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Advances in Modelling and Measuring Environmental Pollution: Connecting Contaminant Behaviour to Ecological and Human Health Effects

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Abstract

Environmental pollution remains a major global challenge due to its complex interactions with ecological systems and human health. Understanding how contaminants originate, move, transform, and exert effects within environmental compartments is essential for effective risk assessment and management. Recent advances in modelling and measurement techniques have greatly improved our ability to characterise contaminant behaviour across air, water, soil, and biota. This review examines current progress in environmental pollution research with a focus on linking contaminant dynamics to ecological and human health outcomes.

Emphasis is placed on process-based models that describe the transport, fate, and transformation of pollutants under environmentally relevant conditions, including the influence of climate variability. The integration of field observations, laboratory experiments, and computational approaches has enabled more realistic predictions of exposure pathways and biological responses. In parallel, developments in analytical and sensing technologies have enhanced the detection of contaminants of emerging concern, such as per- and polyfluoroalkyl substances, microplastics, mercury, and antibiotic resistance determinants, at trace levels in complex environmental matrices.

The review highlights how combined modelling and measurement approaches help to identify critical exposure routes, assess cumulative and long-term risks, and improve understanding of pollutant-induced stress in ecosystems and human populations. Challenges related to data uncertainty, scale mismatches, and environmental relevance are also discussed. Strengthening the connection between contaminant behaviour and observed ecological and health effects is vital for informing evidence-based environmental policy and sustainable pollution management.

Keywords: Environmental pollution; contaminant behaviour; modelling approaches; measurement techniques; ecological effects; human health

Objectives

1. To review recent advances in modelling approaches used to describe the transport, fate, and transformation of environmental contaminants.
2. To examine modern measurement and analytical techniques for detecting pollutants at environmentally relevant concentrations.
3. To explain the link between contaminant behaviour and their ecological effects across different environmental compartments.
4. To assess how contaminant exposure contributes to human health risks through various exposure pathways.
5. To highlight current challenges, knowledge gaps, and future research directions in environmental pollution studies.

1: Identification of Environmental Contaminants in Soil, Air, and Water

Identification of environmental contaminants in soil, air, and water is a critical step in assessing pollution sources, exposure pathways, and risks to ecosystems and human health. Advanced analytical chemistry techniques are widely employed to detect and quantify contaminants at environmentally relevant concentrations, with methods selected according to the characteristics of each environmental medium (Alloway, 2013; Manahan, 2017).

Common Environmental Contaminants by Medium

Air: Air pollutants include particulate matter (PM), nitrogen oxides (NO_x), sulphur dioxide (SO_2), ozone (O_3), carbon monoxide (CO), greenhouse gases such as carbon dioxide (CO_2) and methane (CH_4), and volatile organic compounds (VOCs). These contaminants primarily arise from industrial emissions, fossil fuel combustion, and vehicular traffic, and are associated with respiratory and cardiovascular effects (WHO, 2021).

Water: Aquatic environments are affected by heavy metals such as lead and mercury, pesticides, fertilisers (nitrates), industrial effluents, pharmaceuticals, petroleum hydrocarbons, and microplastics. Agricultural runoff and wastewater discharge represent major contamination pathways, posing risks to aquatic life and drinking water safety (Schwarzenbach et al., 2010).

Soil: Soil contamination commonly involves heavy metals (lead, arsenic, cadmium), pesticide residues, persistent organic pollutants, sewage sludge, electronic waste components, and microplastics. Long-term accumulation in soils can result in food-chain transfer and chronic exposure to humans and wildlife (Kabata-Pendias, 2011).(Table 1).

