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Intelligent Environmental Chemistry: AI-Assisted Detection and Destruction of Persistent Pollutants

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Abstract

Persistent pollutants present a long-term environmental challenge because they resist natural degradation, migrate across environmental compartments and accumulate in organisms and food webs. Per- and polyfluoroalkyl substances, polychlorinated biphenyls, chlorinated pesticides, pharmaceutical residues and brominated flame retardants may occur at trace concentrations within chemically complex water, soil, sediment and biological samples. Conventional environmental analysis provides highly sensitive and selective measurements, but laboratory workflows can be time-intensive, dependent on predetermined target lists and difficult to adapt to rapidly changing contaminant profiles. Treatment systems face a related limitation: fixed operating conditions may remove contaminants from water without completely destroying them, or may generate transformation products whose toxicity and persistence remain uncertain.

Artificial intelligence offers a complementary capability for environmental chemistry. Machine-learning models can support spectral interpretation, chromatographic peak recognition, non-target screening, source attribution, toxicity prediction and treatment-process optimization. This study develops a conceptual architecture connecting AI-assisted pollutant detection with adaptive destruction technologies. The framework integrates sensor data, high-resolution mass spectrometry, chemical descriptors, environmental metadata, mechanistic reaction knowledge and feedback from advanced oxidation, photocatalytic and electrochemical treatment systems.

An author-generated simulation compares conventional fixed-parameter treatment with an AI-optimized hybrid process across five persistent-pollutant classes. Illustrative destruction or mineralization efficiency increases from 58% to 91% for a PFAS mixture, from 63% to 89% for PCB congeners, from 69% to 94% for chlorinated pesticides, from 72% to 96% for pharmaceutical residues and from 61% to 90% for flame retardants. The simulated average increases from 64.6% to 92.0%. These values are illustrative and do not represent measured treatment-plant performance.The study concludes that intelligent environmental chemistry should connect detection, identification, risk prioritization, treatment selection and post-treatment verification within a closed analytical loop. AI should augment rather than replace validated chemical analysis and mechanistic reasoning. Reliable implementation requires representative training data, uncertainty estimation, explainable model outputs,

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transformation-product monitoring, mass-balance verification, cybersecurity and independent laboratory confirmation.

Keywords: environmental chemistry, artificial intelligence, persistent pollutants, PFAS, non-target screening, mass spectrometry, advanced oxidation, photocatalysis, electrochemical treatment

1. Introduction

Persistent chemical pollution is a global environmental concern because certain substances remain in water, soil, sediment, air and biological tissues for extended periods. Their resistance to physical, chemical and biological transformation allows them to travel far from their original sources. Some compounds accumulate in organisms and become increasingly concentrated through food webs, creating exposure risks even where local production or use is limited.Persistent pollutants include historically regulated persistent organic pollutants as well as emerging contaminant groups that exhibit similar environmental behaviour. Important examples include polychlorinated biphenyls, organochlorine pesticides, brominated flame retardants, per- and polyfluoroalkyl substances, selected pharmaceuticals and resistant industrial chemicals. Their environmental behaviour varies according to molecular structure, polarity, volatility, hydrophobicity and resistance to oxidation or reduction.

The Stockholm Convention established an international framework for restricting or eliminating listed persistent organic pollutants because of their persistence, bioaccumulation, long-range transport and harmful effects. Its continuing scientific evaluation process reflects the fact that persistent-pollutant management is not a completed historical issue. New chemicals and transformation products continue to require assessment. Environmental detection is complicated by low concentrations and chemically complex matrices. A water sample may contain natural organic matter, salts, suspended particles, metabolites and industrial contaminants. Soil and sediment introduce additional extraction challenges. Biological samples may contain lipids, proteins and other compounds capable of interfering with analysis. Analytical methods must therefore distinguish target pollutants from a large chemical background.

Conventional methods such as gas chromatography, liquid chromatography, mass spectrometry and immunoassays remain essential. These techniques can provide high sensitivity and chemical specificity. However, traditional workflows often depend on predefined target lists. A laboratory may report accurately on compounds it was instructed to search for while overlooking structurally related chemicals, transformation products or previously unrecognized contaminants. High-resolution mass spectrometry has expanded the possibility of suspect and non-target screening. Rather than searching only for a limited list of known compounds, analysts can examine accurate mass, isotopic patterns, fragmentation spectra and chromatographic behaviour. Hollender et al. (2017) emphasized that high-resolution mass spectrometry can support broader environmental-contaminant identification, although data interpretation remains demanding.

