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Artificial Intelligence-Driven Environmental Pollution Monitoring and Remediation: Advances in Predictive Modelling, Smart Materials, and Sustainable Technologies – A Critical Review

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ABSTRACT: Innovative solutions for contaminant detection, prediction and remediation are needed for a long-term solution to environmental pollution and its effects on ecosystem integrity, public health and sustainable development. AI, especially machine learning and deep learning technologies, are being more widely adopted to enhance the management of pollution through the use of environmental monitoring networks, advanced materials, and treatment technologies. The current review investigates the latest developments in environmental monitoring and analysis using AI, AI-based pollution forecasting, smart remediation materials, and sustainable pollution-control systems. Application studies involving atmospheric pollutants, wastewater contaminants, heavy metals and microplastics, using an emphasis on sensor networks, remote sensing, data fusion and intelligent process optimization. The predictive relationships between material properties and contaminant removal has been shown to be a potential application of AI-assisted material discovery for enhancing adsorbent selection, photocatalytic performance, and biochar-based remediation. Likewise, highly automated wastewater treatment plants provide potential for optimizing their operation, recovering resources, and minimizing energy consumption. However, reported improvements are often from laboratory experiments, retrospective datasets, or simulations, but not from independent validations in the field. Scarcity of data, algorithmic bias, lack of interpretability, lack of uncertainty quantification, lack of durability of the material, and the environmental impact of the computational infrastructure are all significant problems. Moreover, predictive accuracy does not necessarily imply better effectiveness of remediation or sustainability. Physics-informed models, explainable AI, standardised datasets, life-cycle assessment, and prospective field validation should be looked into in future research. The application of AI in the design of materials using environmental responsibility and principles of circular economy can complement pollution prevention and mitigation if technological innovation is accompanied by transparent assessment, regulation and implementation in different environmental contexts all over the world.

1. INTRODUCTION

1.1 Environmental Pollution as a Global Sustainability Challenge

Environmental pollution continues to be a significant issue concerning ecological stability, public health and sustainable development. Industrialisation, urbanisation, intensification of agriculture and increase in material consumption has led to the addition of different contaminants to the atmosphere, water bodies and land. Such contaminants are particulate matter, nitrogen oxides, volatile organic compounds, toxic metals, pesticides, pharmaceutical residues, industrial dyes and microplastics.

Pollution management is not just about the identification of contamination after it's released. The success of environmental protection efforts requires the knowledge of the sources of pollutants, how they are transported and transformed, how they will affect the environment, and how they can be remediated with minimal secondary environmental effects.

Laboratory analyses, regulation monitoring stations, periodic field sampling, and physicochemical measurements are conventional monitoring methods. These methods give useful reference data, but can be costly, geographically restricted, labor intensive, or not responsive enough to the dynamic nature of the environment.

In a similar fashion, traditional remediation technology could be energy intensive, need significant use of chemicals, equipment and facility resources, and involve operation skills. Their performance can vary because of complex interactions between the physical, chemical and biological properties of the environment.

The other solution areas to these challenges through artificial intelligence (AI) include predictive analysis, automated pattern recognition, intelligent control and data-informed material development (Garbagna et al., 2025).

1.2 Emergence of Artificial Intelligence in Environmental Science

AI has computational methods that can detect patterns, predict, assist in decision-making, and adapt to complex data sets. Machine learning is one of the largest applications of AI, and Deep Learning (DL) involves training multilayer neural networks to learn representations from data. Examples of environmental applications are predicting pollutant levels, calibration of sensors, detection of contaminated areas, prediction of treatment effectiveness, and optimisation of operating parameters. Garbagna et al conducted a systematic review on AI-based air pollution modeling and discussed the increasing application of machine-learning and deep-learning techniques in forecasting air pollutants (Garbagna et al., 2025). AI's applications have also evolved from prediction to environmental decision-making, automated treatment and sustainable resource management in recent years. Yet this is not a sign of environmental benefit. A model can be highly accurate on past data, but have poor performance during abnormal pollution events or when applied to a different region.

1.3 Rationale and Objectives

The existing literature focuses on the environmental monitoring or remediation technologies and/or smart materials individually. An integrated assessment is also essential as the effectiveness of AI will rely upon the ability to link accurate observations with effective interventions. This review critically assesses the use of AI in three interrelated fields; environmental monitoring, predictive modelling, and pollutant remediation. Focus on the development of intelligent sensors, remote sensing systems, AI-assisted adsorbents, photocatalysts, biochar materials and wastewater treatment technologies. Sustainability, operational feasibility, model reliability, and the constraints that hinder the implementation of innovations developed on the lab scale to become effective environmental solutions is also discussed in the review.

