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Review

A Bibliometric Perspective on Numerical Simulation to Transport Behaviors of Emerging Pollutants in Soils

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Abstract: The migration of emerging pollutants in soil poses a potential threat to groundwater systems. Numerical simulation can predict the migration behavior of contaminants and reduce experimental costs. In this study, based on the bibliometric analysis method, CiteSpace software was used to perform big data mining and visualization analysis of the relevant research papers in the Web of Science core dataset from 1994 to 2024. This topic has published 417 papers and 9315 citations in the past 30 years and has shown a rising trend of increasing attention. The U.S. is the country and organization that has published the largest number of papers in this area, accounting for approximately 42% (175) of the total papers. Different research teams have formed close collaborations utilizing their respective strengths to conduct in-depth research in this area. Current research hotspots in this topic include emerging pollutant species, transport behavior, transformation mechanisms, and numerical simulations. Future research will likely focus on the risk assessment and management of emerging pollutants in soil. This provides a new perspective for research on the environmental behavior of emerging pollutants in soil and their early warning and control measures.

Keywords: emerging pollutants; soil; longitudinal migration; numerical simulation; CiteSpace

1. Introduction

Emerging contaminants are generally defined as substances that have been detected in the environment but are not yet routinely regulated. There are many types of emerging contaminants, such as perfluoroalkyl substances (firefighting foam, non-stick coatings, etc.), pharmaceuticals (antibiotics, painkillers, hormones, etc.), personal care products (cosmetics, preservatives, fragrances, etc.), microplastics (rayon, nanoplastics, etc.), industrial chemicals (plasticizers, flame retardants, surfactants, gasoline additives, etc.) [1]. In recent years emerging contaminants have been found to remain in soil, and their environmental persistence, biotoxicity, and cumulative nature pose a serious threat to soil ecosystems and may cause adverse effects on human health through the food chain. Therefore, the contamination of soil with emerging contaminants is a matter of concern.

Emerging contaminants remain in soils through a variety of pathways [2]. For example, agroecosystems are a major entry point for microplastics and additives into soils, and annual microplastic loads are estimated to reach 430,000 and 300,000 tons per year on agricultural land in Europe and North America, respectively, which exceeds the total load of microplastics in the ocean [3]. Because soil is a porous medium with large pores and cracks (or fissures), contaminants may migrate vertically through the soil profile [4]. The transport of emerging contaminants in soil is a combination of component diffusion processes and medium flow processes [5]. The transport of

emerging contaminants may pose uncertain hazards. It has been shown that atrazine in soils enters aquatic ecosystems such as surface water, groundwater, drinking water, and other aquatic ecosystems through rainfall, surface runoff, and leaching processes, ultimately posing a range of potential environmental problems [6].

The transport behavior of emerging contaminants is influenced by a variety of factors, such as soil pH, organic matter content, temperature, and microorganisms [7]. The complexity of these experiments limits the development of emerging contaminant research. Numerical simulation is an important means to predict the migration of pollutants in soil, as it is fast, convenient, and cost-effective [8]. Ren et al. used a modeling strategy to predict the potential migration risk of microplastics in soil-groundwater systems [9].

Numerical modeling methods have been shown to have good predictive ability for emerging pollutants in soil transport processes. However, there are fewer systematic reviews on this topic, especially investigations from a bibliometric perspective. In this work, a bibliometric approach was adopted to perform literature big data mining based on the Web of Science (WoS) core database using CiteSpace software (version 6.1) [10]. Countries, institutions, authors, journals, and keywords are selected for data mining and analysis. The visualization presents the general trends, distributions, and hot spot changes in this field, providing a new perspective for studying the migration behavior of emerging pollutants in soil.

