

Review

AI/ML-Enabled Advanced Oxidation for Real Wastewater Treatment: Mechanistic Evidence, Multi-Objective Optimization, and Scale-Up Roadmaps

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Abstract

Advanced oxidation processes (AOPs) are widely applied to degrade recalcitrant organic contaminants in municipal effluents, industrial wastewaters, and water-reuse streams. Their deployment, however, remains constrained by matrix scavenging, high energy or reagent demand, catalyst/electrode ageing, and the possible formation of toxic transformation products. Artificial intelligence and machine learning (AI/ML) have been proposed as tools for prediction, optimization, catalyst discovery, mechanism inference, and process control, but high accuracy on curated laboratory datasets is often confused with actionable knowledge for real treatment systems. This narrative review evaluates AI/ML-enabled AOPs through an evidence-to-deployment framework built on three principles: real wastewater is treated as the primary inference domain; mechanistic claims are graded according to convergent evidence; and AI/ML contributions are linked to explicit decisions rather than to model accuracy alone. We argue that progress depends less on black-box complexity than on standardized reporting, benchmark matrices, curated datasets, uncertainty-aware validation, and pilot-scale demonstrations that satisfy contaminant removal, energy efficiency, byproduct safety, and operational constraints simultaneously. A six-gate decision framework and a targeted research agenda are proposed to guide future studies toward deployment-grade evidence.

Keywords: advanced oxidation processes; real wastewater; machine learning; artificial intelligence; reactive oxygen species; multi-objective optimization; byproducts; toxicity; digital twins; resource recovery

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1. Introduction

This article is a narrative review of AI/ML-enabled advanced oxidation processes (AOPs) for real wastewater treatment. Its purpose is not to recatalogue every UV-, ozone-, Fenton-, electrochemical-, persulfate-, photocatalytic-, or hybrid-AOP variant. Instead, it evaluates what evidence is needed before laboratory AOP results and data-driven models can support engineering claims. The review therefore treats AOPs as coupled chemical, analytical, modelling, reactor, monitoring, and regulatory systems rather than as isolated degradation reactions.

AOPs are attractive because short-lived oxidative species can transform contaminants that resist biological treatment, adsorption, coagulation, and membrane separation. The same reactivity creates the central deployment problem. Bicarbonate, carbonate, chloride, bromide, nitrate, dissolved organic matter (DOM), suspended solids, conductivity, light attenuation, and catalyst or electrode ageing can suppress target degradation, redirect reaction pathways, increase energy demand, or generate oxyhalides and halogenated products. These drawbacks are not secondary details; they define whether an AOP is useful in a real treatment train.

The existing review landscape is extensive but uneven with respect to inference. Foundational and process-specific reviews synthesize AOP chemistry, Fenton and photo-Fenton processes, electrochemical oxidation, persulfate activation, photochemical platforms, and hybrid biological-AOP treatment [1–13]. Recent guidance also calls for more systematic AOP research and better comparability [9]. These works are essential, but they do not fully specify when a mechanistic label is sufficiently supported, when an optimized condition becomes operationally meaningful, or when an AI/ML model has generalized beyond a laboratory interpolation domain. AI/ML-oriented reviews and applications [14–20] similarly demonstrate modelling potential but often leave the link among mechanism, real-matrix validation, uncertainty, and pilot operation underdeveloped.

The specific gap addressed here is therefore not the absence of AOP reviews, but the absence of a consolidated evidence hierarchy for AI/ML-assisted AOP deployment. A removal curve is not mechanistic proof. A scavenger test is not species identification. A random train-test split is not evidence of transfer to another wastewater matrix. A single-objective optimum is not process design. These distinctions are especially important because AI/ML can amplify patterns in the literature, including biased sampling, weak mechanistic labels, missing byproduct data, and unrealistically narrow operating windows.

Because the literature is heterogeneous in process type, target contaminant, matrix composition, model architecture, and endpoint definition, a structured narrative review was selected rather than a formal meta-analysis. The reference set was assembled from iterative searches in Web of Science, Scopus, ScienceDirect, ACS Publications, Royal Society of Chemistry, MDPI, IWA Publishing, and Google Scholar. Searches covered foundational AOP literature and recent AI/ML studies through the manuscript-preparation period, using combinations of terms such as ‘advanced oxidation process’, ‘real wastewater’, ‘matrix effect’, ‘machine learning’, ‘artificial intelligence’, ‘Bayesian optimization’, ‘digital twin’, ‘soft sensor’, ‘reactive oxygen species’, ‘toxicity’, ‘byproduct’, ‘EEO’, ‘pilot scale’, and ‘resource recovery’.