1.4 Scope and Review Approach

A critical narrative-review approach was used based upon 25 relevant publications from PubMed indexed literature on environmental monitoring, AI modeling, remediation materials and sustainable treatment systems. Review articles and research works on air, water and soil pollution are discussed. Research papers are prioritized if they are related to practical applications, technical challenges, and predictive performance and environmental outcomes. The review is not meant to be a comprehensive systematic search nor a quantitative meta-analysis. It aims at synthesizing key developments, identifying methodological shortcomings and research priorities.

2. ARTIFICIAL INTELLIGENCE TECHNOLOGIES FOR ENVIRONMENTAL POLLUTION MONITORING

2.1 Machine Learning and Deep Learning Approaches

The machine learning approach allows environmental scientists to model complex relationships between pollutant concentrations, meteorological parameters, geographic factors, industrial activity, and treatment parameters (Nelson et al., 2026). Some of the commonly used algorithms are random forests, support vector machines, gradient boosting, artificial neural networks, and decision trees. Random forests may be able to detect nonlinear relationships and interactions between the predictors, and to give information on variable importance. SVMs are helpful for certain classification/regression tasks, especially in cases where feature engineering is suitable. Gradient-boosting classifiers are a family of sequentially trained

classifiers that can work well with structured datasets in the environment. Images, spatial data, and temporal observations of pollutant data are used in deep learning architectures such as convolutional neural networks, recurrent neural networks, and long short-term memory networks. Recently, attention-based architectures and graph neural networks have been popular for capturing long-range dependencies and spatial relationships. But there is no one algorithm that is superior in all cases. Performance is related to data quality, sampling frequency, environmental complexity, training procedures and the validity of model evaluations. In 2026, the authors of a thorough review of air-quality modelling highlighted the ability of AI to predict air quality as well as the limitations of interpretability, uncertainty and the lack of data from regions (Nelson et al., 2026).

2.2 AI-Integrated Air Quality Monitoring

One of the mature AI applications in the environment is air pollution monitoring. The traditional regulatory stations are able to make good measurements, but do not have adequate spatial coverage to capture significant variation in the neighborhood (Nelson et al., 2026). The use of low cost sensor networks can be used to enhance spatial coverage, but their measurement may be influenced by humidity, temperature, sensor aging and possible interference from other pollutants. Machine learning can be used to calibrate the sensors to reference instruments and remove systematic measurement errors. Sousan and colleagues explored machine learning methods to enhance the calibration of the cheap air-quality monitor, an example of data-driven methods for environmental sensing (Sousan et al., 2025). The usefulness of these systems is that they can supply more geographically specific data relating to the exposure to pollutants. Under other environmental conditions, however, calibration models developed under this set of conditions may not be reliable. However, sensor networks must undergo reference comparisons, drift detection and periodic recalibration (Sousan et al., 2025).

2.3 AI-Driven Water Quality Monitoring

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2.4 Remote Sensing and Geospatial Monitoring

Satellite observations and aerial imagery and use of unmanned aerial vehicles offer the possibility of carrying out evaluations of environmental conditions over large geographic regions. Remote sensing is able to measure vegetation parameters, land-use, atmospheric parameters, surface temperature, and some water quality indicators. These observations can be used in conjunction with ground observations to estimate pollution distributions using AI algorithms. A systematic review of deep learning for water quality prediction also identified the rising applications of water quality computational modelling using deep learning approaches (Li et al., 2024). One review of the river water quality prediction methods using artificial intelligence models also found that there was a geographical bias in the research published and lack of uncertainty assessment as significant drawbacks (Amin et al., 2026). While remote sensing is a good tool for regional screening, it is not capable of detecting all pollutants directly. Satellite-derived estimates are often based on secondary relationships between the measured surface characteristics and the contaminant concentration. As a result, ground truth measurements are still needed for calibration and validation.

2.5 Detection of Microplastics

Microplastics are difficult to analyze because of the size, shape, polymer composition, colour and weathering of the particles. The common identification methods involve optical microscopy, Fourier-transform infrared spectroscopy, Raman spectroscopy and hyperspectral imaging. AI can help with particle recognition, spectral signatures interpretation and polymer type classification, which can be automated. Jin et al. discussed the applications of AI in microplastic detection and pollution mitigation, highlighting image analysis, spectroscopic approaches, and hyperspectral techniques (Jin et al., 2024). Recent reviews also highlight the capability of multimodal sensing to aid the identification of microplastics in complex environmental samples

(Kumar et al., 2026). However, classification can be influenced by biofilms, degradation of particles, spectral interferences, and inadequate training sets. Clean particles in the laboratory might be very different from weathered particles from sediments or wastewater, and an algorithm trained on clean particles may not work very well when applied to weathered particles. Also, identification of micro-plastic doesn't show successful removal or degradation (Bai et al., 2026).