Table 1: Common Environmental Contaminants by Environmental Medium

Environmental Medium	Major Contaminants	Primary Sources	Key Health / Environmental Impacts
Air	Particulate matter (PM), nitrogen oxides (NO_x), sulphur dioxide (SO_2), ozone (O_3), carbon monoxide (CO), greenhouse gases (CO_2, CH_4), volatile organic compounds (VOCs)	Industrial emissions, fossil fuel combustion, vehicular traffic	Respiratory and cardiovascular diseases, reduced air quality, climate change impacts
Water	Heavy metals (lead, mercury), pesticides, fertilisers (nitrates), industrial effluents, pharmaceuticals, petroleum hydrocarbons, microplastics	Agricultural runoff, wastewater discharge, industrial activities, oil spills	Toxicity to aquatic organisms, bioaccumulation, drinking water contamination, human health risks

Soil	Heavy metals (lead, arsenic, cadmium), pesticide residues, persistent organic pollutants, sewage sludge, e-waste components, microplastics	Agricultural practices, industrial waste disposal, mining, sewage application	Soil degradation, food-chain transfer, chronic exposure to humans and wildlife

1.1 Sampling and Sample Preparation

Standardised sampling methods such as soil coring, water grab sampling, and air filtration are used to ensure representative samples. Sample preparation techniques, including solid-phase extraction (SPE) and liquid–liquid extraction (LLE), are essential for concentrating trace contaminants and minimising matrix interference before analysis (Harris, 2020).

1.2 Analytical Identification Techniques

Chromatographic techniques such as gas chromatography–mass spectrometry (GC-MS) and liquid chromatography–mass spectrometry (LC-MS) are widely applied for identifying complex organic pollutants in environmental samples. Spectroscopic methods, including X-ray fluorescence (XRF), near-infrared (NIR), and laser-induced spectroscopy, provide rapid elemental and chemical characterisation. Molecular approaches such as enzyme-linked immunosorbent assay (ELISA), fluorescence immunosensing, and molecularly imprinted polymers offer high sensitivity and selectivity for specific contaminants, particularly pesticides and metals (Skoog et al., 2018).

1.3 Importance of Contaminant Identification

Accurate contaminant identification supports public health protection, regulatory compliance, and environmental risk assessment. It also guides remediation strategies and informs pollution management policies at local, regional, and global scales (United Nations Environment Programme, 2019).

1.4 Sources of Environmental Contamination

Major sources of contamination include industrial discharge, agricultural runoff, mining operations, fossil fuel use, sewage disposal, and improper waste management. Understanding these sources is essential for controlling pollutant inputs and mitigating long-term environmental impacts (Förstner & Wittmann, 2012).

2: Measurement and Detection Techniques:

Accurate measurement and detection of environmental contaminants at environmentally relevant concentrations are essential for understanding pollution dynamics and assessing risks to ecosystems and human health. Recent advances in analytical tools and monitoring methods have significantly improved sensitivity, selectivity, and reliability across different environmental compartments, including air, water, soil, and biota.

Modern chromatographic techniques such as gas chromatography–mass spectrometry (GC-MS) and liquid chromatography–mass spectrometry (LC-MS) are widely used for detecting organic pollutants, including pesticides, pharmaceuticals, volatile organic compounds, and persistent organic pollutants. High-resolution mass spectrometry (HRMS) has further enhanced the identification of trace-level contaminants and unknown compounds in complex environmental matrices (Richardson & Kimura, 2020).

Spectroscopic methods play a crucial role in elemental analysis and rapid screening. Techniques such as X-ray fluorescence (XRF) allow non-destructive measurement of heavy metals in soils and sediments, while inductively coupled plasma–mass spectrometry (ICP-MS) provides highly sensitive quantification of trace metals in water and biological samples. Laser-based and infrared spectroscopic techniques are increasingly applied for real-time air and water quality monitoring (Skoog et al., 2018).

Advances in sample preparation methods, including solid-phase extraction (SPE), solid-phase microextraction (SPME), and passive sampling devices, have improved the detection of contaminants at low concentrations by enhancing pre-concentration and reducing matrix interference. These approaches are particularly valuable for long-term monitoring of pollutants in aquatic and atmospheric environments (Vrana et al., 2005).