Studies were included when they contributed to at least one of five review domains: real-matrix AOP evidence, reactive-species or transformation-product evidence, AI/ML prediction or optimization, catalyst/electrode discovery, or reactor translation and digital operation. Priority was given to reviews, benchmark or guidance papers, real-wastewater case studies, toxicity/byproduct studies, pilot or continuous-reactor evidence, and AI/ML papers with explicit validation or interpretability. Studies were excluded from detailed synthesis when they only reported parent-compound removal in ultrapure water, lacked matrix or operating descriptors needed for inference, or used AI/ML solely as retrospective curve fitting without a decision-relevant output. After removal of duplicate or duplicate-title records, 123 references were retained. The supplementary literature matrix records the selected references, evidence categories, and first citation locations.

This framing allows AI/ML to be evaluated constructively but conservatively. Tree ensembles, neural networks, Gaussian-process surrogates, active learning, Bayesian optimization, multi-objective evolutionary algorithms, soft sensors, and digital twins can represent nonlinear interactions among pollutant descriptors, matrix composition, catalyst or

electrode properties, light or current distribution, oxidant dosing, hydrodynamics, and material ageing [14–31]. Their value, however, depends on whether they change a treatment decision under realistic constraints. Section 2 defines real wastewater as the inference domain and establishes minimum reporting expectations. Section 3 grades mechanistic and risk evidence. Section 4 examines AI/ML tasks as a chain of prediction, optimization, discovery, mechanism inference, and digital operation. Section 5 addresses reactor translation, soft sensing, digital twins, and circular coupling. Section 6 converts these arguments into decision gates and research priorities (Figure 1).