Artificial intelligence may help manage this analytical complexity. Machine-learning models can classify spectra, detect chromatographic features, distinguish chemical signals from background noise and rank potential molecular structures. Deep-learning systems may learn representations directly from spectra or molecular graphs, while ensemble methods can combine chemical descriptors with

environmental metadata.AI can also contribute to spatial and temporal pollution surveillance. Sensor networks generate repeated observations that can be analysed for anomalies, contamination events and source patterns. Models may combine rainfall, river flow, industrial activity, land use and chemical measurements to identify conditions associated with increased pollutant concentrations.

2. Review of Literature

2.1 Environmental Persistence and Analytical Detection

Persistence is not a single universal property. It may refer to resistance to photolysis, hydrolysis, oxidation, reduction or biodegradation. A chemical may remain stable in groundwater but transform more rapidly in the atmosphere. Environmental persistence must therefore be evaluated in relation to the relevant compartment and transformation pathway.

Hydrophobic persistent pollutants commonly associate with organic matter and sediment. Their apparent disappearance from water may reflect sorption rather than degradation. More polar compounds may remain mobile and move through groundwater or treatment systems. PFAS compounds present a distinctive challenge because carbon–fluorine bonds provide substantial chemical and thermal stability.

Schwarzenbach et al. (2006) observed that aquatic pollution requires attention to contaminant occurrence, environmental behaviour, exposure and treatment. Effective environmental chemistry must connect measurement with an understanding of transport and transformation. A concentration value without information regarding chemical identity, source and fate provides an incomplete basis for intervention.

2.2 Artificial Intelligence in Chemical Identification and Risk Prioritization

Machine learning has become increasingly relevant to chemical science because chemical datasets contain nonlinear relationships between structure, properties and reactivity. Butler et al. (2018) described the potential of machine learning to accelerate molecular and materials research. Environmental chemistry can use similar approaches to predict pollutant properties and prioritize analytical candidates.

Chemical fingerprints and molecular descriptors can represent structural features such as functional groups, polarity, molecular size and bond patterns. Models can then estimate partition coefficients, degradation susceptibility, toxicity or adsorption behaviour. Graph neural networks offer another approach by treating atoms and bonds as a molecular graph.

2.3 Pollutant Removal, Destruction and Adaptive Treatment

Removal and destruction are chemically different outcomes. Activated carbon, ion-exchange resins and membranes can remove a pollutant from water by concentrating it into another phase. These technologies may be effective components of treatment, but the spent material or concentrate still requires management.

PFAS treatment illustrates this distinction. Rahman et al. (2014) reviewed the behaviour of perfluorinated compounds in drinking-water treatment and showed that conventional processes may have limited effectiveness for certain PFAS. Adsorption and membrane processes can reduce water concentrations but produce contaminated residuals.

Ross et al. (2018) discussed remediation and management approaches for PFAS-contaminated sites, emphasizing that treatment selection depends on contaminant composition, media and project objectives. The diversity of PFAS structures makes a single universal treatment unlikely.

3. Objectives

The principal objective of this study is to develop an intelligent environmental-chemistry framework connecting pollutant detection, identification, risk prioritization, treatment optimization and destruction verification. The study treats AI as an analytical and decision-support capability rather than an autonomous replacement for environmental chemists.

A second objective is to distinguish chemical removal from verified destruction. This distinction is essential because adsorption or filtration can reduce water concentration without eliminating the contaminant. The proposed architecture therefore includes post-treatment monitoring of parent pollutants, transformation products and toxicity.

The specific objectives are:

- To examine the analytical difficulties associated with detecting persistent pollutants in complex environmental samples.
- To evaluate the potential role of machine learning in spectral interpretation, chromatographic feature recognition and non-target screening.
- To develop a layered architecture integrating laboratory analysis, field sensors, chemical databases, risk prediction and treatment control.
- To compare conventional fixed-parameter treatment with an AI-optimized hybrid strategy through a clearly labelled simulation.
- To evaluate illustrative destruction efficiency across PFAS, PCB, pesticide, pharmaceutical and flame-retardant pollutant classes.
- To identify the analytical evidence required to distinguish pollutant transfer, transformation and mineralization.
- To examine data-quality, interpretability, cybersecurity, by-product and environmental-justice challenges.

