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Artificial Intelligence-Driven Environmental Toxicology: Predictive Toxicity Modelling, Forensic Pollution Analysis, and AI-Enabled Public Health Surveillance

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Abstract: Rapidly advancing technologies, including artificial intelligence, are needed to tackle environmental health issues. Traditional environmental toxicology has relied on experimental bioassays, epidemiological studies, and statistical models. However, the increasing volume and complexity of environmental data are not well served by existing frameworks. Artificial intelligence and machine learning provide new opportunities to improve environmental toxicology modelling and health surveillance. This article analyses the most promising artificial intelligence and machine learning techniques for modelling environmental toxicology, with a focus on forensic environmental studies and health risk assessment. The article reviews the state of the art in predictive toxicology modelling, quantitative structure-activity relationship models, deep learning, and large-scale data frameworks. In addition, the article explores environmental learning models to identify sources and patterns in environmental data, including the integration of forensic data to support the legal use of environmental data. This study also addresses the use of artificial intelligence in environmental epidemiology, the application of smart technologies in epidemiology, and the assessment of population exposure to environmental toxins. The review discusses key issues such as data negligence, model explainability, legal acceptability, ethical issues, regulatory impediments, and emerging research pathways, including hybrid mechanistic-AI models, federated learning, multi-omics, and global AI-driven monitoring. This review highlights the scope of AI-Environmental Toxicology for improving scientific accuracy, forensic accountability, and proactive data-driven public health advocacy.
Keywords: Artificial Intelligence, Machine Learning, Environmental Toxicology, Forensic Environmental Science, Public Health Risk Assessment, Predictive Toxicity Modelling, QSAR, Explainable AI, Environmental Surveillance, Exposure Analytics.

I. INTRODUCTION

Environmental toxicology is the science of studying the sources, behaviour, and effects of contaminants (chemicals, physical, and biological) on ecosystems and people. Factors such as rapid industrial growth, urban sprawl, technological advancement, and the subsequent greater release of toxic chemicals (such as heavy metals, pesticides, microplastics, Endocrine Disruptors, etc.) have led to increased levels of POPs in the environment. Contaminants disrupt the ecosystem. They are also a major source of exposure and risk to humans through various routes, such as inhalation, the gastrointestinal (GI) tract, and dermal contact, as well as through biomagnification and bioaccumulation in the food chain. Diseases such as cancer, neurodegenerative, reproductive, and developmental disorders and metabolic disorders have been linked to exposure to contaminants in the environment[1]. Environmental toxicology has become a critical and prerequisite discipline for assessing and evaluating risks, as well as for informing the regulation and management of the environment. Environmental toxicology has also become a major research and advocacy discipline in the field of environmental justice. Typically, environmental toxicology has involved laboratory studies, animal bioassays, epidemiology, analysis using chromatographic and spectrometric methods, and statistical modelling. While these methods have provided valuable insights and continue to do so, they have major shortcomings in our current data-rich, data-driven world.

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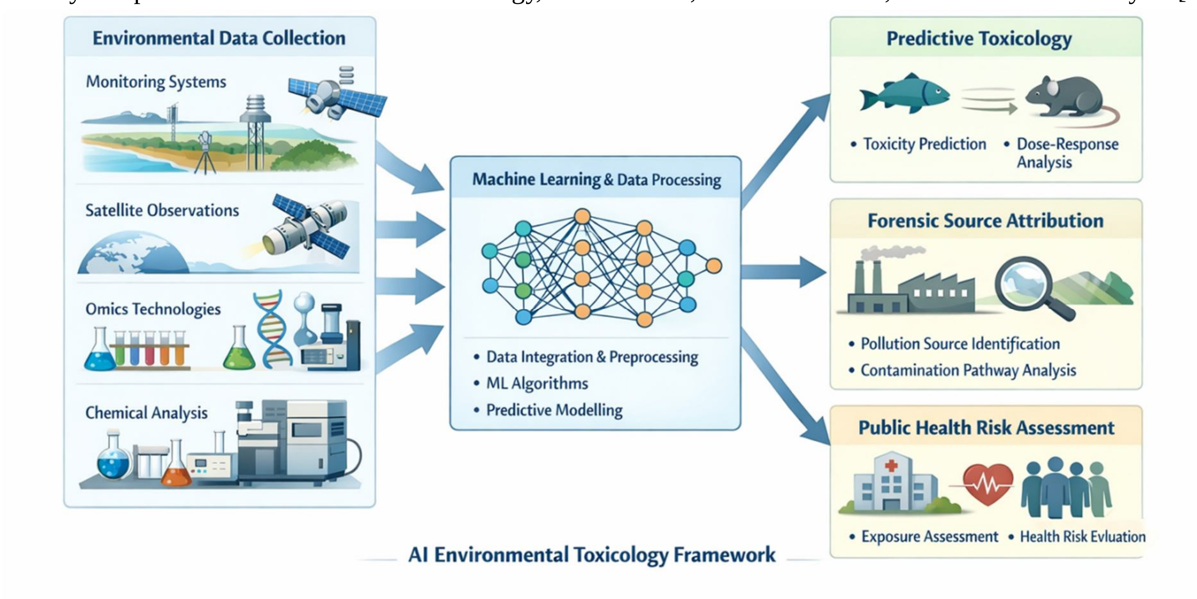
Conventional toxicology methods are time-intensive, expensive, ethically problematic due to animal testing, and unable to evaluate the large number of new chemicals introduced each year. Additionally, the complexity and nonlinearity of interactions among multiple contaminants, genes, and environmental factors render traditional statistical methods inadequate. In forensic situations, it is also difficult to determine the sources of environmental pollutants and the liability for environmental pollution using conventional methods. The same is true in public health: systems without real-time predictive capabilities cannot identify emerging environmental threats (and their potential impacts on the public) before widespread exposure occurs. AI and machine learning (ML) have the potential to address challenges in computational toxicology, including predictive toxicity modelling, rapid hazard classification, and high-throughput chemical screening. Various ML techniques, such as support vector machines, random forests, and deep neural networks, can be used to model, analyse, and predict environmental exposures, as well as to identify and address environmental challenges [2]. Additionally, the use of explainable AI methods makes the predictive model legally and scientifically defensible to the end user, and mechanistic models can be used to explain the toxicology. The use of environmental monitoring systems, integrated satellite imagery, biosensors, and omics technologies can strengthen toxicology.AI's application in environmental toxicology and go beyond predictive modelling. AI can assist forensic environmental scientists in identifying pollution sources, recognizing patterns of contamination, and correlating digital evidence in environmental crime investigations. In terms of public health protection, AI can be used in early warning systems to predict areas of potential harmful exposures, assist in the modelling of disease spread, and facilitate the implementation of targeted interventions. This review focuses on the intersection of Artificial Intelligence and Machine Learning with Environmental Toxicology, specifically on how they have been developed for forensic applications and for assessing health risks from the perspective of the general public. This paper combines the most recent developments, challenges, and innovations from various disciplines. It provides, for the first time, an integrated approach that combines the key components of Environmental Toxicology, Data Science, Forensic Science, and Health Data Analytics[3].



