources for cleanup and remediation are limited, ecological models play a pivotal role in prioritizing areas that are most susceptible or critical for protection. This ensures the efficient allocation of available resources.

Regulatory Compliance: Many countries have environmental regulations and international agreements in place to protect water-sensitive areas. Ecological models provide a scientific basis for assessing compliance with these regulations.

Public Health: Toxic chemical warfare agents (CWAs) can contaminate drinking water sources and affect human health. Ecological models help in understanding how pollutants may enter the food chain and impact human populations, thereby informing public health responses.

Environmental Management: These models are valuable tools for designing and implementing strategies for environmental management and remediation after chemical warfare agent (CWA) contamination events.

Various modeling approaches can be employed to predict how ecosystems respond to anthropogenic interventions. These approaches encompass mechanistic models, statistical models, and machine learning (ML) methods. Our first step will be selecting the approach that best suits our problem. Additionally, we will create an outline for aligning the modeling process with decision-making and identifying the essential requirements to enhance the utility of ecological models in supporting management decisions, particularly when the need arises to justify these decisions to the public (Figure 3).

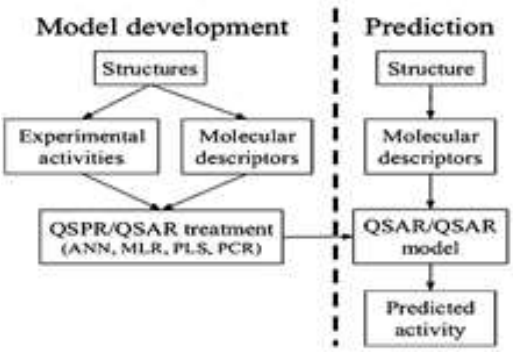

Fig. 3: An Ecological modeling approach

4 Proposed Analysis

In the frame of this proposed analysis, a brief outline of the overall work plan with the required steps is the following:

- The molecular modelling of several nerve agents using molecular dynamic simulation in order to define their molecular structure and to study the thermodynamical, transport and other dynamical properties. Flexible models for nerve agents (GF, GP, GB, GA, VX, VM, Soman, A230, A232 & A234) will be created for molecular dynamics simulations. The new models will test against experimental data for available thermodynamic and other properties. An array of thermodynamic and structural properties will be presented and compared to experimental studies if available. To achieve that, machine learning techniques will be integrated in our approach so that our simulation will take advantage of this powerful tool.
- The modelling of the effects of these substances, by applying a series of QSAR models toxicity, skin permeation, pharmacokinetic aspects as well as the environmental fate of a series of nerve agents. The extraction of reliable information about the toxic effects caused by nerve agents will be performed by using a series of freely available and validated QSAR models that predict the physicochemical, biological, and environmental effects of these substances. The knowledge of the substances' structure is necessary and will be available through the molecular dynamics modelling carried out first hand.
- The modelling of the effects of the release of the nerve agents in water sensitive areas. Simple models will be used to simulate the ecosystems of the water sensitive areas and demonstrate the possible consequences of a release. Water-

sensitive areas that exist in various regions of Greece will be identified, with a special emphasis on Northern Greece. The biodiversity of these specific areas will be analyzed, and their aquatic and mixed ecosystems will be categorized accordingly. Marine and freshwater ecosystems perform many vital functions such as filtering, diluting, and storing water, preventing flooding, maintaining local microclimatic balance, and preserving biodiversity. All types of ecosystems provide natural resources and are available for a wide range of products and services, such as trade, transport routes and recreational opportunities. The protection of these goods requires a broad perspective. Having categorised the various ecosystems, the visual programming language STELLA will be used to model the possible ways nerve agents could be released in a release in water sensitive areas as well as the effects that will be caused in these areas in the event of an incident, [13]. STELLA software is a graphical, icon-based modelling software package that can be used to build relatively complex models. It is constructed to describe and analyse communities of organisms under the influence of random variability in disturbance rates and episodic disturbances. Nerve agents are highly toxic and can rapidly affect exposed subjects. Therefore, the modelling of the chemical warfare toxic agents in water sensitive areas and the possible effects of their release may lead to the creation of an immediate warning mechanism, [14].

5 Discussion

The concept and methodology of the proposed analysis have been set to specifically ensure maximum impact on the scientific, societal, economic, and environmental ecosystems involved by developing, adapting, and integrating dedicated scientific tools and methodologies in an effective way that leads in pushing the current knowledge state to new limits.

The strategic objectives of this study are the following:

- Connecting our research with the solving of challenges and the reinforcement of some of the Sustainable Development Goals (SDGs), adopted by the United Nations, and to the framework of the European Green Deal for an environment without toxic substances.
- In line with the strategy for EU international cooperation in research and innovation, multilateral international cooperation is encouraged.
- Promote scientific and practical approaches to the scientific community for the extreme emergency situations related to chemical warfare agents (CWAs).
- Eradication of chemical weapons and prevention of their re-emergence in accordance with the objectives of the Organization for the Prohibition of Chemical Weapons (OPCW).

