



Mathematical Modelling of Environmental Pollution Dynamics: From Contaminant Transport to Ecological Risk Prediction

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Abstract: Environmental pollution is complex because contaminant transport, chemical transformation, environmental compartments, biological processes, and human activity interact. Mathematical modelling describes these processes and can predict pollutant fate, forming the basis for quantitative ecological risk assessment. This review considers mathematical methods for characterising the spatial and temporal dynamics of environmental contaminants in soil, water, sediment, and atmosphere. It focuses on differential equation modelling, advection–dispersion equations, reaction–transport modelling, compartmental modelling, stochastic modelling, and numerical simulation techniques. It critically assesses the mathematical representation of contaminant sources, movement, adsorption/desorption, degradation, bioaccumulation, and transformation. The discussion focuses on using models to generate pollutant concentration gradients and exposure pathways for ecological risk estimation and environmental management. The review also considers uncertainty and sensitivity analyses as key tools for assessing model reliability and identifying the parameters that most influence environmental outcomes. It also examines optimisation approaches for remediation planning, including source control, contaminant removal, biodegradation, and treatment allocation. The review discusses emerging AI and machine learning applications as complementary tools for parameter estimation, surrogate modelling, nonlinear prediction, and real-time environmental monitoring. The review also considers incorporating mechanistic mathematical models alongside data-driven models to improve predictions in complex,

uncertain environments. The review emphasises the need for multiscale, interdisciplinary mathematical models that connect contaminant dynamics and ecological responses and inform risk-based decision-making. Future research directions include coupled multi-compartment models, uncertainty-aware prediction, hybrid mechanistic–machine-learning models, and optimisation-based environmental remediation strategies.

Keywords: Environmental Pollution; Mathematical Modelling; Contaminant Transport; Ecological Risk; Numerical Simulation

Nomenclature:

ADR: Advection–Dispersion–Reaction
APIs: Active Pharmaceutical Ingredients
AI: Artificial Intelligence
ADRE: Advection–Dispersion–Reaction Equation
CTRW: Continuous-Time Random Walk
PNEC: Predicted No-Effect Concentration
SSDs: Species Sensitivity Distributions
PIML: Physics-Informed Machine Learning
FNO: Fourier Neural Operator

I. INTRODUCTION

Environmental pollution is a multi-scale phenomenon in which chemical, physical, and biological processes occur in soil, water, sediment, and atmospheric compartments. The global burden of chemicals is substantial and continues to increase. More than 100,000 substances are now in use [1.a.1], listed in national and regional inventories, and the total amount of new substances released is claimed to exceed the planet's safe operating space [2]. Other boundary-based arguments have focused on persistent compounds, including per- and polyfluoroalkyl compounds (PFAS) [3]. These pesticide residues are a major component of the global agricultural land base [4], and metal contamination continues to affect agricultural soils and food safety [5]. The resulting burden on human health remains significant [6].

Pharmaceuticals deserve particular attention in pharmaceutical science. A worldwide survey of 258 rivers in 104 countries found the highest cumulative concentrations of active pharmaceutical ingredients (APIs) in rivers in sub-Saharan Africa, South Asia, and South America; the most contaminated rivers were associated with poor wastewater infrastructure and pharmaceutical manufacturing [7]. Pharmaceutical production effluents are known to negatively affect aquatic ecosystems [8], and environmental reservoirs of antibiotics and resistance genes raise added ecological and clinical concerns [9]. However, where these contaminants are likely to be found, how long they will persist, and what they will do to organisms can't be determined from monitoring alone, because monitoring is spotty and time-limited.

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Mathematical modelling fills this gap by translating conservation of mass, transport equations, and reaction rates into equations that can be solved, calibrated, and interrogated. Even today, classical advection–dispersion–reaction (ADR) models continue to be the foundation of contaminant hydrology and are being expanded to incorporate non-linear sorption and time-varying sources and heterogeneous media [10,11]. Regional and global models include compartmental and multimedia models that extend the mass-balance approach to regional and global scales, including projections of chemical exposure under global change [12]. At the same time, with the development of machine learning, the question of how to jointly use existing machine knowledge and knowledge gained during the process has been raised [13,14].

Most current reviews address contaminant transport, ecological risk, uncertainty analysis, remediation optimisation, and artificial intelligence (AI) in isolation. In contrast, this review follows a logical sequence: from transport and transformation mathematics to representations of key processes; from predicted concentrations to ecological risk; from uncertainty/sensitivity analysis to remediation optimisation; and finally from mechanistic approaches to machine-learning approaches. The goals are to present the state of the art in recent developments (2020-2025), highlight the assumptions and limitations that shape these models' reliability, and provide an overview of research needs for coupled, uncertainty-aware, and decision-oriented models.

II. REVIEW METHODOLOGY

We used a structured narrative review to assess recent advances in mathematical modelling of environmental pollution dynamics, including contaminant transport, fate and transformation, ecological exposure, risk prediction, uncertainty analysis, optimisation, and emerging data-driven approaches. A narrative design was deemed suitable because the literature uses a wide range of mathematical frameworks and environmental compartments, as well as computerisation methods, validation strategies, and decision-making applications that cannot be easily combined through quantitative meta-analysis.