The integration of environmental monitoring systems with artificial intelligence for predictive toxicology, forensic analysis, and public health risk assessment is illustrated in Figure 1.

II. BUILDING BLOCKS OF ENVIRONMENTAL TOXICOLOGY AND HEALTH RISK

Environmental toxicology studies the interaction between living organisms and environmental pollutants and the impact these interactions have on public health. For the construction of predictive, AI-based toxicological models, understanding the toxic agent's essence, routes of exposure, and behaviour in tissues is critical—primary Pollutants and Pathways of Exposure. A primary environmental contaminant is an environmental pollutant, including pesticides, heavy metals, and organic pollutants. Heavy metals such as lead, mercury, and arsenic are examples of heavy metals that bioaccumulate and persist in a given environment[4]. Pesticides and herbicides consisting organophosphates, carbamates, and neonicotinoids, as well as industrial pollutants such as dioxins and polychlorinated biphenyls (PCBs), which are known as persistent organic pollutants (POPS), as well as dioxins, resist environmental degradation and can travel long distances in the atmosphere.

Pharmaceuticals, personal care products, and microplastics are emerging contaminants that are not yet fully regulated, raising toxicological concerns. Contaminants can be inhaled through the air, ingested through water and food, and contacted through polluted soil. Direct exposure via the food chain can be critical for chronic toxicity, especially for lipophilic compounds present in animal tissues. People are exposed to complex mixtures of pollutants, making it increasingly difficult to quantify risk due to their synergistic or cumulative effects. Sensitive groups, such as children, pregnant women, the elderly, and the working class, are the most affected by this phenomenon due to their physiological vulnerability and the high exposure context[5].

The term toxicokinetics refers to how a substance is absorbed, distributed, metabolised, and eliminated by the body (the ADME processes). Absorption is influenced by physical and chemical properties, such as solubility and particle size, and distribution is affected by blood flow rate and tissue affinity. For example, lipophilic compounds can be retained by the body and their biological half-life is increased by the accumulation in fatty tissue.[6]. Biotransformation, which is mainly carried out by the liver, can detoxify a substance but can also result in the formation of more toxic metabolites (bioactivation) and is dependent on the cytochrome P450 enzymatic pathways. The metabolism of a compound in the body and its elimination through urine, faeces, sweat, or breath will determine how long it remains active. Toxic dynamics, however, concern toxic substances and their interactions with cellular constituents (receptors, enzymes, DNA, and membranes). The mechanisms of toxicity include disturbances in oxidative stress, the endocrine system, mitochondria, and genes, as well as the induction of inflammation. While the relationship between dose and response is central to toxicodynamics, traditional threshold-based assumptions of toxicity are challenged by the presence of non-linear and low-dose effects, particularly with endocrine disruptors. The approaches are essential in the development of predictive in silico models and the application of artificial intelligence mechanisms to represent biological systems.[6].

A. The Process of Bioaccumulation and Use of Biomarkers

Biomarkers indicate measurable exposure, effects, or susceptibility. Exposure biomarkers can be measured in blood, urine, hair, or tissue, and include chemicals or their metabolites. Effect biomarkers show biological responses, including DNA damage, changes in enzyme activity, or modifications in gene expression. Susceptibility biomarkers examine genetic polymorphisms that may limit detoxification. The fields of genomics, proteomics, and metabolomics have recently improved the efficiency of biomarker discovery, especially in high-resolution analysis of toxic responses. The gradual accumulation of chemicals in living organisms is known as bioaccumulation. In contrast, the increasing concentration of the same chemicals at different trophic levels of the food chain is known as biomagnification. Persistent and lipophilic contaminants are particularly important because of their long biological half-lives and potential relative chronic toxicity. These processes are important to understand in ecological risk assessments and in forensic source attribution.[7].

B. Risk Assessment Frameworks that Assess Human Health

The assessment of risk from health threats involving humans uses a streamlined framework, such as hazard identification, dose-response assessment, exposure assessment, and risk Characterisation. Regulatory risk, through reference doses (RfD), acceptable daily intake (ADI), and slope factors for cancer, assesses dimensions of undesirable outcomes. Conventionally, frameworks rely on a limited dataset and use deterministic models, overlooking a population’s variabilities, mixture toxicity, and new climate change-contaminated risk. Utilising advanced data analytics and Artificial Intelligence (AI) predictive models offers better ways to improve the framework through probabilistic risk assessment, real-time exposure appraisal, and predictive health risk assessment. A sound understanding of rudimentary toxicological principles remains vital, data-driven, biologically rational, and scientifically and legally defensible.[8].

Pollutant Category	Examples	Major Sources	Primary Exposure Routes	Major Health Effects
Heavy Metals	Lead, Mercury, Arsenic, Cadmium	Mining, industrial discharge, contaminated water	Inhalation, ingestion, dermal contact	Neurotoxicity, kidney damage, and developmental disorders
Persistent Organic Pollutants (POPs)	Dioxins, PCBs	Industrial waste, chemical manufacturing	Food chain bioaccumulation, inhalation	Endocrine disruption, carcinogenic effects
Pesticides	Organophosphates, Carbamates, Neonicotinoids	Agricultural spraying	Food contamination, inhalation, and dermal exposure	Neurological disorders, reproductive toxicity
Emerging Contaminants	Microplastics, pharmaceuticals, and personal care products	Wastewater discharge, consumer products	Water ingestion, food chain transfer	Hormonal disruption, inflammatory responses
Air Pollutants	PM2.5, ozone, nitrogen oxides	Vehicles, industries, power plants	Inhalation	Respiratory and cardiovascular diseases

Table 1. Major Environmental Pollutants, Sources, and Human Exposure Pathways

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III. THE EMPLOYMENT OF ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN TOXICOLOGY MODELLING

The complexity of environmental exposure and the rapid growth of chemical data have set Artificial Intelligence (AI) and Machine Learning (ML) as pioneering components in toxicological modelling. Even though traditional statistical methods have long been in use, they remain disappointing for modelling nonlinear relationships, high-dimensional interactions, and large, heterogeneous datasets. Environmental toxicology is complemented by AI methods that offer greater accuracy, efficiency, adaptability, scalability, and predictive capabilities. Artificial Intelligence is the simulation of human cognitive activities by computer systems. Such activities include perception, prediction, classification, and decision-making. A field of study under AI is called Machine Learning. ML studies the training of models without explicitly providing instructions. In toxicological modelling, the ML technique used is typically classified as supervised, unsupervised, or reinforcement learning.[9].