2. Data Mining

The WOS core database was selected, and the retrieval strategy was set as follows: TS = (mathematical model OR numerical simulation OR numerical model OR computational model OR mathematical simulation OR digital simulation OR virtual simulation) AND TS = (transport OR migration OR transfer OR migrate) AND TS = (emerging pollutant OR emerging contaminant OR disinfectant OR surfactant OR flame retardant OR persistent organic contaminant OR pharmaceutical OR pesticide OR antibiotic OR endocrine disruptor OR hormone OR microplastic OR nanoplastic OR personal care product) AND TS = (soil OR ground OR land). The search spanned from 1 January 1994 to 1 March 2024. A total of 417 research papers were ultimately retrieved when conferences, abstracts, and other irrelevant papers were excluded. The data were downloaded and saved as plain text files as samples for bibliometric analysis. These data samples were analyzed by CiteSpace software according to the "country", "institution", "author", "journal" and "keyword" options. The time slice for the literature setting was one year, while the other parameters were system defaults, and all the data were visualized to obtain trends and patterns to identify research frontiers and hotspots.

3. Bibliometric Analysis

3.1. Analysis of Annual Publishing Trend

The annual publication volume can reflect the trend of a research field. The trend analysis of annual publications related to the numerical simulation of the transport behavior of emerging pollutants in soil is shown in Figure 1. A total of 417 papers and 9315 citations were published from 1 January 1994 to 1 March 2024, with an average of approximately 14 papers per year. Although there are some fluctuations in the number of papers and citations each year, the overall trend still shows a yearly increase. The number of papers in 2023 reaches a peak of 28 annually, and the number of citations is the highest at 931. In addition, as of the first quarter of 2024, seven relevant papers have been published. This suggests that research in this field is growing rapidly and is in a continuous upward phase.

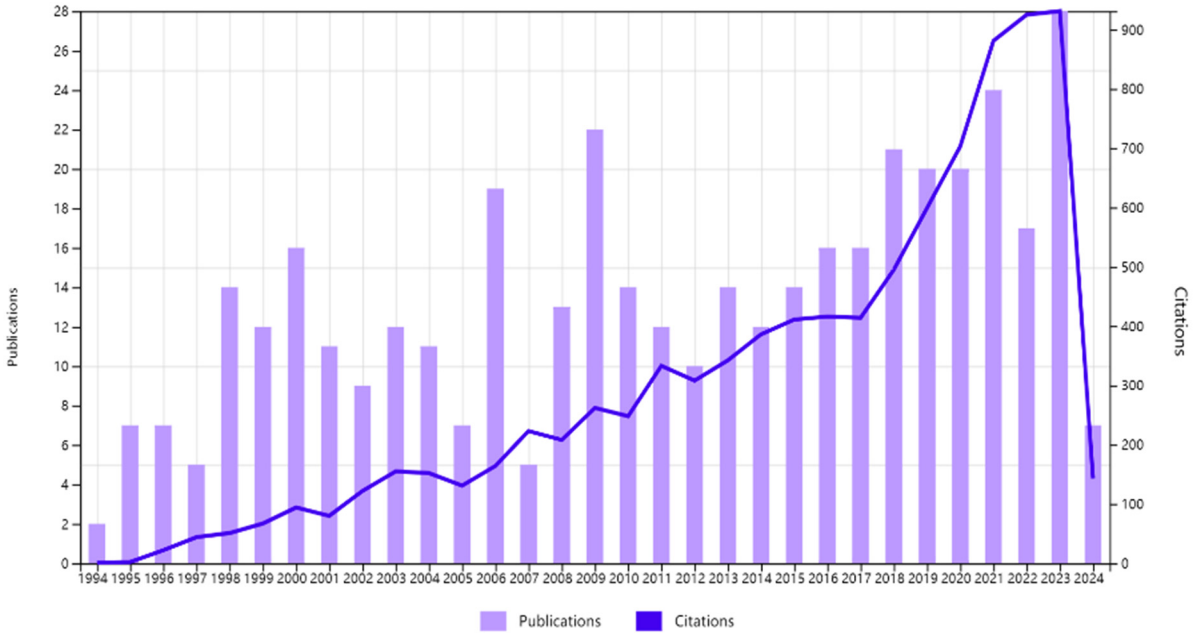

Figure 1. Annual publication trends of relevant literature on the topic.