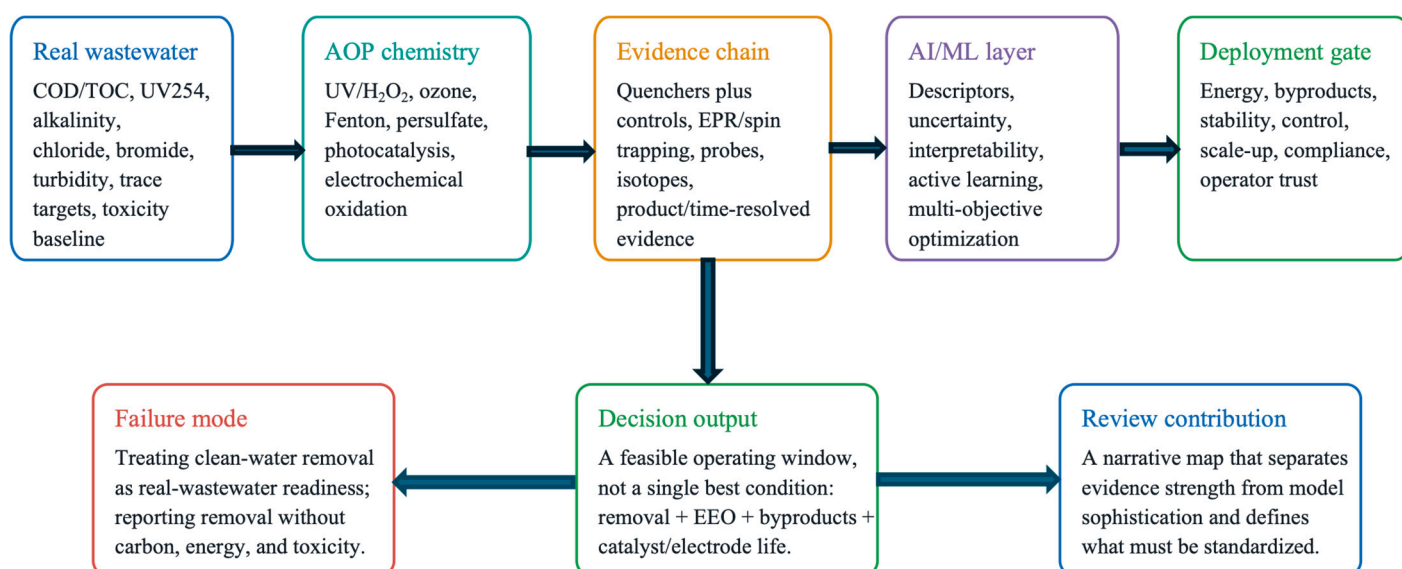


Figure 1. Evidence-to-deployment architecture for AI/ML-enabled advanced oxidation processes. The figure links real-matrix characterization, AOP chemistry, mechanistic and risk evidence, AI/ML validation, and deployment gates into one evidence chain rather than treating them as independent claims.

2. Real Wastewater as the Object of Inference

In this review, real wastewater means a site-derived or pilot/plant-derived aqueous matrix that contains the co-varying organic, inorganic, particulate, and operational features produced by an actual municipal, industrial, reuse, leachate, concentrate, or food-processing source. It differs from synthetic water because the target contaminant is embedded in a variable background of DOM, COD/TOC, UV254, alkalinity, halides, nitrate, sulfate, suspended solids, trace metals, conductivity, pH, and biological or colloidal matter. A synthetic matrix can isolate mechanisms, but it cannot by itself define the target domain for deployment.

This definition sets the boundary for model validity. A model trained primarily on a probe pollutant in deionized water, buffered salts, or a single laboratory recipe may learn controlled-chemistry relationships. It should not be interpreted as a model for municipal effluent, reverse-osmosis concentrate, pharmaceutical wastewater, landfill leachate, textile effluent, or saline industrial discharge unless those matrices are represented or explicitly tested. Real-wastewater evidence therefore includes both the source identity and the matrix descriptors that determine radical exposure, light penetration, mass transfer, electrode potential distribution, catalyst accessibility, and byproduct formation.

Matrix effects should be written as mechanisms, not as background complications. Bicarbonate and carbonate convert hydroxyl radicals into carbonate radicals, altering lifetime and selectivity. Chloride can scavenge hydroxyl or sulfate radicals while producing chlorine-derived radicals and halogenated products. Bromide can introduce bromate or

brominated organics. DOM consumes oxidants, absorbs light, competes for radicals, and generates its own transformation-product pool. Suspended solids scatter light, shield catalyst surfaces, and accelerate fouling. Conductivity alters electrochemical energy demand and current distribution. Reporting the matrix is therefore part of reporting the mechanism [32–36].

Concentration scale is a second boundary condition. Many laboratory studies use target compounds at concentrations convenient for chromatography or UV detection, often far above environmental micropollutant levels. This practice can be useful for product identification and kinetic analysis, but it changes competition with background organic matter and can distort apparent selectivity. A process optimized for milligram-per-litre dye removal may not translate to microgram-per-litre pharmaceutical control in secondary effluent. Conversely, trace micropollutant removal may appear successful while bulk COD remains largely unchanged. AI/ML models must distinguish these regimes rather than pooling them as generic removal efficiency.

A deployment-oriented review must separate water-quality endpoints from engineering endpoints. Water-quality endpoints include parent loss, apparent rate constants, mineralization, COD/TOC reduction, biodegradability, toxicity, and regulated or suspected byproducts. Engineering endpoints include EEO or related energy metrics, oxidant utilization, reagent consumption, catalyst or electrode lifetime, leaching, regeneration, maintenance interval, hydraulic residence time, and treated volume per active area or footprint [37–45]. Parent-compound removal is necessary, but it is not sufficient evidence of risk reduction or deployability.

Weak comparability remains a major limitation. AOP studies use different target concentrations, lamps, electrodes, reactor geometries, catalyst loadings, oxidant doses, analytical endpoints, and definitions of efficiency. Without minimum reporting, even a large AI model learns confounded patterns. It may assign importance to catalyst mass when the hidden driver is light attenuation; infer matrix classes from incomplete descriptors; or learn that a process is efficient because studies used unrealistically low contaminant concentrations. Unreported variables become unmeasured confounders.