A. Literature Search and Identification of Relevant Studies

The papers were identified using Scopus, Web of Science Core Collection, PubMed, ScienceDirect, and Google Scholar, from the end of 2020 to the end of 2025. The search strategy combined keywords and Boolean operators related to environmental pollution and mathematical modelling. The most common search terms were “contaminant transport,” “pollutant fate,” “reactive transport,” “advection–dispersion,” “mathematical modelling,” “numerical simulation,” “compartment model,” “stochastic modelling,” “ecological risk,” “exposure assessment,” “bioaccumulation,” “uncertainty,” “sensitivity analysis,” “optimisation,” “remediation,” “machine learning,” and “physics-

informed modelling.” The authors also reviewed selected, highly cited literature to identify additional relevant studies that provided valuable evidence for the review.

B. Selection of Literature

Studies were deemed to be of relevance if they advanced the understanding, development, application or evaluation of the mathematical/computational approaches to environmental pollution dynamics. We placed special emphasis on peer-reviewed research articles, review papers, perspectives, and scholarly book chapters that focused on contaminant behaviour in soil, water, sediment, or atmospheric systems. We also included studies that combined modelled contaminant exposure with ecological or human health risk assessment. We also included literature addressing uncertainty quantification, sensitivity analysis, optimisation, remediation approaches, and machine-learning or other data-driven approaches used to model environmental pollution.

Studies were not included if they did not include mathematical/computational modelling, did not provide a verifiable DOI for the publication, or were conference abstracts without accessible full text. The review focused on literature from 2020 onwards to reflect the most recent advances, but included older, foundational concepts when needed to provide appropriate theoretical background.

C. Data Extraction and Narrative Synthesis

The selected publications were reviewed, and the information was extracted and organised into major themes relevant to the review's objective. The information extracted consisted of the environmental compartment studied, the mathematical or governing equations used, the analytical or numerical solution method, the representation of the pollutant or contaminant source and the transformation processes, the treatment of uncertainty and parameter sensitivity, the approach used for model validation and the ecological, environmental, or health risk endpoints.

The information was then compiled in narrative form rather than statistical form. Comparisons focused on mathematical formulations, practical environmental applications, the studies' strengths and shortcomings, and opportunities to incorporate them into new computational methods and techniques, including machine learning, optimisation, and physics-informed modelling. The review focused on the shift from traditional contaminant-transport and compartmental models to more comprehensive models that address uncertainty, ecological risk, remediation, and predictive decision-making.

D. Final Literature Base

After conducting a literature search, assessing relevance, discarding irrelevant articles, and evaluating the available evidence, we selected 43 articles as the core literature for this narrative review. The following publications form the basis for discussing mathematical methods in

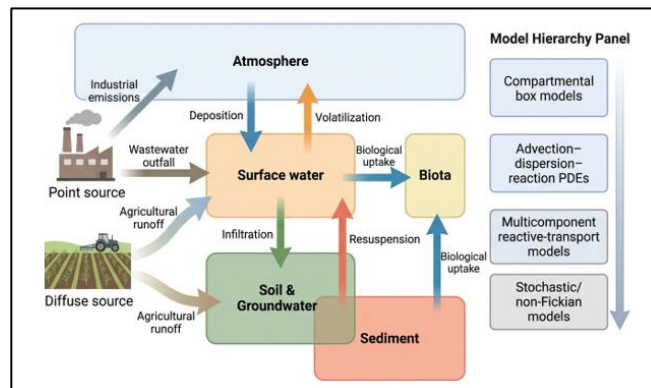


contaminant transport, pollution dynamics, ecological risk prediction, uncertainty and sensitivity analysis, remediation optimisation, and new data-driven or machine-learning approaches.

We selected these 43 articles to represent the evidence, not to create an exhaustive systematic-review dataset. We therefore analysed the results qualitatively and highlighted major methodological advances, recurring trends, “voids,” and future opportunities for mathematical modelling of environmental pollution dynamics.

III. POLLUTION DYNAMICS ACROSS ENVIRONMENTAL COMPARTMENTS

Point sources (industrial discharges, wastewater treatment plants, and spills) and diffuse sources (agricultural runoff, atmospheric deposition, and urban runoff) can introduce contaminants into the environment. They then distribute among air, water, soil, sediments, and biota based on physical and chemical characteristics (such as solubility, vapour pressure, sorption affinity, and persistence). Advection within each compartment, along with molecular diffusion and mechanical dispersion, drives chemical movement. In contrast, volatilisation, deposition, infiltration, resuspension, and biological uptake between compartments control transport. Transformation processes, such as hydrolysis, photo-reduction, oxidation, and biodegradation, eliminate or change the original chemical, sometimes into more significant chemicals. [Figure 1](#) summarises these pathways and the hierarchy of mathematical models.