4. Research Methodology

4.1 Research Design and Literature-Review Procedure

The study applies a conceptual-review and simulation-based design. The conceptual component synthesizes research concerning persistent-pollutant chemistry, high-resolution mass spectrometry, suspect screening, machine learning, advanced oxidation, photocatalysis, electrochemical treatment and remediation verification.

Literature searches were structured around combinations of the terms “persistent organic pollutants,” “PFAS detection,” “non-target screening,” “high-resolution mass spectrometry,” “machine learning environmental chemistry,” “AI water-quality monitoring,” “photocatalytic degradation,” “electrochemical oxidation,” “advanced oxidation processes” and “transformation products.”

Scholarly information was examined through major bibliographic databases, publisher platforms, institutional repositories and authoritative environmental-organization resources. The analytical time

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range was restricted to literature within the permitted publication period. The search and synthesis were completed for preparation of this manuscript.

4.2 Proposed Intelligent Environmental-Chemistry Architecture

The proposed platform contains five integrated layers. The sampling layer collects water, soil, sediment, air or biological material according to a documented protocol. Metadata include time, location, weather, hydrological condition, land use and potential pollution sources.The analytical layer uses sensor measurements, chromatography, high-resolution mass spectrometry and supporting chemical tests. Quality-control samples, blanks, standards and replicate measurements are necessary to distinguish environmental signals from analytical contamination or instrumental drift.

The AI interpretation layer performs feature recognition, spectral classification, candidate ranking, concentration prediction and anomaly detection. It also estimates uncertainty and identifies samples that require expert review.The decision layer combines chemical identity, concentration, persistence, mobility, toxicity and exposure information to prioritize contaminants. It recommends a treatment pathway while accounting for matrix composition, energy requirement and expected by-product formation.

Table 1: Proposed intelligent environmental-chemistry architecture

Functional layer	Representative inputs	Principal AI-assisted function	Required human or laboratory control
Environmental sampling	Location, matrix, time and field conditions	Adaptive sampling prioritization	Validated sampling protocol
Chemical measurement	Spectra, chromatograms and sensor signals	Feature detection and signal classification	Blanks, standards and calibration
Chemical identification	Exact mass, fragments and databases	Candidate ranking and confidence estimation	Expert interpretation and confirmation
Treatment control	Pollutant profile, pH, oxidant and energy data	Parameter and treatment-sequence optimization	Safety constraints and operator approval
Post-treatment verification	Residuals, products, toxicity and mass balance	Failure detection and process learning	Confirmatory chemical analysis

The architecture is closed-loop. Post-treatment results become new evidence for process optimization. However, model updates should occur through controlled validation rather than unrestricted self-modification.

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4.3 Simulation Scenario and Performance Measurement

The simulation compares conventional fixed-parameter treatment with an AI-optimized hybrid strategy for five pollutant classes: a PFAS mixture, PCB congeners, chlorinated pesticides, pharmaceutical residues and brominated flame retardants.The conventional condition represents a treatment system operated using predetermined oxidant dose, catalyst loading, residence time and energy input. The AI-optimized condition uses simulated feedback from pollutant measurements and process sensors to adjust treatment sequence and operating conditions.

The hybrid treatment concept includes an initial concentration or separation stage followed by a pollutant-appropriate destructive process. Depending on the simulated chemical profile, the system may emphasize photocatalysis, electrochemical oxidation, advanced oxidation or reductive treatment.

Destruction efficiency is represented by:

$$\eta D = C0C0 - CR - CT \times 100$$

where C0 is the initial parent-pollutant equivalent, CR is the residual parent compound and CT is the equivalent concentration represented by persistent transformation products. This definition prevents parent disappearance from being treated automatically as complete destruction.