2.6 Soil Contamination Monitoring

Soil contamination is a variable process depending on the spatial variability of soil and affected by land use, industrial processes, agriculture, soil chemistry, and geology. Traditional soil monitoring involves soil sampling and lab testing, which can be costly on a large scale. Machine learning algorithms can combine field measurements, geographic factors and spectral data to forecast potentially toxic element concentrations. An investigation of machine learning applications at industrially contaminated sites reviewed the application of environmental covariates as well as hyperspectral data on metal contamination in soil (Zou et al., 2026). The importance of spatially appropriate validation, uncertainty assessment and explainability in toxic-element concentration prediction was also highlighted in another review (Hawrami, 2026). Spatial validation becomes particularly important when the sampling sites are near each other, as they may have similar environmental characteristics. When such observations are randomly split into a training set and a test set, the performance of the model can be overestimated. Predictions should thus be tested at truly independent sites for environmental decision making.

3. ADVANCES IN AI-BASED PREDICTIVE MODELING

3.1 Pollutant Concentration Forecasting

Predictive modelling is one of the most popular applications of AI in environmental science and has been heavily researched. Pollutant concentration forecasting systems attempt to forecast concentrations from concentration measurements, weather data, emission information and environmental information. The particulate matter with aerodynamic diameter less than 2.5 and 10 micrometers ($PM_{2.5}$ and PM_{10}), ozone, nitrogen dioxide, sulfur dioxide and carbon monoxide are among the pollutants of the atmosphere, which are usually modeled. The traditional statistical methods (autoregressive models) provide useful bases. Machine learning is one subset of these technologies which can model nonlinear interactions and complex temporal patterns. In cases where a large amount of sequential data is available, deep learning models might be especially effective. Better results on past data does not guarantee good performance in scenarios of wildfires, industrial accidents, weather extremes and sudden shifts in emissions though. It is then required to test under extreme conditions and daily changes in the environment for a successful prediction system.

3.2 Spatial Prediction and Pollution Hotspot Identification

AI spatial models can estimate contamination concentration at sites for which there are no direct measurements. These techniques are based on concentrations observed and on geographic, environmental, and anthropogenic predictors. It is used for mapping of soil contamination, for estimating the vulnerability of groundwater resources, estimating exposure to the atmosphere, and for prioritisation of environmental sampling. The 2026 review of machine learning on soil and ground water contamination reviewed the use of environmental data and predictive models and the variables that control pollutant distribution. The potential benefit is to better allocate monitoring and remediation resources.

However, predictions should not be considered as absolute measures, as they are spatial predictions. As there is less training data and the environment that the data has been collected from is different from the environment the model is used for, uncertainty generally increases. Maps with a single predicted concentration can give the false impression of precision. Prediction intervals and uncertainty maps are therefore required, as is a description of the spatial domain of applicability.

3.3 Hybrid and Physics-Informed Models

Algorithms are statistical, based on data only and do not always represent the physical and/or chemical processes controlling pollutant behavior. This reduces their usefulness in varying conditions. The problem is treated by a physics-informed modeling that includes scientific constraints, process knowledge, or mechanistic equations in the computational models. These can be mass-balance relationships, reaction rate equations, hydrodynamic principles, and transport equations, etc. Hybrid systems can include machine learning elements that estimate hard-to-measure parameters and/or correct for systematic errors in prediction by a mechanistic model. In a physics-informed discussion of the transition from proof-of-concept machine learning to trustworthy deployment in natural and engineered water systems, Ma and colleagues emphasized the need for explainability and

for the systems to be integrated into operations (Ma et al., 2026). These are promising models that strike a balance between flex and scientific consistency. However, adding physical constraints does not necessarily mean there are no prediction errors. Performance can still be negatively affected by the wrong assumptions, incomplete mechanisms, and substandard training data.

3.4 Explainable Artificial Intelligence

Limited interpretability is a common criticism for complex machine learning models. Predictions can be less useful to environmental decision-makers because they don't always have a full understanding of the factors that affect them. Explainable AI methods explain the behavior of models by calculating feature importance, partial dependence plots, and using attribution methods like SHAP. These methods can be helpful in making predictions and determining the relationship between the variables used. One important difference is that explaining the behaviour of the model is one thing and establishing causality for the environment is another. A high weight, for example, for temperature in the model when determining pollutant concentrations, does not automatically mean that this is the primary cause of the pollutant concentration. The structure of the model, the presence of correlated variables and the presence of unmeasured confounders can all impact the results of attribution. Mechanistic understanding should then be followed by "explainability".

3.5 Model Evaluation and Uncertainty Quantification

Typical performance measures for environmental AI studies include coefficient of determination, root mean square error, mean absolute error, precision, recall, and classification accuracy. While these are helpful, they are not enough, if they are not reported with adequate validation. A high coefficient of determination does not mean that a model is good for capturing the "pulse" of pollution events, it only indicates that the model captures the general seasonal patterns well. Similarly, a high classification accuracy may be deceiving when the samples are contaminated. Temporal and spatial cross-validation, independent external testing and evaluation with distribution shifts are, therefore, essential. Uncertainty quantification is also important, as the decision threshold and health implications of the environmental decision may be important for public health. For example, if the prediction is very close to the limit of a pollutant allowed then further confirmatory sampling should be required and should not be considered as compliance. The goal of the practical should be something that is reliable environmental decision support and not just optimizing a numeric performance measure.