3.2. Analysis of Publishing Country

The top countries/regions with the greatest number of publications in the field of research from 1994 to 2024 are shown in Figure 2 and Table 1. The United States of America has the highest number of publications in the field, with a total of 175 publications (42% of the total), while Germany and China are in second and third places, with 52 (12%) and 45 (11%) publications, respectively. Other top 10 countries in terms of number of publications include Canada, France, the UK, Australia, Denmark, India, Italy, Spain, the Czech Republic, Japan, and the Netherlands, which indicates that these countries are facing the problem of contamination of soil with emerging pollutants.

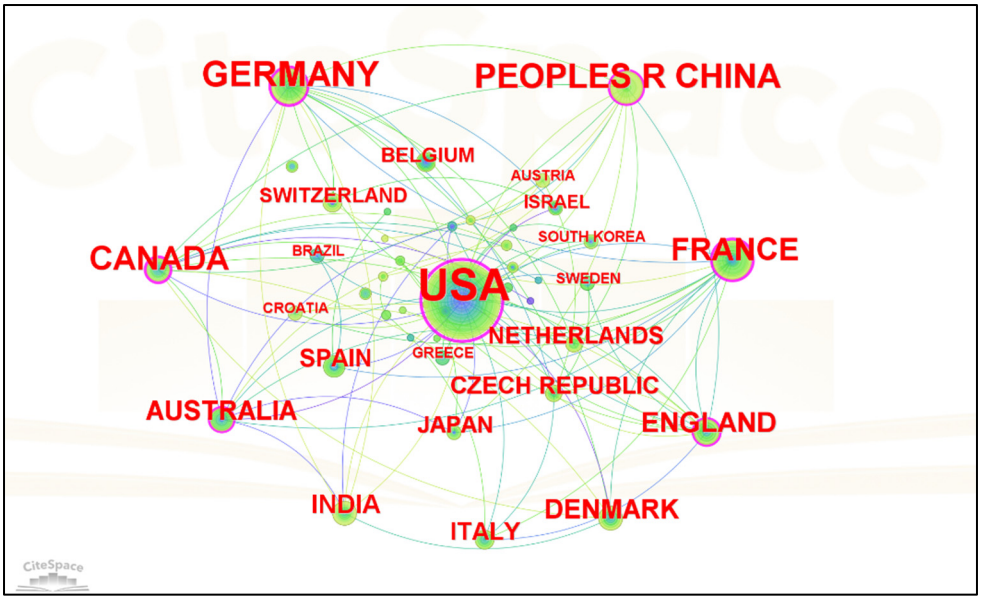

Figure 2. Major country/region co-occurrence network.

Table 1. Number of publications in the country (region).

Queue Number	Country (Region)	Publication Number
1	USA	175
2	Germany	52
3	China	45
4	Canada	40
5	France	32
6	UK	20
7	Australia/ Denmark	18
8	India	16
9	Italy/Spain	15
10	Czech Republic/ Japan/Netherlands	13

3.3. Analysis of Publishing Institution

The major national research institutions conducting research in this field around the world are shown in Figure 3. Among them, the University of California System published the most articles, accounting for 9.8% (41 articles). The United States Department of Agriculture, University of California Riverside, and Center National de la Recherche Scientifique are at the forefront, publishing 24 articles (5.8%), 24 articles (5.8%), and 18 articles (4.3%), respectively. This shows that the migration behavior of emerging pollutants in soil has received widespread attention from American and European research institutions. It is obvious from the vertical and horizontal links that there is close collaboration between the different research institutions. This also illustrates the importance of academic ex-changes to jointly utilize their respective strengths to address the problem of residual emerging contaminants in soil.