Benchmark matrices should therefore contain both chemical and operational descriptors. A minimal benchmark package would specify the water source or surrogate recipe, target contaminant set, radical scavenging capacity or proxies, halide and alkalinity levels, analytical methods, toxicity assays, lamp or electrode geometry, energy accounting, and reporting templates. Such a package would make it possible to compare UV/persulfate, electrochemical, photo-Fenton, and catalytic systems without pretending that all removal percentages are equivalent. It would also support model training by reducing hidden heterogeneity. Recent calls for systematic AOP research and the older EEO literature point in this direction, but the AI/ML era makes standardization more urgent because unstructured heterogeneity becomes model bias [1,9,38,39].

Table 1 is intentionally operational. It does not require every study to measure every possible variable. It identifies the variables without which a deployment-oriented claim becomes underdetermined. Chloride and bromide, for example, are not mandatory because every paper concerns halogen chemistry; they are mandatory because byproduct risk cannot be judged without them. Similarly, catalyst stability and leaching are not optional for heterogeneous AOPs because they determine whether apparent activity survives reuse and whether the process introduces secondary contamination.

Table 1. Minimum reporting scaffold for AI/ML-enabled AOP studies in real wastewater matrices.

Reporting Domain	Minimum Variables or Endpoints	Why It Matters for Inference
Matrix identity	Source, pretreatment history, pH, conductivity, COD/TOC, UV254, alkalinity, chloride, bromide, sulfate/nitrate, turbidity/suspended solids.	Defines the target domain and prevents synthetic-water findings from being overgeneralized [32–36,46–50].
Pollutant and product analytics	Initial and final target concentration, detection limit, transformation-product screen, regulated oxyhalides, AOX where relevant.	Distinguishes disappearance of the parent compound from genuine risk reduction [32,51–61].
Performance and risk endpoints	k _{app} or fluence-normalized kinetics, TOC/COD, biodegradability, acute/chronic toxicity or bioassay panel.	Links oxidation chemistry to water-quality improvement rather than a single removal metric [35,37,38,42–44,62,63].
Engineering accounting	EEO or kWh m ^{−3} per log removal, reagent consumption, hydraulic residence time, catalyst/electrode loading, leaching, regeneration, service time.	Allows comparison of deployable efficiency and prevents unrealistic operating recipes [4,39,41,64–68].
AI/ML provenance	Data source, replicate structure, feature definitions, missing-data handling, train/test split logic, uncertainty calibration.	Prevents leakage, hidden confounding, and overclaiming from random-split accuracy [17–24,26–31,33–36,38,39,46,57,62,69–75].
External validation	Pollutant-family holdout, matrix-class holdout, temporal holdout, or pilot confirmation.	Tests whether the model supports decisions outside the laboratory interpolation domain [22,30,31,47,65,74,76–81].

3. Mechanistic Evidence and Risk Closure

Reactive-species language needs special discipline. Hydroxyl radical is often treated as the default oxidant because it is highly reactive and historically central to AOP definitions. But modern AOPs include sulfate-radical systems, chlorine-radical chemistry in saline matrices, carbonate radicals in alkaline waters, singlet oxygen and surface-bound species in non-radical persulfate activation, superoxide in photocatalysis, and high-valent metal species in Fenton-like or single-atom systems [34,82–86]. These species differ in lifetime, selectivity, diffusion distance, pH dependence, and byproduct profile [7,87,88]. A manuscript that reports only parent removal cannot determine which selectivity regime operated.

The problem is not that scavenger tests are useless. They are useful when framed as stress tests. A robust quenching experiment should include scavenger-only controls, adsorption controls, pH and ionic-strength checks, concentrations high enough to compete kinetically but not so high that they rewrite the matrix, and interpretation based on known rate constants. Even then, the result should be used to generate hypotheses. Recent work on probes and quenchers emphasizes that probes can also be oxidized by multiple species, scavengers can produce artifacts, and apparent inhibition can reflect changes in catalyst surface chemistry rather than direct radical removal [89–92].

Product evidence has two roles. It can support mechanism by showing whether the observed transformation pattern is consistent with electrophilic hydroxylation, electron transfer, chlorine substitution, oxygen addition, ring opening, decarboxylation, defluorination, or other pathways. It can also support risk assessment by identifying intermediates that persist or increase toxicity. These roles are linked but not identical. A product pattern may clarify chemistry while still showing that treatment is incomplete. Conversely, a toxicity reduction may be operationally valuable even when the precise radical pathway remains unresolved. The manuscript should not collapse these two claims.