5. Analysis

5.1 Simulated Detection and Treatment Outcomes

The conceptual platform improves detection through combined interpretation of spectral, chromatographic and environmental information. A conventional workflow may prioritize a limited target list, while the intelligent workflow ranks target, suspect and non-target features according to analytical confidence and environmental significance. The simulation assumes that low-confidence features are not automatically reported as confirmed pollutants. Instead, they are assigned to a verification queue. This reduces the risk of presenting uncertain molecular candidates as definitive chemical identifications.

Treatment performance is evaluated through destruction or mineralization efficiency rather than simple removal from the aqueous phase. The conventional fixed-parameter condition achieves efficiencies ranging from 58% to 72%. The AI-optimized hybrid condition ranges from 89% to 96%.

Table 2: Simulated treatment performance by pollutant class

Pollutant class	Conventional treatment	AI-optimized hybrid treatment	Percentage-point improvement
PFAS mixture	58%	91%	33
PCB congeners	63%	89%	26
Chlorinated pesticides	69%	94%	25
Pharmaceutical residues	72%	96%	24

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Pollutant class	Conventional treatment	AI-optimized hybrid treatment	Percentage-point improvement
Flame retardants	61%	90%	29
Mean performance	64.6%	92.0%	27.4

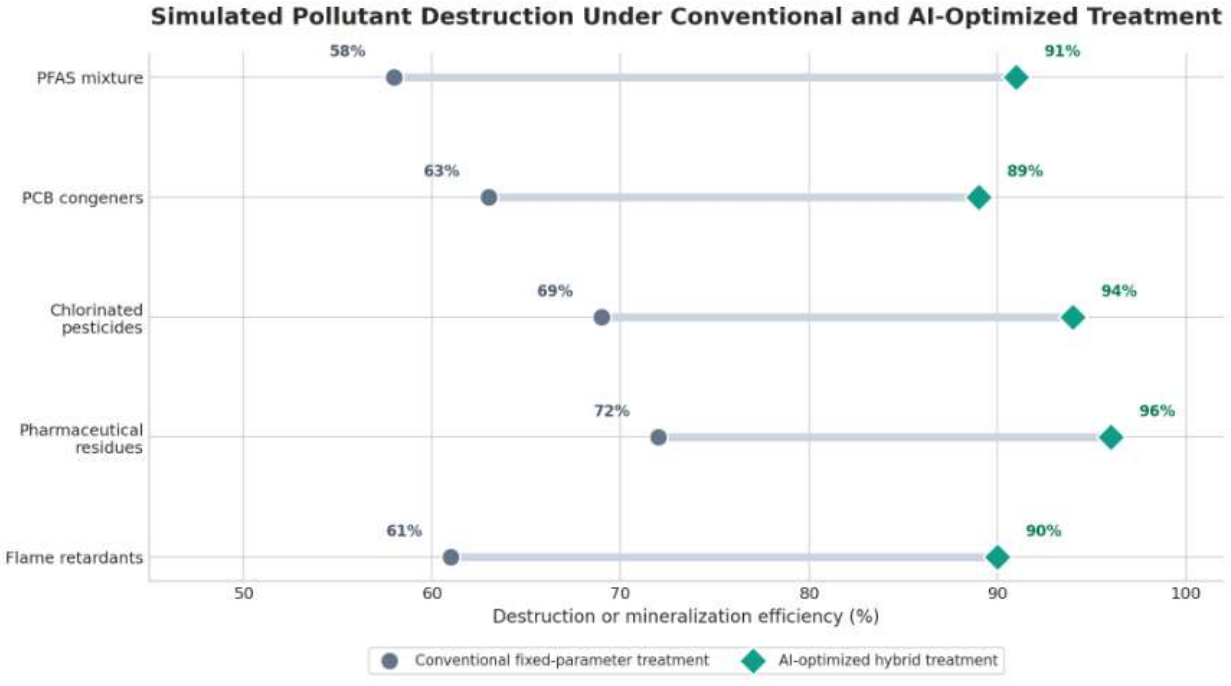
The largest simulated improvement occurs for the PFAS mixture. This result reflects the conceptual advantage of selecting a specialized concentration-and-destruction sequence rather than relying on a fixed process. It does not imply that PFAS destruction is easy or that 91% efficiency can be expected universally.

PCB congeners and flame retardants also show substantial improvements. Their hydrophobicity and matrix association can limit treatment access. The intelligent system therefore considers separation, solvent conditions and catalyst compatibility before destructive treatment.