In addition, biosensors, immunoassays, and molecular techniques such as ELISA and fluorescence-based sensors provide rapid, cost-effective detection of specific contaminants, including pesticides, heavy metals, and endocrine-disrupting chemicals. The integration of these methods with field-deployable sensors supports continuous monitoring and early warning of pollution events (Rodriguez-Mozaz et al., 2015).

Overall, the combination of advanced analytical instrumentation and innovative monitoring strategies has strengthened the ability to measure contaminants at environmentally relevant levels, supporting robust risk assessment and informed environmental management.

3: Transport and Transformation Processes:

Advection and Convection: Contaminants are transported with the bulk movement of fluids, such as river flow, groundwater movement, and atmospheric circulation. This process enables pollutants to spread from local sources to regional or global scales.

Dispersion: Dispersion occurs due to variations in flow velocity and pathways, causing contaminants to spread laterally and vertically. In aquatic systems, mechanical dispersion enhances mixing and dilution.

Volatilisation: Certain contaminants transition from solid or liquid phases into the gaseous phase and enter the atmosphere. Volatilisation is influenced by temperature, vapour pressure, and wind speed.

Leaching and Infiltration: Water-soluble contaminants migrate downward through soil profiles into groundwater. This process is especially important for nitrates, pesticides, and some heavy metals.

Erosion and Suspension: Pollutants attached to soil or sediment particles are transported through erosion by wind or water. These processes contribute significantly to the redistribution of contaminants in terrestrial and aquatic systems.

Sorption and Desorption: Contaminants may bind to soil or sediment particles (sorption) or be released back into water or air (desorption). Sorption reduces mobility but may increase persistence.

Transformation Processes (Changes in Contaminant Form)

Physical Transformation: Photolysis involves the breakdown of contaminants by sunlight, particularly in surface waters and the atmosphere.

Chemical (Abiotic) Transformation: Hydrolysis, oxidation–reduction reactions, and complexation alter contaminant structure and reactivity. These reactions can either detoxify pollutants or form more persistent and mobile products.

Biological (Biotic) Transformation: Microorganisms degrade contaminants through metabolic processes such as respiration and cometabolism. Plants and animals may absorb contaminants, leading to internal transformation or accumulation.

Factors Influencing Contaminant Fate: The fate of contaminants depends on their physical properties (volatility, solubility, particle size), chemical characteristics (reactivity, bond strength, pH sensitivity), biological activity (microbial presence and enzyme function), and environmental conditions such as temperature, moisture, oxygen availability, and sunlight.

Persistence and Environmental Fate: Persistence refers to the length of time a contaminant remains in the environment. Some substances resist degradation and form transformation products that may be more mobile or toxic than the parent compound. Bioaccumulation in organisms can amplify impacts through food webs, increasing risks to ecosystems and human health.

4: Modelling of Contaminant Behaviour in Air, Water, and Soil

Modelling of contaminant behaviour involves the use of mathematical and computational tools to simulate how pollutants are generated, transported, dispersed, transformed, and ultimately removed or deposited within environmental systems. These models are widely used to understand pollution dynamics in air, water, and soil, and they support environmental management, risk assessment, policy development, and the design of pollution control strategies.

Key Processes Represented in Pollution Models: The behaviour of contaminants in the environment is controlled by interconnected physical, chemical, and biological processes. Pollution models describe these processes using mathematical equations based on conservation of mass, energy, and momentum. By representing real environmental conditions, models help explain how pollutants move, change, and persist across air, water, and soil systems. Accurate representation of these processes is essential for predicting exposure, assessing risks, and guiding pollution management strategies (Schwarzenbach et al., 2016; Manahan, 2017).

Transport (Advection): Advection describes the movement of contaminants with the bulk flow of an environmental medium. In the atmosphere, pollutants are transported by wind fields over short or long distances, often crossing national boundaries. In surface waters, advection occurs through river flow and ocean currents, while in soils and aquifers it takes place through groundwater movement. Advection largely determines the direction and speed at which contaminants spread from their sources. This process is a core component of air quality, surface water, and groundwater models (Seinfeld &Pandis, 2016; Bear, 1972).