[Fig.1: Conceptual Framework of Pollution Dynamics Across Air, Water, Soil, Sediment and Biota, with the Corresponding Hierarchy of Mathematical Models (Compartmental, Advection–Dispersion–Reaction, Reactive-Transport and Stochastic)]

Sources: Concept synthesis based on references [2,10-12].

Spatial heterogeneity and temporal variability complicate this. Aquifer properties vary many orders of magnitude, seasonal hydrology changes flow paths, and emissions are not necessarily constant. Even in the relatively simple case of a contaminant in a heterogeneous aquifer, models must simultaneously represent space-dependent velocity and dispersion fields, non-linear sorption, and time-varying boundary sources [10]. At continental to global scales, it is even harder to assess whether model groundwater representations are realistic [15]. Surface-water quality models face similar challenges in hydrodynamics, loading, and in-stream processing [16].

These considerations drive this hierarchy of models, matching complexity to the question. A box model suffices for screening; a site-scale remediation design might require a 3-D reactive-transport simulator; and a regulatory exposure assessment might require a probabilistic framework that propagates uncertainty in a risk metric. [Table I.](#) summarises the key model classes addressed in this review.

Table I: Principal Classes of Mathematical Models used to Describe Contaminant Dynamics and Ecological Exposure

Model Class	Mathematical Basis	Typical Application	Main Limitation	Key Refs.
Advection–dispersion–reaction PDEs	$R \frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - v \cdot \nabla C - \lambda C + S$	Groundwater plumes, soil columns, rivers	Heterogeneity and non-linear sorption require numerical solution; analytical forms limited.	[10,11]
Multicomponent reactive transport	Coupled PDEs with equilibrium and kinetic geochemical relations	Redox fronts, mineral reactions, PFAS retention	High computational cost; large parameter sets	[11,17]
Compartmental / multimedia box models	ODE mass balances with first-order inter-compartment transfer	Regional exposure, chemical screening, pharmaceuticals and pesticides	Well-mixed assumption removes spatial gradients	[2,12]
Stochastic / non-Fickian models	Continuous-time random walk; jump-length and waiting-time distributions	Heterogeneous or fractured aquifers with heavy-tailed breakthrough	Parameter identifiability; calibration data demand	[18]
Probabilistic risk models	Species sensitivity distributions; Bayesian networks	Ecological risk estimation, effects thresholds	Dependence on toxicity data quality and structure	[19,20]
Data-driven and hybrid models	PINNs, neural operators, differentiable models	Surrogates, inverse problems, forecasting	Extrapolation, interpretability, training data	[21,22]

IV. MATHEMATICAL MODELS FOR CONTAMINANT TRANSPORT

A. Advection–Dispersion–Reaction Equation

Consider a dissolved contaminant in a saturated porous medium; combining conservation of mass, Darcy's law, and

Fick's law of dispersion yields the advection–dispersion–reaction equation (ADRE). The general form of the equation is:

$$R \frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - \mathbf{v} \cdot \nabla C - \lambda R C + S(\mathbf{x}, t) \quad (1)$$

where C is the dissolved concentration, $\mathbf{v}$ the seepage velocity, D the hydrodynamic dispersion tensor, λ a first-order decay constant, S a source or sink term and R the retardation factor. Linear equilibrium sorption is described by $R = 1 + \rho_b \cdot K_d / \theta$, where ρ_b is the bulk density, K_d is the distribution coefficient, and θ is the porosity. The dimensionless groups (Péclet number ($Pe = \mathbf{v}L/D$) and Damköhler number ($Da = \lambda L/\mathbf{v}$)) represent the relative importance of transport and reaction [11]. If velocity and dispersion do not change in space and time, analytical solutions can be developed; if they do, a numerical solution is required.

Recent work provides examples of ways to enrich the classical equation. Radha and Singh solved a two-dimensional ADRE with space-dependent velocity and dispersion, time-varying axial inputs, non-linear sorption, decay, and production using Crank–Nicolson and alternating-direction implicit finite-difference schemes, and established stability using the Péclet and Courant numbers [10]. They conclude that source type, bulk density, and sorption non-linearity significantly modify plume geometry, highlighting the need for site-specific parameterisation.

B. Sorption, Retardation and Multicomponent Reactive Transport

Sorption is the main mechanism that delays groundwater flow. Researchers often use non-linear isotherms instead of linear partitioning because they reflect realistic mass-sorbed limits. Both the Freundlich isotherm $S = K_f \cdot C^n$ and the Langmuir isotherm $S = S_{\max} \cdot K_L \cdot C / (1 + K_L \cdot C)$ introduce a non-linear form for the transport equation, and in the former case, R is not bounded, while in the latter case, R saturates at a maximum of $S_{\max}$. If more than one mechanism retains a compound, the representation should be extended beyond this. For instance, PFAS transport in unsaturated soil also involves adsorption at the air–water interface, which other models do not account for, and vadose-zone mathematical models have incorporated it [17]. Field evidence shows that PFAS concentrations in soils are relevant, as reflected in the proposed mechanistic parameterisation [23].