Some supervised learning techniques, such as linear regression, decision trees, random forests, support vector machines (SVMs), k-nearest neighbours (KNN), and gradient boosting, are used for predicting toxicity, classifying hazards, and modelling exposure. These models are created based on labelled datasets, in which the input features (e.g., chemical descriptors, exposure concentrations) and outcomes (e.g., toxic vs. non-toxic, lethal dose values) are paired. Methods under unsupervised learning, including k-means and hierarchical clustering, and principal component analysis (PCA), are used to discover structures in environmental datasets. For example, these techniques could cluster chemicals based on structural similarity, uncover patterns of anomalous exposures, or identify the underlying mixtures of pollutants in environmental samples. The use of ensemble methods, which combine multiple algorithms to enhance prediction accuracy, has become especially relevant in toxicology. The random forest method and boosting methods both improve accuracy and reduce overfitting, making them appropriate for complex environmental datasets that are noisy and exhibit multicollinearity. More and more often, hybrid frameworks that combine statistical modelling and ML algorithms are used to achieve both interpretability and predictive performance.[9].

AI / ML Technique	Type	Key Application in Environmental Toxicology	Example Use
Linear Regression	Supervised	Dose–response modelling	Predict toxicity thresholds
Random Forest	Supervised (Ensemble)	Chemical toxicity prediction	Predict carcinogenic potential
Support Vector Machine (SVM)	Supervised	Hazard classification	Classifying toxic vs non-toxic compounds
K-Nearest Neighbours (KNN)	Supervised	Similarity-based chemical analysis	Predict chemical behaviour
K-Means Clustering	Unsupervised	Chemical grouping	Identifying pollutant mixtures
Principal Component Analysis (PCA)	Unsupervised	Dimensionality reduction	Pattern detection in environmental data
Neural Networks	Deep Learning	Complex toxicity modelling	Mixture toxicity prediction

Table 2. Machine Learning Techniques Applied in Environmental Toxicology Modelling

A. QSAR and Predictive Toxicity Modelling

One of the earliest and most important uses of AI in toxicology is Quantitative Structure–Activity Relationship (QSAR) modelling. In this approach, QSAR models are built to establish mathematical relationships between chemical structure descriptors and a chemical's biological activity or toxicity. Examples of such molecular descriptors include physicochemical parameters such as lipophilicity and molecular weight, as well as electronic and topological descriptors. The models are further improved by the use of machine learning algorithms, which help capture and generalise non-linear relationships over an extensive range of chemical classes. Predictive toxicity modelling is more complex than analysing a single compound and instead involves high-throughput screening of thousands of chemicals. More and more regulatory bodies are relying on in silico models to minimise the need for animal testing and to speed up the assessment of the risks posed by different chemicals. ML-based models can predict a chemical compound's acute toxicity, potential to cause cancer, potential to cause genetic mutations, potential to disrupt the endocrine system, and environmental toxicity. To further enhance the accuracy of these predictions, sophisticated methods, such as molecular docking, are used. Molecular docking, a cheminformatics approach that combines structural biology and computational toxicology, is one such method.[10].

Furthermore, multitask learning models enable the simultaneous prediction of multiple toxicity endpoints, thereby improving efficiency and reliability. Additionally, models utilising transfer learning can be fine-tuned on smaller, specialised datasets after having been trained on large, general chemical datasets. These advancements prominently increase the environmental toxicology assessments' innovativeness and broad application

B. Deep Learning and Big Environmental Data

Deep learning, a subfield of machine learning that mimics artificial neural networks, excels at analysing high-dimensional, unstructured datasets. Increasingly, deep neural networks (DNNs), convolutional neural networks (CNNs), and recurrent neural networks (RNNs) are being used for toxicological data. For instance, CNNs can be used to analyse images of chemical structures or patterns, and RNNs are used to analyse time-series data on environmental exposure. The integration of large datasets in environmental health research, such as remote sensing imagery, real-time environmental sensor networks, omics (genomics, proteomics, and metabolomics), and electronic health records, is reshaping the field. AI can analyse the spatio-temporal aspects of pollution, predict exposure, and determine the relationships between environmental variables and diseases. When compounds are represented as interconnected nodes and edges, Graph Neural Networks (GNNs) improve the modelling of chemical behaviours and structure.

It is worth noting that, unlike traditional models, deep learning models excel at identifying subtle nonlinear relationships. For example, in the case of mixture toxicity, which involves the synergistic or antagonistic interaction of several pollutants, multilayer neural networks provide superior modelling. This phenomenon is especially relevant in urban areas, where people are exposed to multiple pollutants simultaneously [11].

C. Explainable AI in Toxicology

Many AI models, especially deep learning models, may be highly predictive. However, they are still called "black boxes," which is one reason they are hesitant to be used in regulatory and forensic settings. This is the problem that Explainable AI (XAI) is designed to solve. Methods such as SHAP (Shapley Additive Explanations), LIME (Local Interpretable Model-Agnostic Explanations), and feature (or variable) importance provide a means to identify which chemical descriptors or exposure parameters are the most influential in toxicity predictions. For model predictions to be considered biologically plausible and legally defensible, the primary hurdle is producing interpretable toxicity predictions.

In AI applications for risk assessment, especially when the AI is used to inform policy or provide testimony to a court, regulatory bodies seek clear, transparent justification for the AI's predictions. XAI methods align model predictions with established mechanisms of harmful processes, or toxicodynamics, ensuring that model predictions are mechanistically sound. Explainable AI fosters trust among interdisciplinary stakeholders, such as toxicologists, forensic investigators, public health experts, and policymakers.

Explainable AI is a bridge between predictive performance and scientific interpretability. Explainable AI boosts confidence in computational toxicology and its applicability in environmental governance. To conclude, the application of AI and ML techniques in predictive toxicology has been transformative. It has facilitated high-throughput predictions, the recognition of complex patterns, and the integration of disparate datasets.

The evolution of method and theory in environmental toxicology has been significant in the fields of Forensic and Public Health. Environmental toxicology has advanced in both breadth and depth, moving from QSAR-based Hazard Prediction to the application of Deep Learning to the analysis of large datasets.[12].