On the other hand, the operational objectives are the following:

- Design an innovative approach that with the combined use of classical molecular modelling and machine learning techniques will produce the force field used to describe each system.
- Investigate the state-of-the-art predictive models based on quantitative structure-activity relationship techniques for the assessment of substance toxicity.
- Identify the future challenges that impede more reliable risk assessment for environmental risk assessment.
- Design and implementation of an effective and efficient method utilising simple models to simulate the ecosystems of water sensitive areas and demonstrate the possible consequences of nerve agents' release.
- The outcome of this analysis may be useful for the solving of challenges and the reinforcement of some of the Sustainable Development Goals (SDGs), adopted by the United Nations in 2015. These SDGs have been adopted worldwide by governments, industry, and many organisations, with a horizon of realisation by 2030. Specifically, the Sustainable Development Goals (SDGs) of interest are the following:

SDG3 Good health and well-being: Exposure to toxic chemical warfare agents (CWAs) through contaminated water can have severe health implications for communities living in affected areas. Achieving good health and well-being is compromised when populations are at risk of exposure to these hazardous agents. The project may be a key to achieving the 3rd Sustainable Development Goal (SDG), as it will provide a deeper understanding of hazardous chemicals, such as nerve agents, in water, and will provide new solutions for the reduction of hazardous chemical pollution and the impacts on human health.

SDG6 Clean water and sanitation: This goal directly addresses issues related to water quality and access. The presence of toxic chemical warfare agents (CWAs) in water-sensitive areas can severely compromise the availability of clean and safe drinking water, making it difficult to achieve this goal. This analysis may contribute to this Sustainable Development Goal (SGD) by proposing mitigation techniques regarding the pollution of water sensitive areas with hazardous warfare chemical substances (i.e., nerve agents) that may pose a danger to public health.

SDG9 Industry, innovation, and infrastructure: This Sustainable Development Goal (SDG) calls for resilient infrastructure, including disaster risk reduction strategies. Preparing for and responding to chemical warfare agent (CWA) incidents in water-sensitive areas involves innovation in disaster management and infrastructure protection. One of the important aspects of disaster management is the creation of precise ecological models, like the one discussed in this work. Therefore, the project's outcome may be useful for the future of industry and infrastructure, as it will offer insights on how to cope with dangerous situations regarding chemical warfare substances and sustainability.

This project could also be indirectly related with other Sustainable Development Goals (SDGs) as well, such as:

SDG 11: Sustainable Cities and Communities: Urban areas near water-sensitive regions may be impacted by chemical warfare agent (CWA) contamination. Ensuring sustainable, resilient cities and communities requires addressing the potential risks posed by toxic chemical warfare agents (CWAs).

SDG 13: Climate Action: Chemical warfare agents can have environmental impacts, including contributions to climate change if they contaminate soil and water. Addressing chemical warfare agent (CWA) incidents is connected to broader efforts to mitigate climate change and protect the environment.

SDG 14: Life Below Water: Water-sensitive areas, such as wetlands, rivers, and coastal regions, are critical for marine life. Chemical contamination from chemical warfare agent (CWA) can harm aquatic ecosystems and marine biodiversity, making it challenging to meet this goal's objectives.

SDG 15: Life on Land: Chemical contamination, including chemical warfare agent (CWA), can have adverse effects on terrestrial ecosystems, biodiversity, and soil quality. Water-sensitive areas often connect with land-based ecosystems, and the contamination can spread, affecting life on land.

Moreover, seas, oceans, rivers and lakes are a source of natural and economic wealth for Europe. During the next few years extensive water-related investments will take place. The priorities of the European Green Deal include the protection of biodiversity and ecosystems, by reducing air-, water- and land- pollution, and moving towards a circular economy. Working in these key areas, for a toxic-free environment, the European Union will improve the health status and the quality of citizens' lives, as well as help protect the environment from dangerous chemical substances. The toxic chemical warfare agents (CWAs) under investigation in this study are extremely harmful to living organisms. In the framework of the European Green Deal for an environment without toxic substances, modelling of these chemical agents is essential, as well as their effective identification and removal in a limited period of time in order to protect the human health and aquatic ecosystems.

6 Conclusions

In summary, ecological modeling approaches are essential for assessing the potential consequences of chemical warfare agent (CWA) incidents in water-sensitive areas. They provide a systematic and scientific way to understand the ecological and human health risks, which is crucial for developing effective strategies for prevention, response, and recovery in the event of such incidents.

An integrated risk monitoring and forecasting system enables individuals, communities, governments, businesses, and other stakeholders to take timely action in order to reduce disaster risks before hazardous events occur, through several systems and procedures of communication and preparedness activities. One of the basics elements of early warning systems is the knowledge from its system risk of destruction. This is of course based on systematic data collection and simultaneous disaster risk assessments. An additional key element is the ability to detect, monitor, analyse and predict risks and possible consequences. The modelling of toxic chemical warfare agents and the release of such substances in water sensitive areas, may provide useful insights about the structure and possible effects, that could be used by an early warning system, [15].

The results achieved by the proposed study will be the cornerstone of the innovative technologies

that will make the industrial sector prosper in the specific mobility and transportation field. Due to the involvement of multiple related entities, the actions, results and impacts of this project can be further exploited EU wide and globally. Therefore, it is of high importance to create solid communication, dissemination, and exploitation routes of the developed outputs. The identified target groups may involve the industry, the academia as well as the public sector, while stakeholders that may be engaged include professionals (firefighters, emergency medical services, trainers for first and second responders, civil protection administrative and operational staff), members of the scientific community, private sector and public bodies (companies, ministries, EC), as well as the media and the general public.

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-Michail Chalaris was responsible for the Supervision.

The authors equally contributed in the present research, at all stages from the formulation of the problem to the final findings and solution.

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Conflict of Interest

The authors have no conflict of interest to declare.