When several species, mineral phases, and microbial reactions interact, the ADRE becomes a system of coupled partial differential equations linked to geochemical (equilibrium or kinetic) relations. Reactive-transport codes solve these systems numerically, either by splitting the operators or using fully coupled approaches, and require careful attention to numerical dispersion and stability conditions [11]. New approaches for integrating process-based simulations with machine learning are also in development, such as combining these models to address electrokinetic remediation of contaminated groundwater [24].

C. Compartment and Multimedia Models

At regional to global scales, a trade-off exists between understanding fine-scale details and model tractability when all environmental compartments are assumed well mixed. An

ordinary differential equation governs the mass M_i in the compartment,

$$\frac{dM_i}{dt} = E_i + \sum_j k_{ji} \cdot M_j - (\sum_j k_{ij} + k_{\text{deg}, i}) \cdot M_i \quad (2)$$

where E_i is the emission rate, k_{ij} the first-order transfer coefficient from compartment i to j and $k_{\text{deg}, i}$ the degradation rate. These models provide the basis for chemical screening, exposure prediction, and assessments of persistence and long-range transport. Recently, researchers applied a mechanistic exposure model to predict pesticide and pharmaceutical-like chemicals in European farming systems under varying land-use and climate change conditions [12]. The main drawback is the lack of gradients within compartments, so multi-compartment models are often coupled with spatially resolved sub-models, as discussed in Section 10.

D. Stochastic and non-Fickian Approaches

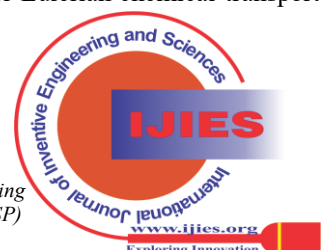
The classical Fickian ADRE cannot account for early arrival and heavy tails observed in breakthrough curves from strongly heterogeneous media. Other particle-transport models include stochastic approaches like the continuous-time random walk (CTRW), which account for mobile–immobile mass transfer and anomalous dispersion through probability functions describing waiting times and jump sizes. Recently, Hansen and Berkowitz proposed a hybrid approach that separates parameters representing macroscopic flow, sub-scale advective heterogeneity, and mass transfer, and explicitly treats the flow velocity field as heterogeneous. At the same time, particle tracking uses CTRW [18]. This is especially applicable in fractured or layered aquifers where site characterisation will never be complete. Descriptions of risk are also central to probabilistic descriptions, as discussed in Section 6.

E. Numerical Solution Techniques

Finite-difference, finite-volume and finite-element methods numerically approximate the governing equations in space and time. Simple schemes are conditionally stable, while implicit schemes like Crank–Nicolson are stable but require linear or nonlinear solvers at every time step; the choice of grid and time step must be based on the Péclet and Courant criteria to monitor numerical dispersion and oscillation [10,11]. Verification determines whether the equations have been solved correctly, and validation determines whether the correct equations have been solved. These tasks differ and cannot be performed by calibration. More recently, there has been growing emphasis on a model's usability, reliability, and feasibility [25].

F. Surface-Water and Atmospheric Systems

Rivers and lakes are commonly modelled with one- to three-dimensional hydrodynamic models coupled to water-quality kinetics for nutrients, dissolved oxygen, sediments, and toxicants; [16] reviews the strengths, data requirements, and typical limitations of these models. Dispersion is usually discussed in Gaussian plume or Eulerian chemical-transport models in the atmosphere, and deep-learning models have successfully predicted pollutant concentrations in the





short term for urban environments with comparable skill [26]. Pharmaceutical contamination of surface water is a case where river transport, wastewater treatment efficiency, and local population determine exposure, and where global monitoring reveals strong socio-economic gradients [7].

Table II: Common Mathematical Representations of key Processes in Pollutant Fate and Transport Models

Process	Common Formulation	Principal Parameters	Notes	Key refs.
Advection	$v = -(K/\theta) \nabla h$ (Darcy flux divided by porosity)	Hydraulic conductivity K , porosity θ , head h	Space-dependent velocity fields increase realism	[10,11]
Hydrodynamic dispersion	$D = \alpha_L v + D_m$	Dispersivity α_L , molecular diffusion D_m	Scale-dependent; possibly non-Fickian in heterogeneous media	[10,18]
Sorption (equilibrium)	Linear (K_d); Freundlich $S = K_f \cdot C^n$; Langmuir $S = S_{max} \cdot K_L \cdot C / (1 + K_L \cdot C)$	K_d , K_f , n , S_{max} , K_L	Non-linear isotherms make R concentration-dependent	[10]
Interfacial adsorption	Additional air–water interface term in vadose-zone transport	Interfacial adsorption coefficient	Important for PFAS in unsaturated soil	[17,23]
Degradation	First-order ($-\lambda C$); Monod-type kinetics	λ , μ_{max} , half-saturation constant	Depends on redox state, temperature, microbial activity	[11]
Source terms	Dirichlet/flux boundary; distributed $S(x,t)$; periodic, exponential or asymptotic input	Source strength, decay constants	Non-point sources better represented as line or area inputs	[10,12]
Biological uptake	One-compartment toxicokinetics (Equation 3)	k_u , k_D , k_e , k_m , k_g	Links environmental concentration to internal dose; microplastics need particle-based treatment	[9,27]