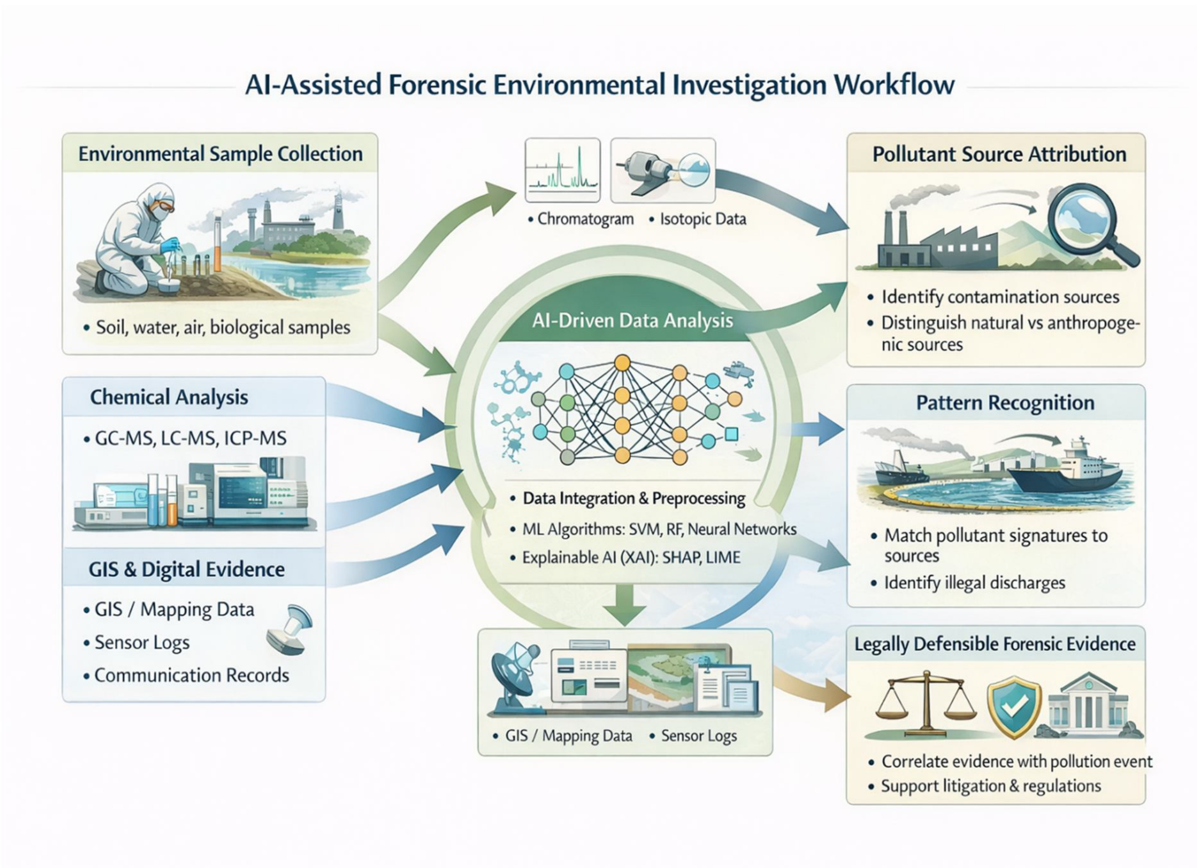
IV. AI-DRIVEN APPLICATIONS IN FORENSIC ENVIRONMENTAL TOXICOLOGY

The application of Artificial Intelligence (AI) in forensic environmental toxicology has facilitated pinpointing contamination sources, interpreting sophisticated environmental evidence, and establishing scientifically defensible causal links between pollutants and polluters.

Environmental crimes such as illegal dumping of waste, violations of industrial discharge regulations, contamination of groundwater, oil spills, misuse of pesticides, and trafficking in hazardous waste often involve complex data structures beyond the reach of traditional investigative techniques. AI applications can analyse chemical signatures, spatial distributions, and temporal patterns systematically, thereby strengthening evidence in environmental litigation and regulatory enforcement.

Application Area	AI Techniques Used	Data Sources	Forensic Outcome
Pollution Source Attribution	Random Forest, SVM	Chemical fingerprints, isotope ratios	Identification of pollution origin
Oil Spill Investigation	Pattern recognition, clustering	Hydrocarbon composition profiles	Matching spill samples to the source
Heavy Metal Contamination Analysis	Machine learning classification	Trace element signatures	Distinguishing industrial vs natural sources
Environmental Evidence Interpretation	Neural networks	Spectrometry, GC-MS data	Automated chemical identification
Environmental Crime Detection	Anomaly detection	Sensor logs, monitoring data	Detection of illegal dumping or discharge
Digital–Environmental Forensics Integration	NLP, remote sensing AI	Satellite images, SCADA logs	Linking pollution to industrial activity

Table 3. AI Applications in Forensic Environmental Toxicology



The integration of environmental sampling, chemical fingerprinting, digital evidence, and machine learning algorithms for pollution source identification and forensic interpretation is illustrated in Figure 2.

A. Pollutant Source Attribution

Identifying the source of environmental pollution is a core problem in forensic environmental toxicology. The technical challenges of source identification include distinguishing the source of contamination(s), whether from ambient (natural) or anthropogenic (artificial) sources, or determining the responsible facility, geographic location, or emission pathway. In the traditional methods, various sources, such as isotope analysis, chromatographic, profiling, and statistical (fingering) methods, provide a basis for documentation. Still, in industrialised settings, pollution sources are too numerous and complex.

Machine learning methods make the most significant contributions to source attribution by interpreting multidimensional fingerprints in chemical data (obtained from spectrometry), isotopic signatures, and trace element data. The trained supervised classification (SC) methods, such as a support vector machine (SVM) or random forests (RF), can detect and interpret the classifications of pollution produced by industrial, agricultural, or mining activities, and can classify all other samples with very high classification accuracy, even if the samples are different in composition and are in trace amounts[13].

Unsupervised clustering methods (UCM) also facilitate the identification of non-obvious groupings and the analysis of latent pollution patterns in environmental data associated with an emission source. In environmental pollution and oil spill (now referred to as EAP) investigations, the HC (hydrocarbon) composition patterns in various samples help identify sources of environmental pollution and EAP, as assisted by AI. In cases of heavy metal contamination, industrial discharge patterns are unmasked, and geogenic (of the Earth's crust) patterns are separated from industrial discharge and geogenic patterns.