The highest final performance occurs for pharmaceutical residues. This class includes diverse molecules, and actual behaviour would vary substantially. The simulated value represents a standardized challenge scenario rather than a claim regarding every pharmaceutical compound.

5.2 Graphical Comparison

Graph 1: Simulated Pollutant Destruction Efficiency Under Conventional and AI-Optimized Treatment Approaches



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The dumbbell graph displays the separation between conventional and AI-optimized treatment for each pollutant class. Conventional results remain between 58% and 72%, whereas the intelligent hybrid process produces simulated efficiencies between 89% and 96%.

The average improvement is 27.4 percentage points. The gain does not arise from AI chemically degrading pollutants by itself. It arises from using chemical measurements and predictive models to select more appropriate treatment sequences, parameter combinations and termination criteria.

Interpretation: AI provides its principal value by adapting treatment to pollutant identity and matrix conditions. The model does not replace oxidation, reduction, catalysis or electrochemistry; it determines how these chemical processes should be combined and controlled.

Key finding: The simulation indicates that connecting detection with adaptive treatment may provide greater value than optimizing either stage independently. Accurate identification supports treatment selection, while post-treatment analysis prevents incomplete transformation from being misclassified as successful destruction.

5.3 Chemical and Operational Interpretation

A high numerical destruction value should be interpreted cautiously. If a parent compound falls below detection limits while persistent transformation products remain, the treatment has not achieved complete environmental resolution. The simulation therefore deducts persistent transformation-product equivalents from apparent destruction.

Energy efficiency is another important consideration. Higher oxidant dose or electrical current may improve destruction but increase operating cost and environmental burden. The intelligent process uses a multi-objective function rather than maximizing destruction regardless of energy.

Matrix conditions may change the optimal treatment. Natural organic matter competes for reactive species, while chloride may produce chlorinated by-products under certain oxidation conditions. Carbonate and bicarbonate can scavenge radicals. AI models must incorporate these chemical relationships or operate alongside mechanistic constraints.

Treatment termination is also an optimization problem. Stopping too early leaves residual contaminants. Continuing treatment unnecessarily consumes energy and may increase by-product formation. Real-time analytical feedback can identify when further treatment produces minimal additional benefit.

An intelligent system can learn from repeated treatment cycles, but learning must remain scientifically controlled. If an unexpected transformation product appears, the system should trigger investigation rather than automatically incorporating the result as acceptable performance.

6. Challenges

6.1 Scarcity of Representative Training Data

Environmental datasets are often small, heterogeneous and geographically uneven. Many pollutant classes lack large collections of validated spectra across diverse matrices. Models trained on purified laboratory solutions may not perform reliably in wastewater, groundwater, sediment extracts or biological samples.

Data sharing is limited by inconsistent formats, proprietary databases and uncertainty regarding chemical identity. Standardized metadata and confidence reporting are necessary before datasets from different laboratories can be combined.

6.2 Chemical Identification Uncertainty

Accurate mass does not uniquely determine molecular structure. Several compounds may share the same molecular formula, and isomers may produce similar fragments. AI can rank candidates but cannot automatically convert incomplete evidence into confirmed identification.

Reports should distinguish confirmed structures, probable structures, tentative candidates and unknown features. Regulatory action should generally rely on confirmatory evidence appropriate to the decision's consequences.

6.3 False Positives and False Negatives

A false positive may direct resources toward a pollutant that is not present. A false negative may leave a hazardous chemical undetected. The relative cost of each error varies with context. Drinking-water safety monitoring may place greater emphasis on minimizing false negatives, whereas broad exploratory screening may tolerate more tentative candidates.

Model thresholds should be selected according to analytical purpose. Independent laboratory confirmation remains necessary for high-impact findings.

7. Discussion

7.1 Connecting Chemical Measurement With Environmental Action

The central contribution of intelligent environmental chemistry lies in connecting analytical evidence with remediation decisions. Conventional monitoring and treatment are often separated institutionally. Laboratories report concentrations, while treatment engineers operate systems under predefined conditions. Information may not circulate rapidly between these functions.

The proposed framework creates a closed loop. Detection identifies the pollutant profile and uncertainty. Risk prioritization determines which compounds require immediate attention. Treatment selection considers molecular structure and matrix conditions. Post-treatment analysis verifies whether the intervention achieved genuine destruction.