A. Contaminant Sources

The sources are represented as initial conditions, Dirichlet or flux boundary conditions, or distributed source terms $S(x,t)$. Point sources are sometimes unrealistic and often easier to number. In contrast, a non-point source from an agricultural field or urban runoff may be better represented by time-varying line or area inputs, such as periodic, exponential, or asymptotic functions [10]. At a larger scale, emissions are estimated from consumption, usage or production data, such as for down-the-drain exposure estimation for pharmaceuticals and agrochemicals [12].

B. Degradation and Transformation

We assume first-order decay, the simplest model, but it hides dependence on temperature, redox state, microbial populations, and substrate availability. We include these dependencies as Monod-type kinetics, multi-step degradation chains, and inhibition terms where relevant. Pharmaceuticals and agrochemicals may form transformation products that are more mobile, more toxic, or both, so the transport equation must be solved for each species in a coupled system [11].

C. Bioaccumulation and Biological Uptake

One-compartment toxicokinetic models are typically used to describe uptake by organisms,

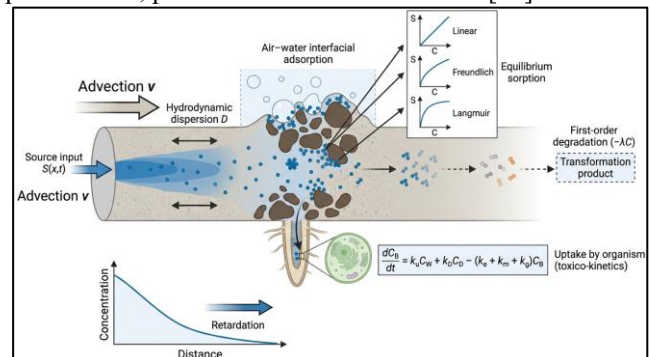
$$\frac{dC_B}{dt} = k_u \cdot C_W + k_D \cdot C_D - (k_e + k_m + k_g) \cdot C_B \quad (3)$$

where C_B is the internal concentration, C_W and C_D the water and dietary concentrations, k_u and k_D the uptake rates and k_e , k_m and k_g the elimination, metabolic transformation and growth-dilution rate constants. Figure 2 summarises the principal process terms fed into a transport model. By extending Equation 3 to food webs, the internal doses relate to the abiotic concentrations obtained from transport models. Similarly, for antibiotics, the mass-balance

V. REPRESENTATION OF KEY PROCESSES

The usefulness and accuracy of any transport model depend on the accuracy of the source, sorption, degradation, and uptake terms that make up the model. Table II collects the most common formulations and the parameters they require.

approach determines which resistance determinants are selected and spread in the environmental reservoir, and the exposure concentration relative to a biomedical threshold is important [9]. For microplastics, particle size, shape, and density distributions should be represented, resulting in a probabilistic, particle-based risk formulation [27].



[Fig.2: Process Representation in Contaminant Transport Models: Source Terms, Advection, Dispersion, Equilibrium Sorption (Linear, Freundlich, Langmuir), Interfacial Adsorption, Degradation and Biological Uptake]

Source: Adapted based on references [9,10,17,27].

VI. FROM CONCENTRATION PREDICTION TO ECOLOGICAL RISK ESTIMATION

An ecological risk assessment integrates exposure risk based on transport modelling with effect data from toxicity information. Tiered practice uses a risk quotient ($RQ = PEC/PNEC$) to compare the PEC with a predicted no-effect concentration (PNEC), where $RQ > 1$ suggests potential concern. This method supports prioritisation, such as ranking APIs according to



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ivers [7], but it does not account for variability, mixtures, or ecological interactions.

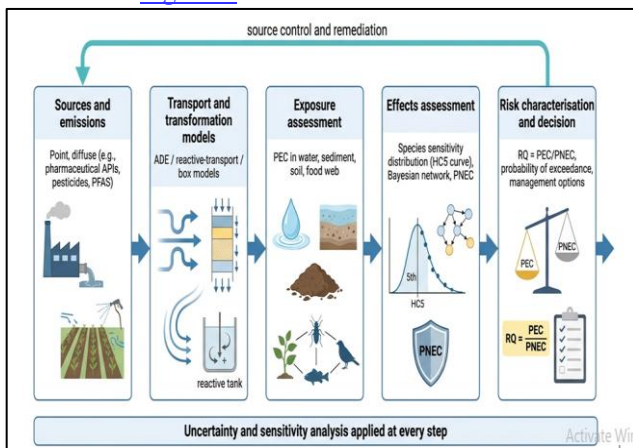
Probabilistic methods overcome these limitations. Species sensitivity distributions (SSDs) model a statistical distribution around toxicity endpoints across species; recent developments include model averaging, censored data, and improved uncertainty intervals [19]. Conditional probabilities link stressors to exposure and endpoints in a framework

complementary to the Bayesian network, allowing different types of evidence to be combined, and the expanded use of such networks has improved environmental risk assessment [20]. Threshold concentrations used in particle-based microplastic risk models are based on particle properties and realistic ecological exposure [27]. Table III. shows the metrics and frameworks used to convert expected exposures to ecological risk.