Quantitative closure is the most underused standard. If a proposed mechanism is correct, it should explain not only that degradation occurred, but why the rate changed with pH, oxidant dose, chloride, bicarbonate, catalyst loading, current density, or light fluence. It should also be compatible with observed oxidant consumption and product

formation. This does not require a complete microkinetic model for every system. It requires enough quantitative reasoning to exclude equally plausible alternatives. Without that step, mechanistic diagrams risk becoming decorative rather than evidentiary.

Risk closure is equally strict. Electrochemical AOPs are particularly powerful but can generate chlorinated products and oxyhalides when halides are present; sulfate-radical and UV/chloride systems can also re-direct radical chemistry; and DOM oxidation can generate complex by-product mixtures that are not captured by parent-compound analysis [32,53–55,57,93]. A review intended for serious publication should avoid the common phrase ‘complete mineralization’ unless TOC data and carbon balance support it [36,52,56,60,94,95]. It should also avoid implying detoxification unless bioassays or toxicological endpoints support it [61].

Mechanistic credibility is the central gatekeeper for AI/ML-enabled AOPs. AI can amplify patterns, but it cannot rescue a dataset built on ambiguous species assignments. The current mechanistic literature makes a clear warning: scavenger experiments, although useful for first-pass diagnosis, are prone to misinterpretation because scavengers are rarely specific, can perturb pH and ionic strength, may react with oxidants or catalysts, and can generate secondary species. Recent reviews and perspective articles have therefore urged the field to move from single-test attribution to convergent evidence involving controls, spin trapping, selective probes, isotope labelling, product distributions, kinetic closure, and theory [7,34,82–91,95–98].

A defensible evidence hierarchy begins with Level 1 evidence: control experiments and inhibition patterns. These tests can rule out trivial explanations and help prioritize hypotheses, but they do not identify dominant reactive species by themselves. Level 2 evidence adds direct or semi-direct detection, such as EPR/spin trapping, time-resolved probes, operando spectroscopy, or targeted transformation-product analysis. Level 3 evidence requires quantitative consistency: radical exposure or flux, isotope or product mass balance, kinetic modelling that reproduces decay and product evolution, and, when appropriate, DFT or microkinetic support. In practice, a mechanism should be described as ‘established’ only when at least one Level 2 line of evidence and one Level 3 closure argument support the same pathway, with products and risk endpoints consistent with that pathway. EPR is valuable but not mandatory in every system; the required direct or semi-direct test should match the species and timescale being claimed. A combination of scavengers and kinetic fitting alone can justify wording such as ‘consistent with involvement of’ but is not sufficient to claim a dominant radical or complete mechanism. Figure 2 formalizes this hierarchy. The conclusion must be scaled to the evidence collected.

Byproducts and toxicity must be embedded in mechanism rather than appended as safety footnotes. Electrochemical oxidation in chloride-containing water can generate active chlorine, chlorinated organics, chlorate, perchlorate, and related species; bromide can introduce bromate and brominated products; UV/persulfate and UV/H₂O₂ can be strongly affected by chloride; dissolved organic matter can yield complex oxygenated byproducts; and pharmaceutical transformation products may differ from parent compounds in persistence and bioactivity [32,53–55,57,99]. These outcomes are not peripheral [52,58–60,93,94]. They determine whether an AOP reduces risk or merely transfers risk from a monitored parent molecule to a less monitored product mixture [36,37,51,56,61,63].

A rigorous narrative review should therefore use mechanistic language sparingly. Statements such as ‘hydroxyl radicals dominated’ or ‘singlet oxygen was the main pathway’ should be reserved for studies where quenching, detection, product analysis, and kinetic reasoning converge. When the evidence is limited, the correct wording is weaker: ‘the results are consistent with involvement of’ or ‘the inhibition pattern suggests but does not prove’. This distinction matters for AI/ML because labels derived from weak mechanistic claims can contaminate training data. A classifier trained to recognize ‘sulfate-

radical-dominated' systems is only as reliable as the evidence that assigned those labels in the first place.