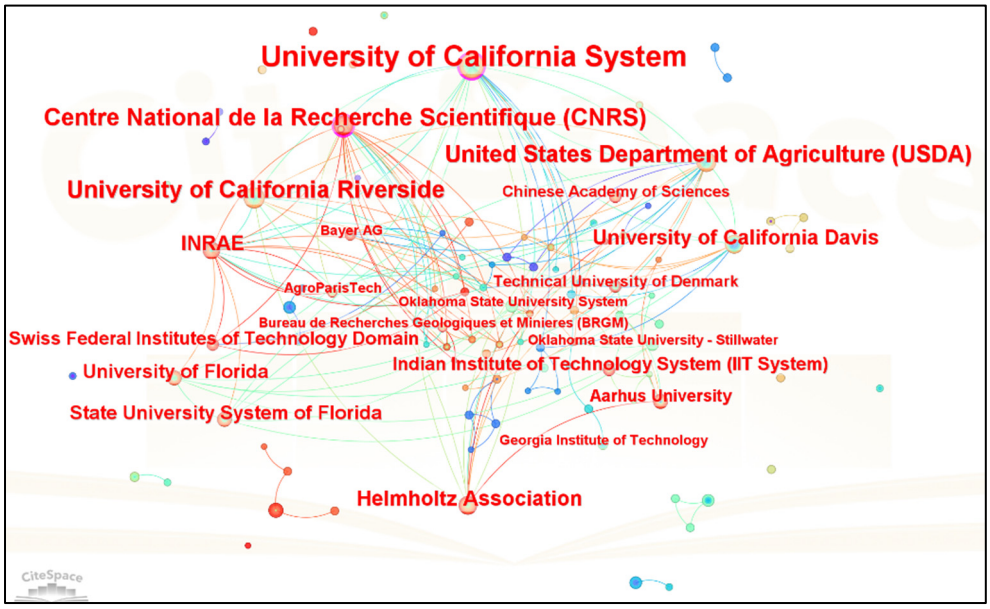

Figure 3. Major institution co-occurrence network.

3.4. Analysis of Publishing Author

In the past 30 years, the authors with the greatest number of publications globally in the field of numerical simulation research on the migration behavior of emerging pollutants in soil are shown in Figure 4. The author who has produced the most documents in this field is Simunek Jirka, who has published a total of 22 papers thus far, accounting for 5.3% of the 417 total papers. For example, Simunek Jirka and collaborators used the unsaturated flow and transport model HYDRUS to evaluate the leaching of per- and polyfluoroalkyl substances (PFAS) from land-applied biosolids used in agricultural practices to determine the impact of PFAS leaching on underlying groundwater resources [11]. In addition, Guo Bo published 8 documents, ranking second. Bradford Scott A and Brusseau Mark L tied for second, both publishing 7 documents. As emerging pollutants emerge one after another,

an increasing number of researchers will explore their environmental behavior in soil, especially by using more convenient numerical simulation methods.