Table III: Metrics and Frameworks Used to Translate Predicted Exposure into Ecological Risk

Metric / Framework	Definition	Typical Use	Limitation	Key Refs.
Risk quotient (RQ)	RQ = PEC/PNEC; RQ > 1 indicates potential concern	Screening and prioritisation of APIs and agrochemicals	Deterministic; ignores variability and mixtures	[7,12]
Species sensitivity distribution (SSD)	Statistical distribution of species toxicity endpoints; HCS derived	Derivation of protective thresholds	Requires adequate, representative toxicity data	[19]
Bayesian network	Probabilistic graph linking stressors, exposure and endpoints	Integrating heterogeneous evidence and expert knowledge	Structure and prior specification influence results	[20]
Particle-based microplastic risk	Threshold concentrations dependent on particle size, shape and density	Microplastic risk assessment	Complex exposure characterisation	[27]
Planetary-boundary framing	Global release or concentration compared with safe operating space	Novel entities and PFAS at global scale	Boundary values remain debated	[2,3]
Health burden	Attributable disease burden from pollution exposure	Policy prioritisation	Coarse resolution for ecological receptors	[6]

Further pathways of exposure exist. A contaminant entering a water body can affect benthic organisms via sediment, pelagic organisms directly, and predators via the food web; humans can be exposed via drinking water or fish consumption, where fish are exposed by drinking contaminated water or by consuming contaminated sediment. Mathematical modelling of these pathways links transport-model concentration fields to uptake/exposure-model concentration fields, and then to population- and community-level endpoints [12]. Global pollution pressures are combined with other pressures; hence, risk is integrated across chemicals, regions, and sectors, and a concept of planetary boundaries [2,3] and health burden [6] is emerging. The entire Linkages between emissions, transport and transformation, exposure pathways, effects models (SSD, Bayesian networks) and risk-based decision-making in a source-to-risk workflow are shown in Figure 3.



[Fig.3: Source-to-Risk Workflow Linking Emissions, Transport and Transformation, Exposure Pathways, Effects Models (SSD, Bayesian Networks) and Risk-Based Decision-Making]

Sources: Based on concepts from references [7,12,19,20].

VII. UNCERTAINTY AND SENSITIVITY ANALYSIS

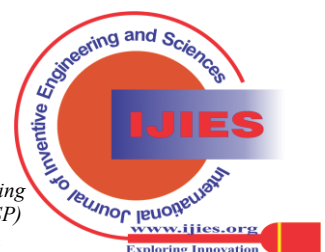
Model predictions are uncertain because of inaccuracies in inputs, model parameters, model structure, and numerical approximation. Uncertainty analysis describes the distribution of outputs resulting from input uncertainty, while sensitivity analysis assigns output variability to its sources. Both are essential for valid risk assessment - indeed, the need for greater transparency and responsibility when using models in policy has begun to be voiced [28], and sensitivity analysis is an essential discipline for systems modelling and for policy support [29].

Local, one-at-a-time analyses are low cost but cannot detect interactions. Global methods address this by partitioning the variance in the output $V(Y)$ into first-order (S_i) and total-order (S_{Ti}) effects.

$$S_i = \frac{V[E(Y|X_i)]}{V(Y)}; \quad S_{Ti} = \frac{E[V(Y|X_{-i})]}{V(Y)} \quad (4)$$

X_{-i} represents all the parameters except X_i . In recent years, open-source software has made computing Sobol-type indices easier, and they can be easily compared with other estimators [30]. In contaminant-transport problems, the dominant factors in global analysis are typically velocity, dispersivity, sorption coefficient, and degradation rate, but this depends on the output metric (peak concentration, arrival time, or cumulative exposure) and the site. These analyses can be performed easily with analytical or semi-analytical models, which is why they remain useful for checking more complicated simulators [10].

Measuring the structural uncertainty is more difficult. Several competing conceptual models of flow, reaction, or





heterogeneity can produce the same forecasts from the same calibration data, and researchers have suggested explicitly modelling perceptual models and knowledge accumulation to mitigate these issues [31]. For machine-learning components, uncertainty can come from the data (aleatoric) and from the model (epistemic); many techniques have been reviewed, such as Bayesian approximations, ensembles, and Monte Carlo dropout [32]. When applying PINNs under parametric uncertainty, parameters can be propagated through the network during training or ensemble training [33]. A suggested workflow is to use global sensitivity analysis to screen parameters, then limit the parameters that data are judged to affect the simulation results, quantify the residual uncertainty, and report risk as a distribution, not a point value.