4. AI-DRIVEN ENVIRONMENTAL REMEDIATION TECHNOLOGIES

4.1 Intelligent Wastewater Treatment

Wastewater treatment is a sequence of physical, chemical, and biological processes, all of which are interdependent and are dependent upon the nature of the wastewater (influent) that is to be treated, microbial activity, wastewater temperature, hydraulic loading, or the operating conditions of the treatment plant. AI can help with effluent quality forecasting, process monitoring, equipment fault identification, and process optimization. Nagpal et al. discussed the use of AI in wastewater treatment, such as forecasting pollutant removal efficiency, tracking water quality parameters, and detecting operational issues (Nagpal et al., 2024). Examples of potential applications are optimizing aeration, chemical dosing, sludge management and treatment scheduling. Predictive models can for instance predict future oxygen demand and help operators to optimize the aeration system. But wastewater treatment plants vary widely in design, in the composition of the wastewater, in the types of microbes present, and in the conditions of operation. An algorithm created for a specific treatment facility could, therefore, be sub-optimal for another treatment facility. Implementation will need to be calibrated locally, have operational safeguards and be compared to conventional control strategies (Nagpal et al., 2024).

4.2 AI-Assisted Biological and Physicochemical Treatment

Biological treatment systems rely on dynamic microbial processes which are sensitive to fluctuations in nutrient concentrations, toxicity, oxygen levels and environmental conditions. The coagulation, adsorption, membrane separation, oxidation, and precipitation are examples of the processes that occur in physicochemical systems. These interactions can be modeled using AI, and better combinations of operating variables can be discovered. Behera and colleagues examined the use of AI in wastewater and waste-gas treatment processes, such as monitoring and controlling them, and recovering resources (Shishir Kumar Behera et al., 2024). AI can work alongside existing treatment technologies to minimize unnecessary testing and help for more responsive operations. However, even with computational optimization, some basic treatment limitations cannot be overcome. AI won't magically develop the capability to remove a specific contaminant if it doesn't have it in the first place. The process's suitability for the underlying treatment process is foremost.

4.3 Deep Learning and Automated Process Control

Deep learning is able to model complex interactions between the wastewater properties, microbial processes, operating conditions, and treatment results. Potential application: Soft Sensors- prediction of variables that are hard to measure from those that can be measured regularly. This can help to reduce the need for regular lab testing for certain operations. A critical review of deep learning for wastewater treatment was performed and the relationship between data-driven and traditional mechanistic models was highlighted (Alvi et al., 2023). Predictive control and automatic control are included in developed systems. For instance, reinforcement learning can discover control strategies that take into account effluent quality, energy consumption, and chemical usage. But there are risks of operations with automated decisions for treatment. An error in control action can be a problem for biological treatment, can result in emissions problems or failure to meet regulations. Therefore, safety limitations, human control and controlled testing must be done before deployment.

4.4 Digital Twins and Smart Treatment Facilities

A digital twin is a representation of a real world system via a computer model that can be updated with real world operational data. In wastewater treatment, digital twins can integrate data from various sensors, process models, and predictive algorithms to simulate and control the treatment processes. They can be used as a resource for operators to use for testing alternative treatment conditions without having to make changes. A smart wastewater treatment review for 2026 called out physics-informed modeling, optimization, and advanced control as all of them as ways to more reliable AI-assisted operation. Digital twins are particularly promising in situations where treatment systems have sufficient monitoring systems and a good history. However, the reliability of a digital twin is dependent on the basis of truth of the data, any assumptions that have been made and calibration. Poor maintenance of sensors and/or obsolete process representation can lead to incorrect operational recommendations.

4.5 Energy Optimization and Carbon Emission Reduction

Significant energy can be needed for the aeration, pumping and sludge processing in a wastewater treatment plant. Optimization using AI could be used to cut down on energy usage without compromising the effectiveness of treatment. Possible solutions involve optimizing aeration control, load forecasting, chemical dosing and scheduling of energy consuming processes. Zhang et al. summarized the various approaches that can be adopted to decrease the emission and optimize the wastewater treatment process using artificial intelligence, and highlighted the importance of coupling treatment performance with energy consumption and carbon emissions to develop an overall optimization strategy (Zhang et al., 2026). But, the savings in energy should be calculated by means of actual operating values. Reduced electricity consumption in a simulation does not mean the same will be the case during long-term plant operation. Any extra sensing equipment and the energy needed to power the computing equipment must also be part of the equation when measuring environmental benefits (Zhang et al., 2026).