The mechanistic standard also affects reactor design. If chloride-derived radicals contribute substantially, the process may be more selective but also more prone to halogenated byproducts. If carbonate radical is dominant, rates against electron-rich moieties may differ from those expected for hydroxyl radical. If non-radical pathways or surface-bound oxidants dominate, catalyst descriptors and mass-transfer features become more relevant than bulk radical probes. Table 2 translates these points into practical evidence tiers, controls, and failure modes.

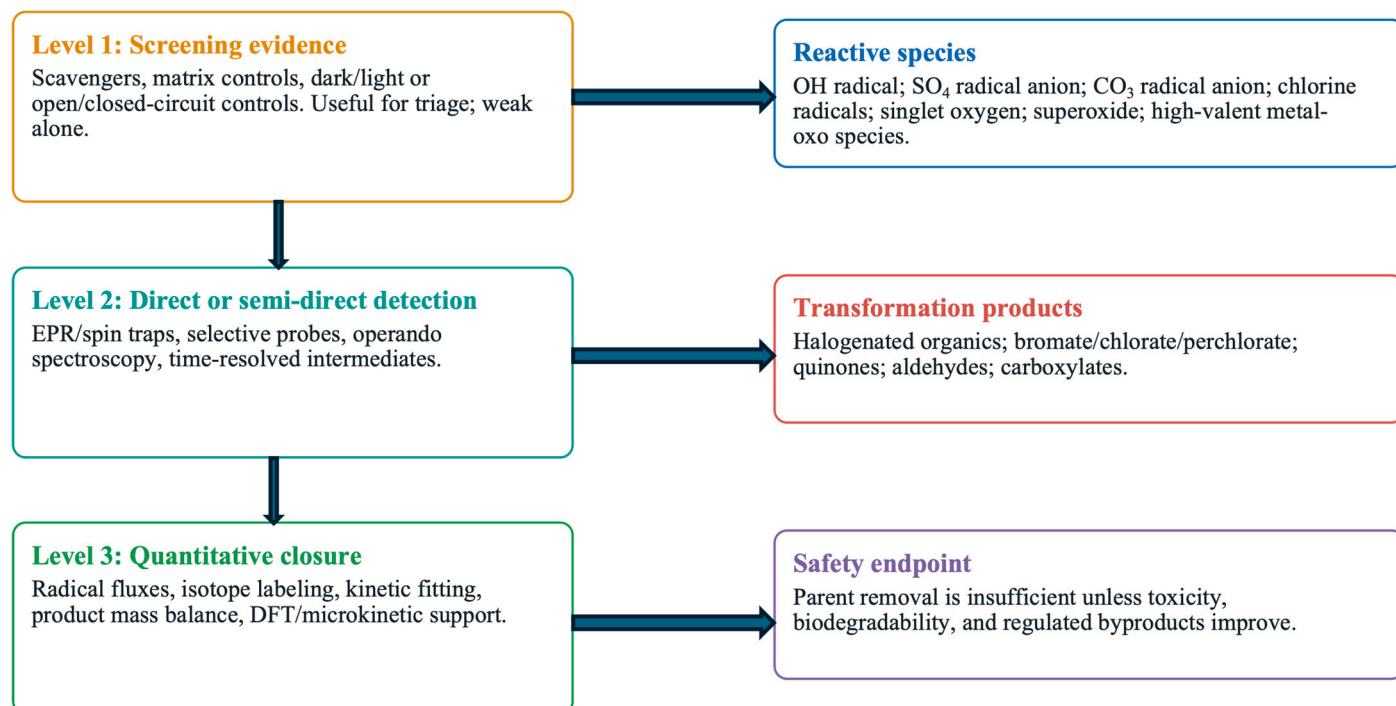


Figure 2. Mechanistic evidence hierarchy and risk-assessment logic. Level 1 evidence supports hypothesis screening; stronger mechanistic claims require direct or semi-direct detection, quantitative closure, and byproduct/toxicity endpoints consistent with the proposed pathway.

Table 2. Mechanistic evidence tiers, common failure modes, and controls for AOP reactive-species claims.