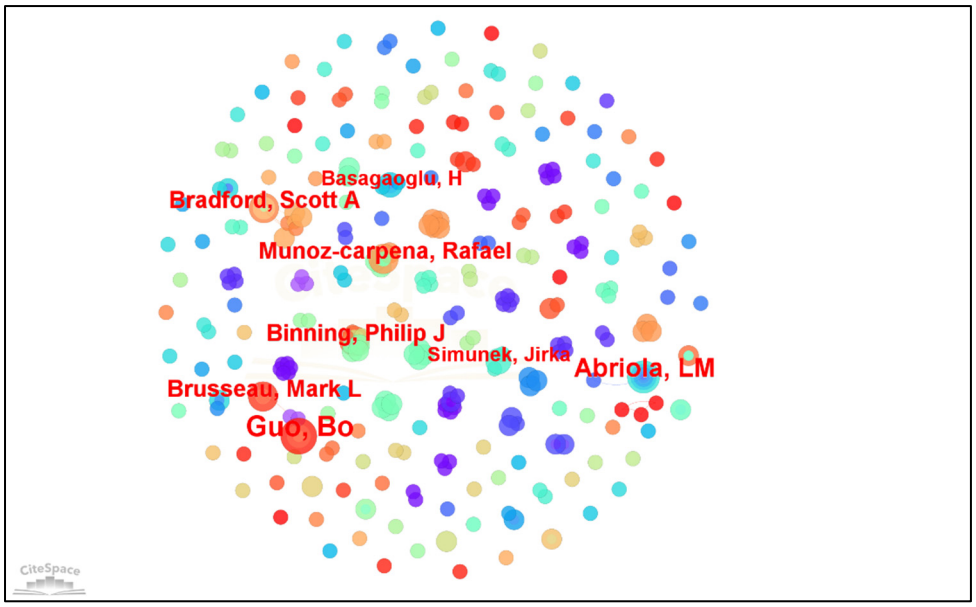

Figure 4. Major author co-occurrence network.

3.5. Analysis of Publishing Journal

A total of 417 papers related to the use of numerical simulations of the migration behavior of emerging pollutants in soil were retrieved from January 1994 to March 2024. The top 10 journals with the most publications are shown in Table 2. The journal with the largest number of publications is the Journal of Contaminant Hydrology (34 articles, 8.2%); Environmental Science Technology ranks second, with 25 publications (6.0%); and Water Resources Research ranks third, with 20 publications (4.8%). Other major journals that also published articles on this topic include Science of the Total Environment (18 articles), Vadose Zone Journal (16 articles), Journal of Hydrology (15 articles), Water Research (10 articles), Journal of Environmental Quality (10 articles), Pest Management Science (9 articles), Soil Science Society of America Journal (9 articles), Environmental Pollution (7 articles), Environmental Science and Pollution Research (7 articles), Journal of Hazardous Materials (6 articles), Soil Science (6 articles) and Water (6 articles).

Table 2. The number of publications in the journal.

Queue Number	Journal Title	Publication Number
1	Journal of Contaminant Hydrology	34
2	Environmental Science & Technology	25
3	Water Resources Research	20
4	Science of The Total Environment	18
5	Vadose Zone Journal	16
6	Journal of Hydrology	15
7	Water Research/ Journal of Environmental Quality	10
8	Pest Management Science/ Soil Science Society of America Journal	9
9	Environmental Pollution/ Environmental Science and Pollution Research	7
10	Journal of Hazardous Materials/ Soil Science/ Water	6

3.6. Analysis of Keyword

Keywords are the refined core of an article. Keyword clustering can provide information about the hotspots of current research. The clustering of the frequency of occurrence of the main 10 keywords in the published articles in this field is shown in Figure 5. The main keywords included diazinon, fate, flow, mechanism, mobility,

multiphysics simulation, numerical simulation, surfactant, transport parameters, and unsaturated flow. These keywords illustrate that the research focuses on pollutant types, transport behavior, transformation mechanisms, and numerical simulation processes.