4.6 Wastewater Reuse and Circular Resource Management

Where conditions are right, treated wastewater is suitable for uses in agriculture, industry and selected nonpotable applications. AI can help with tracking reclaimed water quality, forecasting treatment outcomes, and planning re-use cycles. AI for wastewater treatment and agricultural re-use was explored by Liu and colleagues, who found potential for further optimisation of wastewater treatment operations but significant gaps between the water quality requirements for re-use and the water quality focus of wastewater approaches (Liu et al., 2025). This distinction is significant since the quality of water acceptable for discharge may not meet the needs of a specific reuse use. Therefore, the reuse system must take into account intended uses, standards for contaminant removal, the risk of contamination by microorganisms, and long-term environmental impacts when using AI systems. Predictive accuracy is not enough to assure sustainable reuse, there needs to be risk management and regulatory compliance.

5. SMART MATERIALS AND AI-ASSISTED REMEDIATION

5.1 Concept of Smart Remediation Materials

The idea of smart remediation materials (SRM) is presented.Concept of smart remediation materials (SRM) is introduced. Smart materials are materials that can be designed to behave differently in response to changes in their environment, selectively interact with contaminants, or can be controlled or monitored to perform functions. For pollution remediation, examples are functionalized adsorbents, photo catalysts, magnetic composites, responsive membranes, and sensor-integrated materials. Smart

needs to be used sparingly. Not all nanomaterials and advanced adsorbents are intrinsically responsive or autonomous. AI can be used to aid material development by predicting material properties, finding promising material compositions and optimizing the conditions for their synthesis. Generally, the intelligence is in the computational design or control system, not the material. This distinction is significant for assessing claims about remediation using AI.

5.2 AI-Guided Biochar Development

Biochar is a carbon rich material that is created by thermochemical conversion of biomass in the absence of oxygen. Its properties are a function of feedstock composition, pyrolysis temperature, residence time, activation method and surface modification. Biochar has the ability to bind some contaminants via adsorption, ion exchange, surface complexation, precipitation, and other processes. Machine learning can simulate the relationships between the production conditions, material properties and pollutant removal performance. A machine learning applications review paper on biochar research revealed that prediction of adsorption efficiency and biochar properties related to environmental remediation are possible (Oral et al., 2024). This can decrease the need for trial and error experimentation and assist in prioritizing potential feedstocks. Lab adsorption capacity does not always correlate to natural waters and contaminated soils. Competing ions, dissolved organic matter, variable pH, and complex mixtures of pollutants may affect adsorption (Oral et al., 2024).

5.3 Sustainable Adsorbents and Biomass-Derived Materials

Advantageously, biomass can provide their source of adsorbents which may be agricultural residues, forestry byproducts, or other forms of renewable feedstocks. The environmental benefits they offer are related to their production energy, activation by chemicals, transportability, durability and end-of-life management. Biochar for water pollution mitigation was reviewed, in which biomass materials were modified, and the usage of machine learning for optimizing the properties of the biochar was introduced (Laishram et al., 2025). AI can help in the determination of feedstocks, preparation temperature and surface treatment combinations that are related to better adsorption. However, a material that can adsorb a lot does not necessarily have to be very environmentally friendly if it uses a lot of energy and/or toxic chemicals in its production. When choosing materials, it is important to take into account the environmental performance and production impacts of materials.

5.4 Machine Learning for Organic Pollutant Removal

Dyes, pharmaceuticals, pesticides and endocrine disrupting chemicals are all examples of organic contaminants that pose challenges for treatment. The removal of these depends upon the molecular structure, the nature of the adsorbent, the chemistry of the solutions and conditions of contact. The removal efficiency can be predicted with AI models and influential operating parameters can be determined. A biochar review on the application of organic wastewater treatment revealed that machine learning could be used for material design, process optimization and pollutant removal prediction (Chu et al., 2025). Removal percentage, however, should be considered in conjunction with the initial concentration of the contaminant, adsorbent dosage, contact time, and solution composition. The high removal percentage obtained in laboratory conditions may not be applicable to industrial effluents with complex effluents and contaminants. Furthermore, adsorption may also be a process of transferring pollutants from water to solid phase, and may not necessarily destroy the pollutants. The need for regeneration, safe disposal and the potential for desorption of contaminants can also not be neglected.

5.5 AI-Assisted Soil Remediation Materials

The remediation of contaminated soil is a complex process due to the interaction between soil contaminants and minerals, organic matter, microorganisms, and soil porewater. The treatment methods can include immobilization, extraction, stabilization, or separation of the heavy metals (Wu et al., 2026). AI can predict the effectiveness of remediation amendments and choose optimal amendment materials. Design, conditions and treatment performance prediction of soil remediation by machine learning was reviewed in 2026 (Fu et al., 2026). These can be used to develop biochar amendments, to design using the optimal stabilizing agent, and to predict changes in metal mobility. But the reduction of the bioavailable fraction of a metal does not mean that the metal has been eliminated from the environment. Long-term monitoring is required to identify whether immobilized contaminants stay stable when soil conditions are changing (Wu et al., 2026).