VIII. OPTIMISATION APPROACHES FOR REMEDIATION PLANNING

Optimisation transforms a predictive model into a decision tool. A generic remediation problem seeks to determine control variables u , such as well locations and pumping rates, injection doses, excavation volumes, or treatment allocations, to minimise cost while satisfying concentration requirements at compliance points.

$$\min_u \sum_k C_k \cdot u_k \text{ subject to } C(x_r, t; u) \leq C_{std}, u_{min} \leq u \leq u_{max} \quad (5)$$

where the transport model calculates C . This simulation–optimisation structure links the physical model to metaheuristics, mathematical programming, or surrogate-assisted search, and critical reviews explain the components, practical limitations, and potential for incorporating uncertainty and surrogate models [34]. Because the simulator

does not require gradients, researchers widely use genetic algorithms, particle swarm optimisation, and multi-objective evolutionary methods, while gradient-based and adjoint methods are preferred when the number of control variables is large.

The major bottleneck is computational cost because each candidate design requires a full forward simulation. Surrogate models, such as neural operators, provide a fast approximation of the simulator and have been shown to work for groundwater contamination across different climatic scenarios [22]. Process-based reactive transport coupled with machine learning has also aided the design of electrokinetic remediation [24]. Another component of remediation decision is also source control, biodegradation and soil amendment; for agricultural soils contaminated with metals, immobilisation, phytoremediation and bioremediation will be selected based on the mobility, bioavailability and cost of the metals [5]. Uncertainty-aware (chance-constrained or robust) formulations are desirable because designs should be compliant when the parameters vary plausibly [34].

IX. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

Machine learning offers complementary benefits: speed, flexibility for high-dimensional data, and the ability to learn relationships that are not easily expressed as equations. Its applications in water-quality assessment have been reviewed, and it is increasingly used to predict, classify, and monitor water quality. However, data quality, interpretability, and transferability remain challenges [35]. Table IV shows the Machine-learning and hybrid approaches relevant to pollution dynamics modelling.

Table IV: Machine-Learning and Hybrid Approaches Relevant to Pollution Dynamics Modelling

Approach	Primary Role	Example Application	Strengths and Limitations	Key refs.
Physics-informed neural networks	Forward and inverse solution of PDEs; data assimilation	Parameter learning and multiphysics assimilation in subsurface transport	Low data demand and physical consistency; optimisation can be difficult	[33,36,37]
Theory-guided neural networks	Embed governing equations and constraints in training	Subsurface flow prediction	Improved generalisation; needs known governing physics	[21,38]
Neural operators (FNO, U-FNO, DeepONet)	Fast surrogates of parameterised PDEs	Groundwater flow and contaminant transport under varying recharge	Very fast predictions; require substantial simulation training sets	[22,39,40]
Differentiable and hybrid models	Learn process closures inside mechanistic structure	Hydrological and geoscientific modelling	Conservation retained; implementation complexity	[14,41]
Data-driven water and air quality models	Prediction, classification, monitoring	Water-quality evaluation; urban air pollution forecasting	Flexible; limited interpretability and transferability	[26,35]
Uncertainty quantification for ML	Bayesian approximations, ensembles	Reliability of ML predictions	Quantifies epistemic and aleatoric uncertainty; added cost	[32]

A. Physics-Informed Learning

Physics-informed machine learning (PIML) incorporates governing equations or conservation constraints into the learning problem, reducing data needs and improving physical plausibility [21]. In physics-informed neural networks (PINNs), the loss function combines data misfit with the residuals of the PDE and its boundary and initial conditions,

$$L(\theta) = \lambda_d \cdot L_{data} + \lambda_f \cdot L_{PDE} + \lambda_b \cdot \frac{L_{BC}}{IC} \quad (6)$$

and the same network can be used to solve forward problems or to infer parameters, as shown for scientific machine learning in general [37]. Tartakovsky and colleagues demonstrated PINNs' ability to estimate

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parameters and constitutive relationships for subsurface flow from sparse measurements [36], and He and colleagues used PINNs for Multiphysics data assimilation in subsurface transport [33]. Theory-based neural networks have also been used to learn subsurface flow [38] and incorporate governing equations and engineering constraints. Reported limitations include difficulty optimising stiff or advection-dominated problems and sensitivity to loss weighting; therefore, PINNs should complement, not compete with, existing solvers [37,42].

B. Neural Operators and Surrogate Modelling

Neural operators are trained to predict solutions to a function-space mapping for a given parameter space and/or boundary conditions, so the network does not need to be retrained for the same mapping problem with different boundary conditions or parameter spaces. DeepONet [39] and the Fourier neural operator (FNO) with a U-Net enhancement for multiphase flow [40] laid the foundation for operator learning theory and practice. Meray et al. modified a U-FNO for groundwater flow and contaminant transport, adding a loss function to enforce physical constraints, and found that the surrogate captured spatiotemporal variations in concentration, hydraulic head, and Darcy velocity under various recharge conditions [22]. These surrogates are appealing for optimisation and uncertainty analysis, where thousands of forward runs are required.