Integrating Spatial Machine Learning Techniques and Geographic Information Systems (GIS) data, pollutant concentration maps, and meteorological, hydrological, and land-use data flow models, and GIS data improve attribution accuracy while aiding probabilistic source identification models; an ever-growing attribution source/model tool in more and more legal cases that require quantitative proof of causation.[14].

B. The Recognition of Patterns in Environmental Evidence

Compositional complexity is a defining characteristic of environmental evidence. AI-enabled Environmental Evidence Pattern Recognition is a machine-learning approach to addressing the problem of toxicity in mixtures of environmental evidence. With the help of a neural network, patterns of co-occurring substances that lead to the identification of a source or pathways of transformation are identified.

A particular class of predictive models that can serve as a basis for early warning systems is neural networks with recurrent connections. Examples of their use include identifying fluctuations in pollutant concentrations associated with illegal discharges or accidental releases.

The analysis of data produced by the intersection of chromatographic spectroscopy (spectroscopy) and gas chromatography-mass spectrometry (GC-MS) is a resource-intensive and sophisticated task that is often assigned to people. The automation of data analysis reduces subjectivity, increases reproducibility, and decreases the potential for error in interpreting data by forensic scientists.[15].

Additionally, more and more anomaly detection algorithms are being employed to detect changes in environmental baselines. AI systems can learn normal background patterns and detect atypical signatures of contaminants, which may indicate illegal activity. This ability enhances environmental surveillance systems, making them more proactive. AI in Forensic Laboratory Toxicology: AI in forensic laboratories supports automating processes, improving workflow accuracy, and enhancing workflows. For instance, machine learning models can assist with spectral interpretation, peak detection and matching, and the quantification of toxic agents found in samples (biological and/or environmental). Automated detection of toxic agents helps maintain analysis accuracy and reduces laboratory turnaround time. \par In instances of environmental exposure-related death or injury, AI can combine toxicological information from biological samples and environmental concentrations to aid in reconstructing the scenario of exposure. Bayesian models can assist with estimating exposure duration (e.g., time, intensity, and/or direction of exposure). This is important information to support the medico-legal determination of exposure. \par Add AI-based decision support systems to provide expert testimony and support about the statistical confidence level of the contaminant source matching and/or explainable AI to support the statistical level of confidence and the explainable AI that is used so that the forensic findings can be explainable and defensible from a scientific standpoint to be in support of the legal admissibility emerging Integration of Digital Forensics and Environment Contamination. The integration of digital forensics and environmental forensics is a new and rapidly developing area of inquiry. The digital footprint is found in almost all environmental crimes. It can include the logging of sensors, supervisory control and data acquisition (SCADA) systems, satellite and other imagery, shipping and other transport communications, and logs of electronic communications. AI can assist in analyzing these disparate digital datasets related to chemical or biological evidence, thereby enabling the construction of temporal and causal links between the two [16].

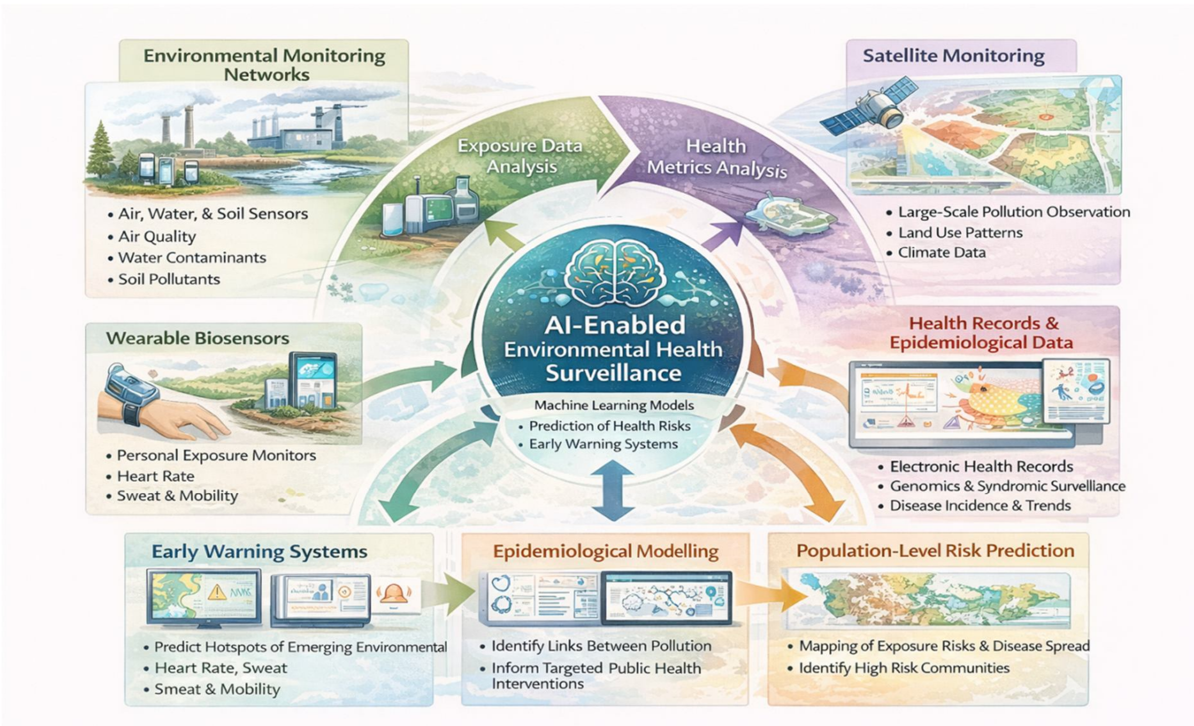
For example, the extraction of illegal mining and deforestation activities from remote sensing images can be performed using machine learning models, which can then be linked to the extraction of heavy metals and their contamination of nearby water bodies. An example of this is the unauthorised disposal of waste in an environmentally harmful way, which an anomaly detection system in industrial process logs can detect.

Examples of this include detecting patterns in Corporate Social Responsibility (CSR) documents, regulatory submissions, and intercompany communications that suggest a breach of an environmental regulation using natural language processing (NLP) technology. Moreover, this multidisciplinary approach is valuable when evaluated with the chemical fingerprinting results.

Artificial Intelligence (AI) applications in environmental forensic toxicology improve source identification, evidence interpretation, laboratory productivity, and analysis of the digital and environmental nexus. The application of Artificial Intelligence (AI) technology improves the reliability of the science and the strength of the legal arguments in environmental forensics investigations.[17].