5.6 Photocatalytic Nanomaterials

Photocatalysis is the application of light activated materials to drive chemical reactions that can reduce organics. Titanium dioxide is the most studied photocatalyst, along with other semiconductor composite materials modified. They are dependent

on surface characteristics, light intensity, charge separation, catalyst composition and water chemistry. AI can help to predict degradation rates and suggest compositions of promising catalysts. Recently, the use of machine learning to photocatalytic nanomaterials in the degradation of environmental pollutants was studied (Gonfa & Soromessa, 2026). Computational screening could speed up the discovery of materials by identifying sets of properties that correlate with better performance. Pollutant disappearance does not necessarily mean complete mineralization, however. Photocatalytic treatment may result in the formation of transformation products with toxicity properties that can differ from that of the original contaminant. Remediation studies will therefore need to assess the degradation pathways, mineralization, byproduct toxicity, catalyst stability, and potential for release of nanoparticles.

5.7 Material Regeneration and Environmental Safety

In order to be applied practically, smart materials need to have a useful life and end-of-life management is needed. The adsorbers may be regenerated via heat treatment, solvent, acids or other chemicals. Fouling in membranes can be caused and photocatalysts can lose activity or components in repeated operation. AI might be able to forecast material deterioration and optimize maintenance or regeneration schedules. However, it is necessary to test the efficiency of regeneration. A material is not sustainable if it is only derived from biomass or has a high removal efficiency in a laboratory. Raw material sourcing, synthesis, operating energy, recovery of contaminants, secondary waste generation and disposal should be included in comprehensive assessment.

6. INTEGRATION OF AI, SMART MATERIALS, AND SUSTAINABLE TECHNOLOGIES

6.1 From Environmental Detection to Remediation

The final transected area is for the remediation of the environment.The last transected area is for remediation of the environment. One of the most significant challenges in environmental engineering is the challenge of integrating the use of monitoring, prediction and treatment in integrated systems. Typical pollution management approaches tend to dissociate environmental monitoring from plan and operational control of remediation. These capabilities could be integrated into a system powered by artificial intelligence, which gathers data on the environment, forecasts contamination threats, suggests remediation steps, and assesses treatment results. For instance, in a water treatment plant, a continuous measurement of the water quality parameters can be used to estimate the quality variations of the water that flows into the plant and to forecast the treatment demand and suggest operating adjustments. Likewise, soil contamination maps could be used to prioritize the remediation sites and to select appropriate treatment materials. Reliable communication between the sensors, databases, models, and operational equipment, however, is required for integration of these functions. Failure of one component could impact the entire decision making process. Thus, a quality assurance, fault detection and procedures for human interventions are required for integrated environmental systems.

6.2 Predictive Maintenance and Resource Efficiency

Pumps, membranes, reactors, aeration systems, and sensors are all parts of environmental treatment systems that need to be regularly maintained. Predictive maintenance is a form of maintenance that tries to predict expected patterns of equipment deterioration before a major failure event happens, which is achieved through the use of AI. These benefits may include decreased downtime, optimized maintenance scheduling, and consistent treatment reliability. Likewise, information-driven optimization can be used to minimize over-dosing chemicals or even wasting energy. But, these advantages rely on the availability of enough representative operational data. Unexpected equipment failures, influential changes, or lack of maintenance records can reduce predictive reliability. To evaluate the usefulness of predictive maintenance, it is not only necessary to have a model that is accurate but also to reduce equipment failure, operational costs and environment noncompliance.

6.3 Sustainable Technology Assessment

The sustainability of AI technologies needs to be considered across the entire lifecycle. Factors that are important include: energy, raw materials, emissions from the manufacturing process, chemical resources, transportation, durability of equipment, waste disposal. Life-Cycle Assessment (LCA) is a method of quantification of the environmental impacts of a system. Along with LCA, a techno-economic assessment of the capital expense, operating costs, maintenance requirements and economic viability can be performed. They are particularly relevant when assessing the impact of AI-driven technologies against the traditional approach. The deeper the contaminant removal in an advanced treatment process, the more energy it consumes,

expensive materials it utilizes or waste management problems it may cause. But in some circumstances, simpler technology will be more overall environmentally harmful. Thus, the demonstration of sustainability should be achieved by evidence, comparative, not postulating from the newness of technology.

6.4 Circular Economy and Resource Recovery

Value-of-material/resource value and waste minimisation are key to circular-economy solutions. The use of AI to enhance process control, resource recovery, and material usage can contribute to these goals. These can be employed to recover nutrients from wastewater; the wastewater can be reused; they can help lower the usage of treatment chemicals; and they can help identify opportunities for reusing industrial waste. Resource Recovery does require more quality and safety requirements, however. Recycled materials may end up being contaminated and recycling operations will not generate new environmental exposure pathways. Besides recovery efficiency, there needs to be a selection of AI decision systems that also consider product quality and the potential for contaminants and regulatory conditions.