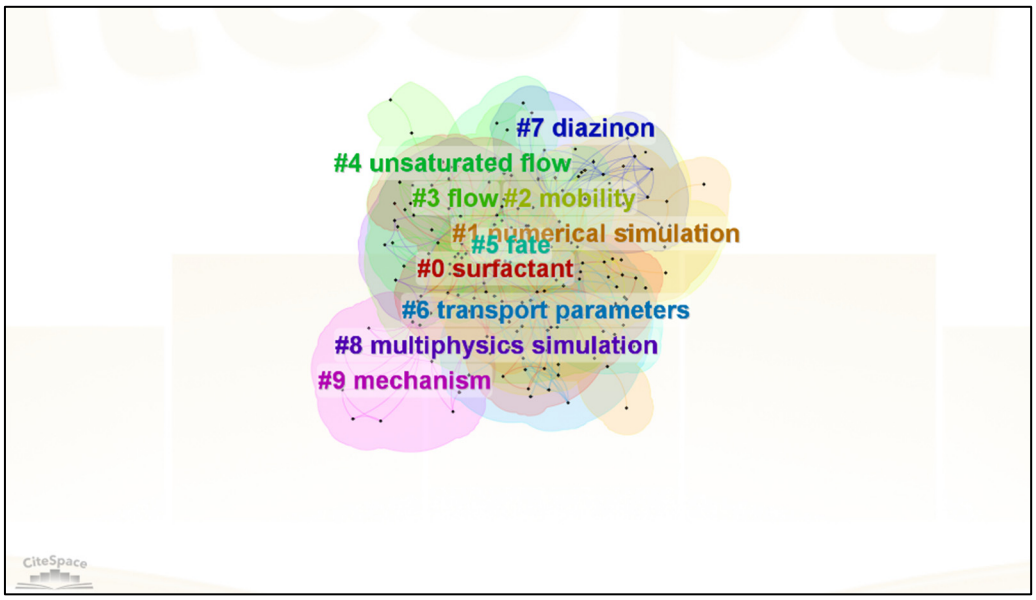

Figure 5. Major keyword co-occurrence network.

Burst citations can represent keywords that appear more frequently in a short period of time and can reflect the cutting-edge direction of current research topics. Figure 6 shows that the 15 keywords with the highest frequency of occurrence include bromide, degradation, fate, movement, pesticides, pesticide transport, pharmaceuticals, preferential flow, retention, residual dodecane, risk assessment, soils, soil columns, solution transport, and water. Among them, the strongest value of burst intensity was in the "soil columns", with a value of 5.08, indicating that soil pollution has always been a research hotspot. This is followed by "retention" and "pesticides", which have emergent intensity values of 4.22 and 4.20, respectively. This shows that the problem of pesticide residues has also attracted much attention from researchers. In addition, "fate", "risk assessment" and "pharmaceuticals" have also been key areas of exploration since 2017 and reflect the possible transformation and potential harm of emerging pollutants during migration.

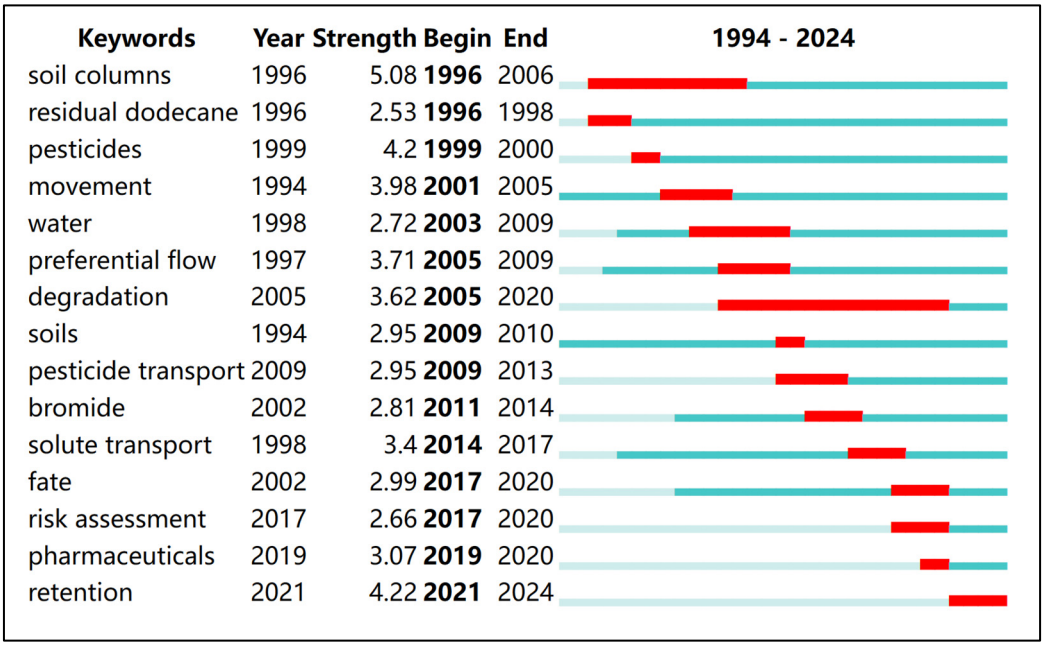

Figure 6. The main 15 keywords with the strongest citation bursts.