Dispersion and Diffusion: Dispersion and diffusion control the spreading and mixing of pollutants in the environment. Dispersion results from turbulence and variations in flow velocity, causing contaminants to spread both horizontally and vertically. Diffusion occurs when pollutants move from areas of higher concentration to lower concentration due to molecular motion. Together, these processes influence dilution, mixing, and spatial distribution of contaminants. They are particularly important in rivers, estuaries, atmospheric boundary layers, and subsurface environments (Fischer et al., 1979; Holmes & Morawska, 2006).

Chemical Transformation: Chemical transformation refers to reactions that alter the structure and concentration of contaminants in the environment. In the atmosphere, photochemical reactions driven by sunlight lead to the formation of secondary pollutants such as ozone and secondary aerosols. In water and soil, contaminants undergo hydrolysis, oxidation–reduction reactions, and complexation with other substances. These transformations may reduce toxicity or generate transformation products that are more persistent or mobile than the parent compound. Accurate modelling of chemical reactions is critical for realistic risk assessment (Schwarzenbach et al., 2016; Fenner et al., 2013).

Deposition and Removal: eposition and removal processes determine how pollutants are eliminated from environmental media. Wet deposition involves the removal of gases and particles by rain or snow, while dry deposition occurs through gravitational settling or surface uptake. In aquatic systems, sedimentation removes particle-bound contaminants from the water column. In soils, biological and chemical degradation contribute to long-term removal. These processes regulate contaminant residence time and environmental loading, making them essential components of pollution models (Wesely & Hicks, 2000; Mackay, 2001).

Inter-media Transfer and Partitioning: Inter-media transfer describes the movement of contaminants between air, water, soil, sediment, and biota. Partitioning processes determine how a pollutant distributes between different phases, such as dissolved, particulate-bound, or gaseous forms. Volatilisation transfers contaminants from water or soil to air, while sorption binds pollutants to solids. These processes control bioavailability, persistence, and long-range transport potential. Multimedia modelling approaches rely heavily on accurate partitioning parameters (Mackay & Fraser, 2000; Schwarzenbach et al., 2016).

Types of Pollution Models

Dispersion Models: Dispersion models estimate pollutant concentrations at specific receptor locations based on emission sources and environmental conditions. Gaussian plume models are widely used for simple, steady-state scenarios involving industrial stacks. More advanced models, such as AERMOD and CALPUFF, incorporate complex meteorology, terrain, and time-varying emissions. These models are commonly applied in regulatory assessments and air quality management (Holmes & Morawska, 2006; U.S. EPA, 2017).

Multimedia Fugacity Models: Multimedia fugacity models describe the distribution of contaminants across interconnected environmental compartments using the concept of fugacity, or chemical escaping tendency. These models are particularly useful for assessing the environmental fate of persistent organic pollutants. They help evaluate long-term accumulation, inter-media transfer, and exposure pathways at regional and global scales. Fugacity models provide valuable insights where monitoring data are limited (Mackay, 2001; Mackay & Fraser, 2000).

Water and Soil Quality Models: Water and soil quality models simulate contaminant behaviour in rivers, lakes, groundwater, and soils. Models such as SWAT and WASP are used to assess nutrient and pollutant transport in surface waters, while MODFLOW-based frameworks simulate groundwater flow and contaminant transport. These models are widely applied in agricultural, industrial, and urban pollution studies. They support watershed management and groundwater protection strategies (Arnold et al., 2012; Zhang et al., 2016).

Receptor Models: Receptor models use chemical composition data measured at monitoring sites to identify pollution sources and estimate their relative contributions. Unlike source-oriented models, receptor models do not require detailed emission inventories. They are especially useful in urban environments with multiple pollution sources. Common receptor modelling approaches include positive matrix factorisation and chemical mass balance models (Hopke, 2016).