V. AI FOR PUBLIC HEALTH SURVEILLANCE AND RISK PREDICTION

The fusion of Artificial Intelligence (AI), environmental toxicology, and public health has, for the first time, enabled the determination of the likelihood of an adverse event and the prevention of disease on a large scale. Historically, public health systems have relied on post-event epidemiological studies. Public health systems have identified environmental health problems only after the population has been exposed and the disease has developed. However, models that use Artificial Intelligence (AI) enable real-time observation of an exposed population, risk assessment in an environment, and the shift toward preventive public health systems.[18].



The integration of environmental monitoring networks, wearable biosensors, satellite observations, and health datasets with artificial intelligence models for environmental health surveillance and risk prediction is illustrated in Figure 3.

A. *Early Warning Systems*

Early warning systems using AI are being developed to identify emerging environmental threats that could become public health emergencies. These systems combine environmental detection systems with machine learning, enabling them to identify anomalies and predict surges during public health emergencies. Environmental detection systems combine data from various environmental monitoring methods. These data may include air quality measurements, water contaminants, weather data (meteorological variables), and satellite data. Certain time-series forecasting methods, such as recurrent neural networks (i.e., RNNs) and long short-term memory (i.e., LSTMs), are particularly useful for modelling temporal pollutant data. These systems rely on historical data to predict short-term exposure. These short-term data-exposure predictions may include particulate matter (PM), ozone, and other industrial emissions. Predictive or modelling systems for air quality (or critical pollutants) are of great benefit to health authorities, as they enable time-sensitive exceedance notifications, preventive pollution source controls, and targeted pollution mitigation.

Imminent threats to environmental health can be easily captured and alerted to regulatory agencies for inspection. AI systems serve as important health protection measures for potentially vulnerable members of the population. Surveillance forecasting models are recognising the role of extreme weather, such as flooding, as well as extreme temperatures, in contaminant movement. The use of climate-sensitive AI models, combined with environmental toxicology, will further enhance preparedness frameworks in impacted areas.[19].

B. Epidemiological Modelling

Epidemiology tries to determine the linkages between a population's health and the environment. Traditionally, epidemiology has explained health outcomes and their correlations with the environment despite the presence of outliers and irrelevant factors, large, complex, non-linear relationships, and high-dimensional data. Machine learning addresses many of these concerns because it is designed to uncover relationships and interactions that are not visible to traditional regression models.

The incidence of illness, as predicted by supervised learning algorithms, is influenced by external environment, age, sex, and genetic factors. Machine learning models have shown associations between air pollution and respiratory illness, cardiovascular disease, and neurodevelopmental disorders. The presence of multiple algorithms in a prediction ensemble method improves prediction accuracy while also reducing bias and variance.[20].

The combination of a causal inference approach and artificial intelligence enhances the reliability of epidemiological research. AI also improves the estimation of causal relationships rather than correlational ones through counterfactual modelling and propensity score matching. AI can also be used to identify causal pathways by integrating multi-omics data, as well as to identify pathways of environmental factors to disease.

Predictive models in epidemiology aid in developing policies and facilitating public health initiatives, including directing efforts to appropriate interventions in communities that are more susceptible to health risks and improving the allocation of public health resources.

C. Smart Environmental Sensors and Integrated Internet of Things

Environmental sensors and IoT devices have significantly increased both the quantity and quality of data available for exposure monitoring. Air quality monitors, water quality sensors, exposed wearables, and exposure-monitoring satellites create continuous environmental data streams. High-frequency data streams are processed in real time using AI algorithms that identify patterns and predict risks.

The combination of edge computing and AI in the cloud enables rapid data analysis and decentralised monitoring. Chemical leak exposure in industrial settings, for example, is automatically reported to regulatory agencies by sensor networks. In smart cities, integrated AI can predict the dispersion of urban pollutants by analysing traffic volume, industrial activity, and weather conditions.

Wearable biosensors have enabled a new level of exposure monitoring. AI can assess and estimate exposure-response relationships by monitoring individual biosensors and environmental parameters. This is the foundation for a shift away from generalised health risk assessments and toward person-centred risk assessments that support the precision public health model.[21].

D. Risk Assessment on a Population Scale

Large-scale risk assessment uses multiple datasets to monitor different types of health risks. The risks are caused by a combination of environmental hazards, demographics, economy, and social and health behaviours, which AI captures. The combination of AI and Geographic Information Systems (GIS) enables the development of spatial risk models, which, in turn, allow exposure risks and patterns of environmental injustice to be modelled and detected.

Exposed communities can be quantified using predictive risk-scoring models that integrate factors related to mixture toxicity, exposure timing, and indices of susceptible exposure. This type of assessment is valuable in poor communities, where risk assessment must be prioritised to assist them.[22].

Additionally, risk modelling across different institutions while preserving data privacy can be achieved using federated learning. Public health agencies improve the predictive capability of their models in compliance with privacy regulations by using AI models trained on a decentralized dataset. Public health surveillance systems based on Artificial Intelligence (AI) enhance the identification of environmental risks, improve epidemiological modeling, and enable population-scale risk assessment. Furthermore, AI, in combination with the Internet of Things (IoT) and advanced analytical systems, supports the integration of toxicology and health care into more proactive management of health risks.[23].

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VI. CHALLENGES, ETHICAL AND REGULATORY CONSIDERATIONS

Challenge	Description	Potential Solution / Research Direction
Data Bias	Limited geographic or pollutant representation	Global environmental data sharing initiatives
Model Explainability	Black-box AI models difficult to interpret	Explainable AI techniques (SHAP, LIME)
Legal Admissibility	Lack of standards for AI forensic evidence	Development of validated regulatory frameworks
Privacy Concerns	Integration of environmental and health data	Federated learning and secure data sharing
Model Generalizability	Poor performance on unseen pollutants	Cross-regional validation datasets
Ethical Concerns	Environmental justice and biased predictions	Inclusive datasets and ethical governance

Table 4. Challenges and Future Research Directions in AI-Driven Environmental Toxicology

The potential impact of Artificial Intelligence (AI) across environmental toxicology, forensic science, and public health is immense. However, there are significant methodological, ethical, and regulatory challenges that need to be addressed for implementation to be responsible and sustainable. The AI models that integrate into decision-making, such as in the judicial system and/or within public health, need to be justified and balanced with respect to data, transparency, equity, and regulatory compliance.

A. Data Bias and Model Reliability

AI systems depend on the quality, variability, and representativeness of the data used to train them. For example, in the field of environmental toxicology, data may be skewed geographically – data used may be limited to a certain developed region or to well-studied, well-known contaminants. This creates a scenario in which models may be less effective for unknown pollutants or for underrepresented demographics. Moreover, the absence of data, measurement variability, inconsistent protocols within a laboratory, and environmental sampling across heterogeneous environments may significantly limit the reliability of a model. Overfitting is when a model performs well on previously studied data but poorly on new data, and it is a significant concern, especially with complex, deep learning models. AI's predictions regarding the toxicity of tested substances may lack generalizability, as the AI system lacks external validation and has not undergone cross-regional testing.[24].