6.5 Responsible Implementation

A multidisciplinary approach involving environmental scientists, environmental engineers, data scientists, regulators and affected communities is required for implementation. Use AI tools for solving problems in the environment, rather than for data or computing power. The factors that determine feasibility are paramount and include cost, maintenance, technical training, cybersecurity and monitoring infrastructure. The impacts of environmental management decisions can be high level and/or significant to the community and ecosystem. As such, AI should not replace the decision-making skills and the regulatory oversight of decision-makers, nor should it be used to make opaque or opaque decisions.

7. CRITICAL EVALUATION OF CURRENT EVIDENCE

7.1 Predictive Accuracy Versus Environmental Effectiveness

One of the recurrent challenges with the field of environmental AI is the focus on the statistical performance without showing the associated environmental benefits. A model might be able to predict concentrations well for instance and provide little information on what impact it has on the remediation decision. Similarly, if a reliable algorithm of the adsorption capacity is used, the capacity might be overrated and the material that can be used in the field may not be captured. So prediction and intervention are key concepts in distinguishing themselves. The criteria to judge predictive models are: If it helps in environmental decision making, if it helps to reduce contamination, if it helps to comply with regulation or if it helps in resource consumption.

7.2 Laboratory Performance Versus Field Validation

The majority of AI-supported remediation research is conducted in laboratory settings with controlled data sets. These data sets might present a limited range of temperature, pH, contaminant concentration and material composition. Real environmental systems show more variability and may have more than one interacting pollutant. Materials designed to be effective for the removal of a specific dye from synthetic water can have different performances when used in industrial effluent which contains salts, organic matter and other competing contaminants. Similarly, a predictive model developed from one treatment facility may not be readily applicable to another facility. Claims of practical effectiveness can only be substantiated after independent field validation.

7.3 Model Transferability and Data Quality

Model transferability is the ability of an algorithm to retain useful performance on new locations, operating conditions and datasets. Often, environmental systems have distribution shifts as a result of seasonal effects, industrial operations, climatic fluctuations, or variations in treatment processes. It is possible for models to be less effective in the future as a result of being trained with a historical data set. There's another issue with data quality. Environmental data can be incomplete and/or lack consistently sized data points, lack geographical uniformity and have data measurement quality issues. Data which are not of high quality can lead to potentially strong statistical relationships that are not transferable. In their critical review on machine learning for adsorption of emerging contaminants, researchers identified a few key challenges that hinder the ability of a machine learning model to reliably predict adsorption: data scarcity, bias, inadequate feature representation, and limited external validation. The restrictions are more widespread in the context of environmental AI (Fan et al., 2026).

7.4 Explainability and Regulatory Confidence

Environmental regulators need reliable, transparent, and well-documented methods. When there is uncertainty in the underlying assumptions, and they are not revealed, black-box predictions can be difficult to integrate into regulatory decisions. Explainable AI can help to understand the behavior of the model, but it cannot replace direct validation or causal analysis. Documented data provenance, version control, performance monitoring and incorrect prediction investigation procedures should be included in the regulatory applications. In addition, AI-driven estimates should not be used in lieu of standardized analytical techniques if direct measurement is required as part of legal compliance.

7.5 Environmental Equity

While AI-powered monitoring systems can help enhance environmental protection, disparities in technology access can exacerbate existing inequalities. High-quality datasets are more likely to be generated in regions with dense sensor networks and laboratory facilities and computational capacity. Communities lacking monitoring infrastructure may be under-represented in model development. This means that the algorithms that are trained mostly from well-monitored areas could yield less accurate forecasts in disadvantaged areas. Self-sampling, training techniques, available tools, and information-sharing procedures must all be developed and shared to enable equitable deployment. The goal should be enhancing environmental protection in various communities, not focusing technological gains in already well-supplied areas.

8. LIMITATIONS OF EXISTING EVIDENCE

Although much work has been done in this area of artificial intelligence based environmental monitoring and remediation (EMR), there are still some weaknesses that limit the reliability and usefulness of the current studies. One of the most noticeable issues is that most of the models are retrospective and most of the investigations are carried out in a laboratory scale. The datasets used in many studies show high accuracy but there is less evidence of good predictive accuracy when operating in variable environments.

The other important limitation is data quality. Environmental data often features missing data, uneven sampling periods, measurement errors, and geographical biases. Such issues may lead to bias and lower generalizability of the model. Spatially and/or temporally correlated observations treated as independent observations can also lead to overestimation of predictive performance in random training–testing divisions.

Interpretability of algorithms is still difficult, especially for complex deep learning architectures. Explainability techniques can be used to determine the influential predictors, but they do not necessarily show causal relationships between environmental variables and pollution outcomes.