Evidence Tier	Typical Methods	Claim Strength	Main Failure Modes
Level 1: screening	Scavengers, gas purging, dark/light controls, open/closed-circuit controls, pH or ionic-strength checks.	Suggests involvement of candidate species or pathways; does not identify dominance alone.	Scavenger non-specificity, matrix perturbation, secondary radical generation, adsorption artifacts [82,89–92].
Level 2: detection	EPR/spin trapping, selective probes, operando spectroscopy, time-resolved intermediates, LC-MS/HRMS.	Provides direct or semi-direct evidence for reactive species and transformation routes.	Spin-trap artifacts, probe selectivity limits, low temporal resolution, detection under non-representative conditions [41,82,83,90,95–98].
Level 3: quantitative closure	Radical flux/exposure, isotope labeling, product mass balance, microkinetic fitting, DFT-supported pathways.	Supports mechanistic attribution strong enough for model labels and reactor design decisions.	Incomplete mass balance, overfitted kinetics, theoretical pathways not linked to measured products [7,34,85–88,90,91,96].

Byproduct and toxicity closure	AOX, chlorate/perchlorate, bromate, transformation products, bioassays, biodegradability tests.	Shows whether the proposed pathway reduces net risk.	Parent removal masks toxic intermediates or regulated oxyhalide formation [32,37,38,51–55,57,59–61,63].
Model-compatible mechanism labels	Evidence scores attached to each mechanism label; uncertainty retained in datasets.	Allows ML models to learn from graded evidence instead of binary but weak labels.	Training labels inherit literature overstatement and become self-reinforcing [14–17,20,24,26,28,69,92,100].

4. AI/ML Task Chain: Prediction, Optimization, Discovery, Inference, and Control

Performance-prediction models should be evaluated against the decision they are supposed to inform. A model used for preliminary screening may tolerate broader uncertainty if it reliably rejects clearly poor options and prioritizes a small experimental set. A model used for compliance control has a much higher burden: it must be calibrated near thresholds, detect drift, and provide conservative recommendations when uncertainty grows. A model used for catalyst discovery has yet another burden: it must avoid exploiting literature artifacts such as inconsistent catalyst doses, unreported adsorption corrections, or selective publication of successful materials. The validation design should match the decision role.

Feature engineering is not a mundane preprocessing step in AOP modelling. It is where chemical knowledge enters the model. For pollutants, meaningful features may include ionization state at process pH, electron-donating or withdrawing substituents, aromaticity, halogenation, bond energies, and known second-order rate constants where available. For matrices, features should encode scavenging demand and optical/electrochemical context rather than only water-source labels. For catalysts and electrodes, features should include not only composition but oxidation state, surface area, morphology, conductivity, band gap, defect density, active-site environment, and stability indicators. Recent catalyst and materials ML literature makes clear that descriptor quality often limits transferability more than algorithm choice [21,27,28,69,70,86].

Algorithm choice should be pragmatic. Random forests and gradient boosting are strong baselines for heterogeneous tabular datasets because they handle nonlinear interactions and mixed feature scales with relatively limited tuning [23,73]. Gaussian-process models and Bayesian optimization are valuable when experiments are expensive and uncertainty guides acquisition [29,71]. Neural networks and graph models become attractive when structured molecular or spectral data are abundant, but they are data-hungry and vulnerable to uncontrolled extrapolation. Multi-objective evolutionary algorithms are useful for Pareto exploration, yet they can generate unrealistic optima if constraints are weak [72]. In a high-quality AOP paper, a simpler interpretable model that passes external validation should be valued above a complex model that performs well only on random splits.

Uncertainty is not optional. AOP decisions involve asymmetric costs: under-dosing may fail to remove contaminants; over-dosing may waste energy or generate byproducts and wrong catalyst recommendations may consume months of synthesis and characterization. Reporting point estimates alone hides these risks. Model outputs should include confidence or prediction intervals, applicability-domain checks, ensemble disagreement, or conservative decision rules. In operational settings, uncertainty should increase when influent composition moves outside the training domain or when sensors drift. If the uncertainty cannot be quantified, the model should not be used as a control authority.

Multi-objective optimization also requires careful language. A Pareto front is not a proof of optimality in the plant. It is a model-based representation of trade-offs under

specified assumptions. The credible claim is that a set of candidate operating conditions performs well under a validated surrogate and merits confirmation. Strong studies should therefore report the objective functions, constraints, search bounds, acquisition strategy, uncertainty treatment, and experimental confirmation of selected Pareto points. They should also show dominated alternatives so that the reader can understand the magnitude of trade-offs. A single optimized condition without the rejected trade-off space is difficult to evaluate.