Machine Learning Models: Machine learning models use data-driven approaches to predict pollutant concentrations and assess environmental risks. Techniques such as neural networks and random forests are effective in handling large datasets and complex non-linear relationships. These models complement traditional process-based models, particularly when system behaviour is difficult to represent mechanistically. Their use is rapidly increasing with advances in computing power and data availability (Reichstein et al., 2019).

Applications and Model Validation: The choice of an appropriate pollution model depends on the study objective, spatial and temporal scale, data availability, and pollutant characteristics. Model outputs are commonly validated by comparison with field monitoring data to assess accuracy and uncertainty. Validation improves confidence in model predictions and helps refine understanding of environmental processes. Reliable models are essential tools for environmental policy development and sustainable pollution management (Jakeman et al., 2006).

5: Ecological Exposure and Effects:

Environmental contaminants interact with organisms and ecosystems through multiple exposure pathways, including water, air, soil, and food chains. Once released, pollutants enter biological systems via direct contact, ingestion, or inhalation, leading to internal exposure at the cellular, organismal, and population levels. The magnitude and duration of exposure depend on contaminant concentration, persistence, and bioavailability, as well as species-specific sensitivity. These interactions can disrupt normal biological functions and alter ecosystem structure and processes (Newman, 2015; Schwarzenbach et al., 2016).

At the physiological level, contaminants can interfere with metabolic pathways, enzyme activity, and hormonal regulation. Heavy metals may inhibit enzymatic reactions, while organic pollutants such as pesticides and endocrine-disrupting chemicals can alter growth, reproduction, and development. Chronic exposure often leads to oxidative stress, immune suppression, and reduced fitness, making organisms more vulnerable to disease and environmental change (Walker et al., 2012; Landis & Yu, 2018).

Bioaccumulation and biomagnification further intensify ecological impacts. Persistent contaminants accumulate in tissues over time and increase in concentration at higher trophic levels. Top predators are therefore exposed to the highest contaminant burdens, which can result in reproductive failure, behavioural changes, and population decline. These effects have been widely documented for persistent organic pollutants and mercury in aquatic and terrestrial food webs (Mackay & Fraser, 2000; Lavoie et al., 2013).

At the community and ecosystem levels, contaminant exposure can reduce species diversity and alter species composition. Sensitive species may decline or disappear, allowing more tolerant species to dominate. Such changes disrupt predator–prey relationships, nutrient cycling, and energy flow, leading to ecosystem imbalance. In extreme cases, pollution can cause habitat degradation and loss of ecosystem services essential for human well-being (Fleeger et al., 2003; Suter, 2016).

Climate change can further modify ecological exposure and effects by altering contaminant transport, bioavailability, and toxicity. Rising temperatures and changing hydrological conditions may enhance contaminant uptake and stress responses, increasing ecological vulnerability. Understanding these combined pressures is critical for effective ecosystem protection and management (Noyes et al., 2009).

6: Human Exposure Pathways and Health Effects:

Humans are exposed to environmental contaminants through multiple pathways that link pollution in air, water, soil, and biota to adverse health outcomes. Exposure may occur over short or long periods and can involve low-level chronic contact or high-level acute events. The nature and severity of health effects depend on contaminant type, concentration, duration of exposure, and individual susceptibility. Understanding these exposure pathways is essential for accurate health risk assessment and effective public health protection (WHO, 2021; Landrigan et al., 2018).

One of the most important exposure pathways is the food chain. Contaminants such as heavy metals, persistent organic pollutants, and microplastics accumulate in crops, livestock, and aquatic organisms. Through bioaccumulation and biomagnification, these substances reach higher concentrations in food consumed by humans, particularly fish, meat, and dairy products. Long-term dietary exposure is associated with neurological, developmental, and endocrine disorders (EFSA, 2012; Lavoie et al., 2013).

Drinking water represents another major exposure route. Pollutants including nitrates, pesticides, industrial chemicals, pharmaceuticals, and heavy metals can enter groundwater and surface water sources. Inadequate treatment or infrastructure failure may result in human consumption of contaminated water, leading to gastrointestinal illness, kidney damage, and increased cancer risk. Vulnerable populations, such as children and pregnant women, are particularly at risk (Schwarzenbach et al., 2010; WHO, 2017).