This architecture changes the role of measurement. Analytical chemistry becomes an active control input rather than a retrospective reporting function. At the same time, treatment performance becomes a new source of chemical evidence. Unexpected resistance or transformation can reveal limitations in the initial identification or reaction model.

The simulated improvement across all pollutant classes illustrates the value of this integration. However, it should not be interpreted as evidence that AI universally increases treatment efficiency by the reported amount. Actual improvement depends on the quality of measurements, available treatment technologies and the chemical domain represented in model training.

7.2 Human–AI Collaboration and Analytical Accountability

AI can process more spectral features than a human analyst can examine manually. It can detect multivariate patterns and rank thousands of molecular candidates. These advantages are particularly useful in non-target screening. Nevertheless, chemical identification remains an evidentiary process requiring expert judgement.

Environmental chemists evaluate sample history, laboratory blanks, isotopic patterns, fragmentation behaviour and plausible sources. They also recognize when a result conflicts with environmental context. AI should organize and prioritize this evidence rather than conceal it behind a single confidence score.

Human oversight is equally important in treatment control. An AI system may recommend increasing oxidant dose, irradiation or current density. Operators must confirm that the recommendation remains within equipment, worker-safety and by-product constraints. Automated adjustments should occur only inside validated operating envelopes.

Accountability requires complete records. The system should preserve the raw measurement, preprocessing method, model version, candidate ranking, treatment recommendation, operator decision and verification result. This record enables independent review and correction.

7.3 From Pollutant Removal to Verified Destruction

Environmental treatment reports frequently use “removal” and “degradation” as though they were interchangeable. Adsorption can remove a pollutant from water but transfer it to a solid phase. Transformation can eliminate the parent compound while leaving persistent intermediates. Mineralization implies a more complete conversion to inorganic products.

Intelligent treatment should explicitly classify its claimed endpoint. If a process only concentrates the pollutant, the system must track the residual stream. If partial degradation occurs, transformation products require assessment. A claim of destruction should be supported by chemical evidence appropriate to the pollutant.

The simulation uses destruction or mineralization efficiency rather than water-phase disappearance. This improves conceptual validity but does not eliminate the need for experimental mass balance. Real treatment evaluation would require parent-compound quantification, product analysis, appropriate inorganic-ion measurement and toxicity assessment.

Hybrid treatment may be particularly useful for persistent pollutants. A separation process can first reduce the volume requiring destructive treatment. The concentrated residual can then undergo energy-intensive oxidation, reduction, electrochemistry or thermal treatment. AI can help determine when this sequence is more efficient than direct treatment.

8. Conclusion

Persistent pollutants are difficult to manage because they resist natural degradation, occur in complex environmental matrices and may generate hazardous transformation products. Conventional analytical chemistry remains essential for their measurement, but target-based workflows can overlook unexpected contaminants. Fixed treatment conditions may also perform inconsistently when pollutant composition and water chemistry change.This study developed an intelligent environmental-chemistry framework

linking sampling, chemical measurement, AI-assisted interpretation, risk prioritization, treatment control and post-treatment verification. The framework preserves the authority of validated analytical methods while using machine learning to manage spectral complexity, prioritize candidate structures and optimize treatment decisions.

The author-generated simulation indicates higher illustrative destruction efficiencies under AI-optimized hybrid treatment than under conventional fixed-parameter operation. The mean increases from 64.6% to 92.0%, with improvements observed across PFAS, PCB, pesticide, pharmaceutical and flame-retardant challenge scenarios. These values are simulated and should not be interpreted as measured performance or expected universal outcomes.The most important implication is that AI does not destroy a pollutant independently. Chemical destruction remains dependent on reaction mechanisms, catalysts, electrodes, energy and operating conditions. AI contributes by interpreting measurements, selecting treatment pathways, controlling parameters and identifying incomplete performance.

Reliable implementation requires representative datasets, transparent confidence levels, transformation-product monitoring, toxicity assessment, mass-balance verification and secure data management. Human analysts and treatment operators should remain responsible for high-impact decisions. When these conditions are satisfied, AI can strengthen environmental chemistry by transforming isolated measurements and treatment operations into a coordinated evidence-based system.

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