4. Conclusions

In this work, a systematic bibliometric analysis of the literature related to numerical simulations of the transport behavior of emerging contaminants in soil was conducted on the Web of Science core database and CiteSpace software, and the following main conclusions were obtained:

(1) A total of 417 papers and 9315 citations have been published on this topic during the nearly 30-year period from 1994 to 2024, indicating that this field is attracting increasing attention from scholars, and the number of relevant papers published continues to show an upward trend;
(2) Although the largest number of papers published by U.S. institutions is 175, accounting for 42% of the total, different research teams have been working closely together and utilizing their respective strengths to carry out in-depth investigations in this field;
(3) The current research hotspots in this field mainly focus on the types of emerging pollutants, transport behavior, transformation mechanisms, and numerical simulation processes, while the risk assessment and management of emerging pollutants in soil will be a future research trend.

Author Contributions

Conceptualization, B.F.; Data curation, F.C.; Formal analysis, P.W.; Methodology, F.C.; Project administration, B.F.; Resources, B.F.; Software, F.C.; Validation, P.W.; Visualization, F.C.; Writing—original draft, F.C.; Writing—review & editing, P.W. and B.F. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement

Data can be provided upon request for collaboration purposes.

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Conflicts of Interest

The authors declare no conflict of interest.

References

1. Teodosiu, C.; Gilca, A.-F.; Barjoveanu, G.; et al. Emerging pollutants removal through advanced drinking water treatment: A review on processes and environmental performances assessment. *J. Clean. Prod.* **2018**, *197*, 1210–1221.
2. Mishra, S.; Sundaram, B. Fate, transport, and toxicity of nanoparticles: An emerging pollutant on biotic factors. *Process Saf. Environ. Prot.* **2023**, *174*, 596–607.
3. Ren, Z.; Gui, X.; Xu, X.; et al. Microplastics in the soil-groundwater environment: Aging, migration, and co-transport of contaminants–a critical review. *J. Hazard. Mater.* **2021**, *419*, 126455.
4. Bläsing, M.; Amelung, W. Plastics in soil: Analytical methods and possible sources. *Sci. Total Environ.* **2018**, *612*, 422–435.
5. Fang S, Hua C, Yang J; et al. Combined pollution of soil by heavy metals, microplastics, and pesticides: Mechanisms and anthropogenic drivers. *J. Hazard. Mater.* **2025**, *485*, 136812.
6. Chang, J.; Fang, W.; Chen, L.; et al. Toxicological effects, environmental behaviors and remediation technologies of herbicide atrazine in soil and sediment: A comprehensive review. *Chemosphere* **2022**, *307*, 136006.
7. Luo, S.; Zhen, Z.; Zhu, X.; et al. Accelerated atrazine degradation and altered metabolic pathways in goat manure assisted soil bioremediation. *Ecotoxicol. Environ. Saf.* **2021**, *221*, 112432.
8. Tong, X.; Mohapatra, S.; Zhang, J.; et al. Source, fate, transport and modelling of selected emerging contaminants in the aquatic environment: Current status and future perspectives. *Water Res.* **2022**, *217*, 118418.
9. Ren, Z.; Gui, X.; Wei, Y.; et al. Chemical and photo-initiated aging enhances transport risk of microplastics in saturated soils: Key factors, mechanisms, and modeling. *Water Res.* **2021**, *202*, 117407.

10. Chen, C. *CiteSpace: A Practical Guide for Mapping Scientific Literatur*e; Nova Science Publishers: Hauppauge, NY, USA, 2016.
11. Silva, J.A.K.; Guelfo, J.L.; Šimůnek, J.; et al. Simulated leaching of PFAS from land-applied municipal biosolids at agricultural sites. *J. Contam. Hydrol.* **2022**, *251*, 104089.