Airborne exposure occurs through the inhalation of particulate matter, gases, and toxic vapours. Air pollution is strongly linked to respiratory and cardiovascular diseases, lung cancer, and premature mortality. Occupational settings may further increase exposure to hazardous substances such as solvents, metals, and dusts. Prolonged occupational exposure is associated with chronic respiratory illness, neurological damage, and increased cancer incidence (Pope & Dockery, 2006; ILO, 2019).

Overall, the interaction between environmental contamination and human health highlights the need for integrated monitoring, exposure assessment, and preventive policies to reduce health risks and protect public well-being.

7: Implications for Policy and Future Research:

Improved understanding of contaminant behaviour, ecological exposure, and human health effects has significant implications for environmental policy, regulation, and sustainable management. Scientific evidence from monitoring, modelling, and laboratory studies provides the foundation for setting environmental quality standards, emission limits, and safe exposure thresholds. By linking contaminant dynamics to ecosystem and human health impacts, policymakers can prioritise interventions and allocate resources effectively (Landrigan et al., 2018; Newman, 2015).

Integrated risk assessment, combining environmental monitoring with models of transport, transformation, and exposure, allows for proactive identification of high-risk pollutants and vulnerable populations. This approach supports regulatory frameworks such as water and air quality directives, chemical safety regulations, and waste management policies. It also enables the development of early-warning systems and mitigation strategies for emerging contaminants, including microplastics, PFAS, and antibiotic-resistant genes (Schwarzenbach et al., 2016; EFSA, 2012).

Future research should focus on filling knowledge gaps in pollutant behaviour, bioavailability, and long-term ecological and health effects. Advances in analytical techniques, remote sensing, and computational modelling can improve detection of low-concentration contaminants and predict complex interactions under changing environmental conditions. Additionally, interdisciplinary studies that link pollution with climate change, biodiversity loss, and socio-economic factors are crucial for sustainable environmental management (Noyes et al., 2009; Reichstein et al., 2019).

Promoting sustainable pollution management requires collaboration between scientists, industry, and policymakers. Evidence-based regulations, combined with public awareness and technological innovation, can reduce environmental contamination and its impact on human and ecosystem health. Research outcomes can also guide remediation strategies, resource management, and long-term monitoring programs, contributing to resilience and sustainability at regional and global scales (Jakeman et al., 2006; Suter, 2016).

Conclusion

Environmental pollution is a complex, multifaceted problem affecting air, water, soil, ecosystems, and human health. Understanding contaminant behaviour through transport, dispersion, transformation, deposition, and intermedia transfer is essential for predicting exposure and assessing risks. Advanced modelling approaches, including dispersion, multimedia fugacity, water and soil quality, receptor, and machine learning models, provide valuable tools for simulating pollutant dynamics and informing management decisions.

Ecological exposure to contaminants can cause physiological stress, bioaccumulation, biodiversity loss, and ecosystem imbalance. Persistent and bioaccumulative pollutants magnify through food webs, altering species composition and ecosystem functions. Human exposure occurs via food, water, air, and occupational contact, with health risks ranging from acute toxicity to chronic effects such as neurological, reproductive, and cardiovascular disorders. Vulnerable populations, including children, pregnant women, and workers in high-risk environments, are particularly susceptible.

The integration of contaminant behaviour modelling, ecological and human health assessments, and monitoring data supports effective environmental regulation, risk assessment, and sustainable pollution management. It enables the identification of high-risk pollutants, prioritisation of interventions, and development of early-warning and mitigation strategies. Future research should focus on emerging contaminants, environmentally relevant concentrations, climate change interactions, and interdisciplinary approaches to safeguard ecosystems and human well-being.

Ultimately, combining robust scientific understanding with evidence-based policies, technological innovation, and public engagement is critical for reducing environmental contamination, protecting health, and ensuring the sustainability and resilience of ecosystems at local, regional, and global scales.

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