Further research on the use of remediation materials that have been designed through the use of AI is also hindered by a lack of data on the regeneration, long-term stability, secondary pollutant production, and field scale effectiveness of remediated materials. Laboratory removal rates do not necessarily reflect the removal that might occur in the field.

Comparative life-cycle assessments and techno-economic evaluations also are often inadequate. Therefore, there is no direct correlation between reported treatment efficiencies and reduced environmental impacts.

The narrative design of this review is limited and the 25 selected PubMed-indexed publications were also limited. Does not offer a comprehensive systematic search, formal risk of bias assessment or quantitative meta-analysis. In addition, not all relevant literature in environmental engineering and computer science is cited in PubMed.

These constraints highlight the need for independent validation, consistent reporting, multi-disciplinary evaluation, and more evidence on the link between computational performance and measurable environmental benefits.

9. FUTURE PERSPECTIVES

Future research should progress from proof-of-concept algorithms to more reliable, explainable, and environmentally friendly AI systems that can help in the real world in managing pollution. An important goal is to build up and make available a set of standardized, publicly available environmental datasets that include a variety of geographical regions, pollutant classes and monitoring conditions.

Physics-informed machine learning and mechanistic–data-driven models can offer opportunities to improve scientific consistency and transferability. They could potentially be integrated with uncertainty quantification to help make more reliable environmental predictions and make regulatory decisions.

The second approach is to deploy an intelligent sensor network, digital twins and automated treatment systems. Integration can allow for seamless monitoring, timely alerts in case of contamination, predictive maintenance, and process optimization. However, autonomous control should be phased in gradually, and be accompanied by safety limits and a human presence.

When utilizing AI, material discovery assessments also need to increasingly take environmental aspects and the efficiency of contaminant removal into account. To identify truly sustainable remediation solutions, predictive models can be applied to assess material synthesis, regeneration, durability, toxicity and life cycle effects of the materials.

Emerging contaminants (pharmaceutical residues, microplastics and mixtures of pollutants in particular) have to be addressed specifically. The use of multimodal sensing, and advanced analysis techniques, can be used to enhance their detection and characterization capabilities and reliability.

The following is recommended for further research: Prospective field trials, independent external validation and techno-economic comparison. There is a need for interdisciplinary synergy, from Environmental engineers, Material scientists, Computer scientists, Community members and policy makers. Monitoring infrastructure and computational resources should continue to be a main concern with regard to equitable access. Finally, the next generation of environmental AI should be judged on its proven ability to decrease pollution, conserve resources, safeguard ecosystems and provide sustainable public health benefits.

10. CONCLUSION

AI is transforming environmental pollution monitoring and remediation, by helping to build sophisticated predictive models, automate data analysis, design smart materials for pollution detection and even optimising treatment strategies. Specially, the use of machine learning and deep-learning techniques has been used to enhance environmental information and decision support for various applications such as air pollution prediction, water quality monitoring, soil contamination assessment or micro-plastic detection.

Also there are opportunities to use AI based remediation technologies. Biochar-based adsorbents, engineered treatment materials, and photocatalytic nanomaterials can be assisted in their development by predictive models. Within the wastewater treatment plant, an intelligent monitoring and process optimization process may be able to optimize the operation of the plant and reduce unnecessary energy consumption, as well as resource recovery (Yiting et al., 2026).

Where there is evidence it has to be critically interpreted. Predictive accuracy is not guaranteed, nor is the accuracy of laboratory work in the field, so remediation can be successful without predictive success. However, there is a big challenge in the shape of model bias, transferability, lack of interpretability and uncertainty quantification. AI-driven environmental technologies must also be considered from a holistic perspective when assessing sustainability. These can impact their environmental value as a result of their energy needs, material production, chemical usage, secondary waste generation and end-of-life management. Thus, AI should be seen as a scientific and engineering tool to complement, not supplant, other measures in fighting environmental pollution. These will be crucial to the future evolution of computational innovation, mechanisms, careful experimental testing, life cycle assessment, and responsible governance. Environmental monitoring, predictive modeling, smart materials and sustainable treatment systems can be used to coordinate efforts that will help to improve pollution prevention and remediation. But real progress should be realised on the basis of measurable decrease in environmental pollution, ecological risk, use of resources and human health impacts.

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AUTHOR CONTRIBUTIONS

Dr. Khushboo Mohammed: Conceptualization, Investigation.

Akshaj Jindal: Literature review and analysis

Akashaj Jindal: Manuscript Drafting

Dr. Khushboo Mohammed: Supervision, Writing—Review & Editing.

CONFLICT OF INTEREST

The author declares no conflicts of interest to disclose.

Ethics Statement

This manuscript is a literature-based review of previously published research and does not involve the recruitment of human participants, collection of primary patient data, or experimentation on animals. Therefore, institutional ethics committee approval and informed consent were not required for the preparation of this review.

Data Availability Statement

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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