To improve reliability, a set of standardised data collection protocols should be established, along with transparent documentation of the model and clearly articulated computational pipelines so that the model may be replicated. The incorporation of uncertainty quantification and the justification of confidence intervals also supports defensibility in a scientific context.

B. Legality of AI Evidence in Forensics

In Environmental Forensics and Toxicology, AI-generated evidence must also meet admissibility criteria. Scientific evidence must be transparent, reproducible, peer-reviewed, and widely accepted within the discipline. A Black-box AI model is difficult because the reasoning or process behind its conclusions is unknown. The absence of XAI (eXplainable AI) is a limitation, but XAI techniques explain the model's reasoning and the importance of key features. The legal system may have concerns about algorithms, including the legal tolerance for erroneous conclusions and the potential for bias. It is therefore essential that AI forensic toxicology be standard in validation, and that experts establish a system for accountability. The use of AI in Environmental Litigation is also a result of extensive methodological approaches and a lack of clarity regarding the methods used [25].

C. Environmental Justice and Privacy

AI-based public health surveillance has been developed. AI-based surveillance and public health have used various open-access, uncontrolled sources of environmental exposure data and integrated them with health records, demographics, and geography. While integrating data sources improves predictive ability, it poses challenges related to data privacy, informed consent, and data security. Unauthorised access or misuse of the data may erode the public’s trust in the surveillance system.

Additionally, environmental justice must be considered. Communities that have been historically marginalised have a larger share of environmental issues. If systems that use AI are trained with bias, inequities will be perpetuated by the underrepresentation or misclassification of exposed at-risk populations. As a result, ethical governance of AI systems must include components of fairness, inclusivity, and community involvement[26].

D. Regulatory Barriers

Regulators' acceptance of AI use in toxicology is slow due to the lack of unified global standards. Most agencies use traditional risk assessment models, and those models tend to have well-defined validation requirements that highlight methodology. For AI models to be used, new policies will need to be created that identify the regulators' requirements for the acceptable balance of transparency, validation thresholds, and accountability built into models. Overall, the use of AI in environmental toxicology and public health is promising. Still, it must be implemented with appropriate focus on data integrity, the law, ethics, and regulations. This will ensure that AI use is trustworthy and equitable.

Future research in this area must focus on developing new, fully integrated, intelligent analytical systems that can connect both biologically and computationally on a global scale. New hybrid AI–toxicology models can represent a new approach to this, as they integrate both data-driven, or 'machine learning', models and toxicological data and may leverage mechanistic explanations to improve model use in AI.

By using complex coding for toxicokinetics and toxicodynamics, the AI models will be better accepted by the biological and regulatory communities. Improvements in the mechanistic understanding of neural network frameworks' predictive capability, as well as in the predictive guidance of more classical physics-based models, will enhance the use of 'augmented' or 'guided' machine learning models. Another option for improving the future of toxicology lies in the use of federated machine learning, especially in the relationships between prospective public health and forensic toxicology involving sensitive data. Decentralised federated learning, or collaborative learning without data sharing, respects data privacy and enables learning from potentially diverse data for both environmental and health datasets. This model could support toxicological surveillance across multiple countries while improving global health security. The predictive capability of information on toxicity provided to countries, while respecting current data-use limitations, can be improved.

Multi-omics (genomics, transcriptomics, proteomics, and metabolomics) integrated with Artificial Intelligence (AI) will improve the precision of predictive models for the exposure-response relationship, as it can provide early biological signatures indicative of toxicity. When integrated with environmental data, AI will provide a more precise, tailored approach to public health.

The combination of global environmental monitoring systems that use AI and real-time sensor networks will be beneficial to monitoring transboundary pollution and forecasting climate exposure. Dynamic global risk maps can be generated by merging satellite data, IoT sensors, and predictive models, enabling rapid action and joint environmental governance. These lines of research aim to implement, for the first time, a proactive ecosystem of data-based toxicology.[27].

VII. CONCLUSION

The combination of artificial intelligence (AI) and machine learning (ML) with environmental toxicology is revolutionising the field by reshaping the processes of detection, interpretation, and management of environmental dangers. This review outlines the present state of the field. It demonstrates that, in the AI paradigm, predictive toxicological modelling improves predictive performance, enhances the efficiency of chemical risk evaluation, supports forensic source attribution, and supports public health surveillance initiatives. AI systems, when used in conjunction with the other methodologies, provide the most thorough risk assessment and the most advanced predictive capacity. Despite the obstacles, the most substantial research gaps remain unaddressed. The forensic and regulatory community is still developing standardised frameworks for validating AI-based toxicology models. The scarcity of uniform, high-quality datasets and the fact that models, not the data, comprise the geographic and demographic framework limit the generalizability of models. Moreover, achieving a balance between scientifically rigorous toxicology and legally defensible AI will require considerable refinement of methodologies to integrate the two. Implementing AI technologies in environmental toxicology also has significant potential to improve environmental governance, legal analytics, and public health planning. AI technologies can be employed for predictive modelling, population-level risk assessment and analytics, and risk exposure analytics. These tools can help decision makers and provide the basis for evidence-based policymaking and targeted intervention strategies. AI, when used in a principled and legally compliant manner, will provide the tools for a flexible, robust approach to protecting the public's health and to forensic accountability for the environment.

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REFERENCES

[1] T. H. Tulchinsky and E. A. Varavikova, "Environmental and Occupational Health," *The New Public Health*, p. 471, 2014, doi: 10.1016/B978-0-12-415766-8.00009-4.

[2] F. Faiola, N. Yin, and R. Yang, "Environmental Toxicology: The Importance of Disease-Specific In Vitro Models," *Environment & Health*, vol. 2, no. 2, p. 65, Feb. 2023, doi: 10.1021/envhealth.3c00186.

[3] "Frontiers | Explainable Artificial Intelligence in Toxicology: Building Trust in Predictive Models." Accessed: Mar. 07, 2026. [Online]. Available: https://www.frontiersin.org/research-topics/74573/explainable-artificial-intelligence-in-toxicology-building-trust-in-predictive-models

[4] E. Demir and S. Kacew, "Environmental Toxicology and Human Health," *Int. J. Mol. Sci.*, vol. 25, no. 1, p. 555, Jan. 2023, doi: 10.3390/ijms25010555.

