frontiers | Frontiers in Environmental Science

TYPE Editorial
PUBLISHED 08 October 2024
DOI 10.3389/fenvs.2024.1502134

OPEN ACCESS

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RECEIVED 26 September 2024
ACCEPTED 30 September 2024
PUBLISHED 08 October 2024

CITATION
Wu Q, Wang X, Xia P, Zhang X and Zhang R (2024) Editorial: Modeling for environmental pollution and change.
Front. Environ. Sci. 12:1502134.
doi: 10.3389/fenvs.2024.1502134

Editorial: Modeling for environmental pollution and change

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KEYWORDS

environment pollution, environment modeling and simulation, computational simulation, machine learning, environmental computing

Editorial on the Research Topic
Modeling for environmental pollution and change

The predictions of environmental pollution and its changes, as well as the formulation of pollution control strategies involve many variables with nonlinear, time-varying, multi-source and multi-objective characteristics, such as real-time monitoring data, population activity data, pollutant exposure data, meteorological data, etc. (Liu et al., 2022). In addition, complex relationships exist between many variables (Zhu et al., 2023). They make it extremely difficult to achieve expected prediction performance. Improved computational methodologies, algorithms and models, such as density functional theory, microkinetic modeling, classical molecular dynamics, continuum modeling, and machine learning (ML), provide a good solution to solve this complexity (Wong et al., 2024). For example, artificial intelligence (AI) technologies can automate analyses by making inferences from data and identifying patterns without explicit programming by humans, thereby providing new opportunities to integrate and analyze large volumes of data (Heacock et al., 2022). ML algorithms, as a subfield of AI technology, can help analyze and model large amounts of complicated data more robustly and efficiently than traditional statistical models (Taoufik et al., 2022).

These advanced computational and data analytical approaches have been employed to tackle complexities of uncertain from interactive and dynamic environmental problems, playing a leading role in modeling, optimization, prediction and control (Ye et al., 2020). However, the current application is mainly based on the direct use of existing functions or commands. Very few models have been developed specifically for environmental Research Topic, which ignore the complexity and specificity of environmental problems. We hope that researchers try to construct environment-specific models including ready-to-use tools or source code to make predictions, which truly integrate the computational and data science methods into traditional environmental modeling to reveal hidden patterns or correlations, thereby promoting environmental management and pollution control. In addition, the complexity of environmental problems leads to an added challenge regarding the interpretation of the modeling results due to the complicated or black-box relationships between input and output variables.

Therefore, this Research Topic aims to feature Original Research articles and Reviews on the developments and applications of modeling and computing technologies in scientific studies on the sources, environmental behavior, fate, transformation, toxicity, risk and removal of pollutants. A series of articles have been published under this Research Topic, involving the important applications of modeling and computing technology in addressing environmental pollution and change, as follows.

Islam et al. investigated the exposure levels of trace elements (Cr, Cu, Ni, As, Zn, Cd, Mn, Fe and Pb) in a long-term banana cultivation field's soil and different tissues of the banana plant (*Musa* spp.). Then the pollution status and potential ecological and health risks of the trace elements were evaluated using various established models and chemometric approaches.

Based on the proposed possible degradation routes of a next-generation propellant HFO-1234ze(E) for pressurized metered-dose inhalers (pMDIs) devices in the atmosphere, Tewari et al. quantified the yield of trifluoroacetic acid (TFA) from HFO-1234ze(E) in the range of 0%–4% using a box-modeling approach under Europe-relevant different atmospheric conditions. Then they estimated an annual rainwater concentration of TFA to be about 0.025 μg/L in France, which could be a negligible level. This work further supports its suitability as a non-persistent, non-bioaccumulative, and non-toxic future propellant for pMDI devices to safeguard access for patients to these essential medicines.

Halama et al. characterized the spatial and temporal patterns of daily and interannual tire road wear particle (TRWP) deposition and associated fate and transport of 6PPD-Quinone in an urbanized watershed, using a process-based ecohydrological model Visualizing Ecosystem Land Management Assessments (VELMA). The modeled daily average 6PPD-Quinone concentration was generally consistent with the observed grab sample concentrations. The results demonstrated the capabilities of VELMA for prioritizing the locations, amounts, and types of green infrastructure that can most effectively reduce 6PPD-Quinone stream concentrations to levels protective of coho salmon and other aquatic species.

Neira-Albornoz et al. developed a comprehensive contextualization of Quantitative Structure-Activity Relationships (QSAR) and Pedotransfer Functions (PTF) models by evaluating the validity of their assumptions and procedures from an evidence-based perspective using empirical results of pesticides as a representative globally relevant model organic pollutant from the literature. They noted that the explicit analysis of contextualization parameters is key to improve the reliability, interpretation and applicability of predictive models. Their findings addressed the apparent incompatibility between the two models and between model assumptions and empirical knowledge. Their work would assist scientists and environmental agencies in interpreting and improving current QSAR and PTF models, and in adapting the development and use of future predictive models to specific environmentally relevant circumstances for regulatory purposes.

Arciszewski et al. used an extensive dataset available from 1997 to 2019, including modelled atmospheric deposition data, assembled fish dataset, additional stressor information, and spatio-temporal modelling to determine if changes in sentinel fishes collected in streams from Canada's Oil Sands Region were associated with oil sands industrial activity. The results suggested some negative (and persistent) effects of atmospheric deposition at some locations on the gonadosomatic index (GSI), etc. in sentinel fish. The mean GSI and body condition estimates have improved throughout the oil sands region investigated since the beginning of these Research Topic in the late 1990s, and mean liver-somatic indices have also slightly increased but remain low. Their work indicated that spatio-temporal modeling provides a novel opportunity to gain deeper insights into to the influence and effects of oil sands development at both local and regional scales.

In summary, the articles in this research theme demonstrate the important role of modeling and computational techniques in the study of pollutant environmental behavior and risk assessment in the fields of soil, atmosphere, hydrology, and other environmental fields, as well as the great potential for future development of modeling techniques. We hope that this research theme can serve as a useful resource for modeling research on environment issues by the academic community, thereby achieving more and greater discoveries and helping us better understand and solve complex environmental problems.

Author contributions

QW: Writing–original draft, Writing–review and editing. XW: Writing–review and editing. PX: Writing–review and editing. XZ: Writing–review and editing. RZ: Conceptualization, Writing–original draft, Writing–review and editing.

Funding

The author(s) declare that financial support was received for the research, authorship, and/or publication of this article. This Research Topic was supported by the National Natural Science Foundation of China (42177260 and 42377408), the Youth Innovation Team Program of Shandong Higher Education Institution (2023KJ108), the Scientific Research Startup Fund for Shenzhen High-Caliber Personnel of SZPT (6023330013 K), Shenzhen Science and Technology Program (KCXST20221021111609022), and Shenzhen Key Research Base of Humanities and Social Sciences (Shenzhen Innovation and Development Research Center of Carbon Peak and Carbon Neutrality Technical Talent).

Acknowledgments

We appreciate all authors, reviewers, and journal editors who have contributed to this Research Topic.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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