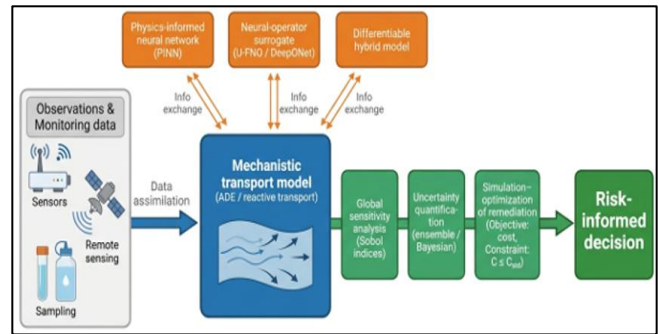
C. Hybrid and Differentiable Modelling

Hybrid modelling can range from using ML techniques to estimate process-model parameters to fully differentiable models, where a neural network replaces the process model within the structure for uncertain process closures. From a modelling perspective, geosciences can learn from vast amounts of available data while maintaining mass and energy conservation and interpretability of state variables [41]. In environmental systems, knowledge-guided machine learning approaches include physics-guided loss functions, hybrid architectures, residual modelling, and physics-informed initialisation, as catalogued in knowledge surveys [14]. Case studies in weather and climate show similar benefits and challenges [42]. The contribution to the debate on the role of hydrological science in the era of machine learning (ML) highlights the importance of process understanding for assessing the generalizability of data-driven models across regimes [13], and cautious perspectives remind us that process understanding remains relevant in the era of ML [43].

D. Real-Time Monitoring and Early Warning

Sensor networks and remote sensing provide continuous streams of water- and air-quality data. Deep-learning forecasters use these streams to predict urban air pollution in the short term [26], and ML-based water-quality evaluation is increasingly linked to monitoring programmes [35]. One promising direction is to use data assimilation methods to update a mechanistic model's states and parameters continually, and PINNs and related methods provide

differentiable assimilation pathways [33]. However, real-time systems need uncertainty quantification to prevent false alarms [32]. Figure 4 presents a hybrid framework integrating a mechanistic transport model, machine-learning surrogates, and physics-informed elements.



[Fig.4: Integrated Hybrid Framework Combining a Mechanistic Transport Model, Machine-Learning Surrogates and Physics-Informed Components with Global Sensitivity Analysis, Uncertainty Quantification and Simulation–Optimisation for Remediation]

Sources: Concept based on references [14,22,29,33,34,41].

X. CHALLENGES AND FUTURE RESEARCH DIRECTIONS

Several problems recur across the topics examined. First, data scarcity: many areas most affected by pharmaceutical and chemical pollution have the least monitoring data [7], and models should accommodate sparse, uncertain inputs. Second, scale bridging: a single framework cannot easily capture pore-scale processes, field-scale heterogeneity, and exposure at catchment/global scales, and comparing groundwater representations at larger scales remains an open problem [15]. Third, chemical diversity: more substances are in commerce [1] than compounds that can be parameterised one-by-one, making a generic, property-based, or ML-assisted approach advantageous. Fourth, transformation products and mixtures complicate the transport equations and risk metrics [11,19].

Four lines of research seem promising. Consistent exposure forecasting under climate and land-use change using coupled multi-compartment models linking spatially resolved transport in groundwater, rivers and soils with an exposure assessment in the regional multimedia models [12]. (2) Uncertainty-aware prediction, where global sensitivity analysis, Bayesian inference and ML uncertainty quantification are common parts of the model workflow [29,32]. (3) Hybrid mechanistic–machine learning models such as neural operators and differentiable models that can preserve conservation laws while learning from poorly known processes [14,22,41]. (4) Optimisation-based remediation, where surrogate models and robust and/or chance-constrained formulations are used to enable cost-effective and risk-informed remediation decisions [24,34]. Across all four, open data sharing, benchmark problems, and transparent reporting are needed, consistent with calls for more responsible model use [28].





XI. CONCLUSION

Mathematical modelling provides the quantitative language that connects emissions to concentrations, concentrations to exposure and exposure to ecological risk. Appropriate scales, data, and decision context are important for applying the different perspectives provided by advection–dispersion–reaction equations, reactive-transport formulations, compartmental mass balances, and stochastic models. Predicted concentrations must be translated through probabilistic effect models, and uncertainty and sensitivity analyses must be performed to estimate confidence in the predictions and provide ecological risk estimates. Optimisation translates predictive ability into remediation strategy, and machine learning, particularly physics-informed, operator-learning and differentiable forms, is increasing the speed and breadth of these tasks. The best progress will come from integrated approaches in which mechanistic understanding constrains the flexibility and uncertainty of the data and informs risk-based decisions.

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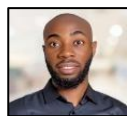


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