[5] T. R. Fagundes, C. Coradi, B. G. L. Vacario, J. M. B. de Morais Valentim, and C. Panis, "Global Evidence on Monitoring Human Pesticide Exposure," *J. Xenobiot.*, vol. 15, no. 6, p. 187, Dec. 2025, doi: 10.3390/jox15060187.

[6] J. Pauluhn, "Toxicokinetic Tests," *Regulatory Toxicology*, pp. 1–26, 2021, doi: 10.1007/978-3-642-36206-4_38-2.

[7] I. of M. (US) C. to A. the S. B. for T. H. Reduction, K. Stratton, P. Shetty, R. Wallace, and S. Bondurant, "Exposure and Biomarker Assessment in Humans," 2001, Accessed: Mar. 08, 2026. [Online]. Available: https://www.ncbi.nlm.nih.gov/books/NBK222378/

[8] N. R. C. (US) C. on A. of T. T. to P. Toxicology, "Overview of Risk Assessment," 2007, Accessed: Mar. 08, 2026. [Online]. Available: https://www.ncbi.nlm.nih.gov/books/NBK10201/

[9] M. Yu, M. Fang, Z. Tian, B. Wang, and D. Walker, "Artificial Intelligence and Machine Learning for Environmental Health Study," *Environment & Health*, vol. 3, no. 10, p. 1115, Oct. 2025, doi: 10.1021/envhealth.5c00324.

[10] T. J. Choi, H. E. An, and C. B. Kim, "Machine Learning Models for Identification and Prediction of Toxic Organic Compounds Using Daphnia magna Transcriptomic Profiles," ., vol. 12, no. 9, p. 1443, Sep. 2022, doi: 10.3390/life12091443.

[11] I. H. Sarker, "Deep Learning: A Comprehensive Overview on Techniques, Taxonomy, Applications and Research Directions," *SN Comput. Sci.*, vol. 2, no. 6, p. 420, Nov. 2021, doi: 10.1007/s42979-021-00815-1.

[12] G. Chaudhary, "UNVEILING THE BLACK BOX: BRINGING ALGORITHMIC TRANSPARENCY TO AI," *Masaryk University Journal of Law and Technology*, vol. 18, no. 1, pp. 93–122, 2024, doi: 10.5817/MUJLT2024-1-4.

[13] L. J. Zhang, L. Qian, L. Y. Ding, L. Wang, M. H. Wong, and H. C. Tao, "Ecological and toxicological assessments of anthropogenic contaminants based on environmental metabolomics," *Environmental Science and Ecotechnology*, vol. 5, p. 100081, Jan. 2021, doi: 10.1016/j.ese.2021.100081.

[14] "(PDF) Analysis of Pollution Patterns Using Unsupervised Machine Learning Algorithms." Accessed: Mar. 08, 2026. [Online]. Available: https://www.researchgate.net/publication/234555819_Analysis_of_Pollution_Patterns_Using_Unsupervised_Machine_Learning_Algorithms

[15] L. Huang *et al.*, "Artificial intelligence: A key fulcrum for addressing complex environmental health issues," *Environ. Int.*, vol. 198, no. 4, p. 109389, Apr. 2025, doi: 10.1016/j.envint.2025.109389.

[16] M. Nikravan, M. H. Kashani, and S. B. Abkenar, "Anomaly detection with artificial intelligence," *Handbook of AI-Driven Threat Detection and Prevention: A Holistic Approach to Security*, pp. 59–78, Jun. 2025, doi: 10.1201/9781003521020-4.

[17] J. G. Maturano, J. D. M. Santana, A. L. Aguilar-García, and M. S. Hernández, "REMOTE SENSING OF ILLEGAL DUMPS THROUGH SUPERVISED CLASSIFICATION OF SATELLITE IMAGES: APPLICATION IN OAXACA, MEXICO," *Geographical Research Letters*, vol. 50, no. 2, pp. 157–177, Dec. 2024, doi: 10.18172/cig.6273.

[18] D. B. Olawade, O. J. Wada, A. C. David-Olawade, E. Kunonga, O. Abaire, and J. Ling, "Using artificial intelligence to improve public health: a narrative review," *Front. Public Health*, vol. 11, p. 1196397, 2023, doi: 10.3389/fpubh.2023.1196397.

[19] I. Villanueva-Miranda, G. Xiao, and Y. Xie, "Artificial intelligence in early warning systems for infectious disease surveillance: a systematic review," *Front. Public Health*, vol. 13, p. 1609615, 2025, doi: 10.3389/fpubh.2025.1609615.

[20] "Guidelines on studies in environmental epidemiology," p. 351, 1983.

[21] F. C. Andriulo, M. Fiore, M. Mongiello, E. Traversa, and V. Zizzo, "Edge Computing and Cloud Computing for Internet of Things: A Review," *Informatics 2024, Vol. 11, Page 71*, vol. 11, no. 4, p. 71, Sep. 2024, doi: 10.3390/informatics11040071.

[22] H. R. Dastjerdi, S. Mohammadi, M. Saeidi, and M. Koohikamali, "Developing a Population-Density-Weighted Community Health Vulnerability Index for Heat and Air Quality to Support Targeted Public Health Interventions: A Multihazard Assessment Using Remotely Sensed and Socio-economic Data in Los Angeles," *Sustain. Cities Soc.*, vol. 14, no. 9, p. 107274, Mar. 2026, doi: 10.1016/j.scs.2026.107274.

[23] A. Horst *et al.*, "Federated learning: a privacy-preserving approach to data-centric regulatory cooperation," *Frontiers in Drug Safety and Regulation*, vol. 5, p. 1579922, 2025, doi: 10.3389/fdsfr.2025.1579922.

[24] H. Xu *et al.*, "Trusted artificial intelligence for environmental assessments: An explainable high-precision model with multi-source big data," *Environmental Science and Ecotechnology*, vol. 22, no. 14, p. 100479, Nov. 2024, doi: 10.1016/j.ese.2024.100479.

[25] C. E. Pratap and D. Harini, "1 Government Advocate (Criminal Side," *Jindal Global Law School, O.P. Jindal Global University*, doi: 10.51244/IJRSI.

[26] "(PDF) AI for Public Health Surveillance." Accessed: Mar. 08, 2026. [Online]. Available: https://www.researchgate.net/publication/384732109_AI_for_Public_Health_Surveillance

[27] J. de P. Souza *et al.*, "Advancing the implementation of artificial intelligence in regulatory frameworks for chemical safety assessment by defining robust readiness criteria," *Front. Artif. Intell.*, vol. 8, p. 1738770, Jan. 2026, doi: 10.3389/frai.2025.1738770