For catalyst discovery, active learning should be tied to experimental feasibility. The acquisition function may suggest an exotic composition or synthesis condition, but the laboratory must consider precursor availability, toxicity, cost, phase stability, leaching, and regeneration. If an AI workflow optimizes activity only, it may select materials that fail under real water or are unacceptable for deployment. The more defensible objective combines activity, selectivity, stability, leaching, regeneration, and byproduct suppression. Recent electrochemical and persulfate studies show that active sites, support structure, and matrix ions can jointly determine whether radical or non-radical pathways dominate [7,20,85–88,98].

Mechanism inference from high-dimensional data should be presented as hypothesis prioritization unless independently validated. Clustering HRMS features may reveal product families; autoencoders may compress fluorescence or spectral data; and graph models may predict likely attack sites. These are valuable tools, but they do not replace chemical confirmation. The correct workflow is iterative: the model proposes a pathway, targeted experiments test it, failed predictions update the model, and uncertainty is retained. This is closer to active scientific learning than to one-pass prediction. The value of explainable AI lies in making that iteration inspectable by chemists and engineers.

The field also needs negative data. Published AOP datasets overrepresent successful degradation, attractive catalysts, and optimized operating ranges. Failed materials, high-byproduct conditions, catalyst deactivation, poor real-water performance, and unstable sensors are less often reported, yet they are essential for decision models. Without negative data, an optimizer learns where researchers have looked, not where a process is feasible. Supplementary datasets should therefore include unsuccessful trials, censored measurements, and reasons for exclusion. A high-level review should explicitly reward such reporting because it is foundational for generalizable AI.

AI/ML papers should distinguish interpolation, extrapolation, and transfer. Interpolation asks whether the model predicts similar pollutants or matrices inside the training distribution. Extrapolation asks whether it behaves sensibly outside that space. Transfer asks whether a model trained in one laboratory, reactor, or water class can be adapted to another. Real deployment requires transfer. That requires metadata, calibration samples, drift monitoring, and perhaps hierarchical or site-adaptive models. The soft-sensor and wastewater-control literature provides useful precedents, but AOPs add stricter chemical and safety constraints [22,30,47,74,78,80,81].

AI/ML applications in AOPs can be organized into five linked tasks: performance prediction, multi-objective optimization, material or catalyst/electrode discovery, mechanism inference, and soft sensing or digital operation. Treating these as one generic ‘AI application’ obscures their different data needs and validation standards. Performance prediction asks whether removal, rate constants, mineralization, byproduct indicators, toxicity, or energy can be forecast from pollutant, matrix, process, and material descriptors. Optimization asks which operating conditions define a Pareto-acceptable envelope. Discovery asks which catalysts, electrodes, immobilization strategies, or activation routes deserve experimental testing. Mechanism inference asks whether high-dimensional analytical or sensor data can prioritize reactive pathways. Digital operation asks whether online measurements can support state estimation, drift alarms, maintenance

decisions, or conservative control recommendations. Each task can benefit from modern modelling, but each has different failure modes [14–18,20,21,23–29,31,59,69–73,86].

For performance prediction, the most defensible input space combines chemically meaningful descriptors with process and matrix variables. Molecular descriptors may include functional groups, aromaticity, ionization state, frontier-orbital proxies, bond-dissociation energies, fingerprints, or graph representations. Matrix descriptors should include pH, alkalinity, chloride, bromide, COD/TOC, UV254, conductivity, suspended solids, radical scavenging capacity where available, and source category. Process descriptors should encode oxidant dose, fluence, lamp spectrum, current density, electrode material, catalyst loading, surface area, hydraulic residence time, and reactor mode. Models trained without these variables can still fit published datasets, but their apparent accuracy is likely to reflect interpolation among hidden experimental conventions rather than transferable chemistry.

Validation is the decisive issue. Random splits are weak when the dataset contains related pollutants, repeated catalyst families, or multiple observations from the same reactor. A model may appear accurate because analogues of the test compound remain in the training set or because all high-removal cases come from a single laboratory protocol. Stronger tests include leave-one-pollutant-family-out validation, leave-one-matrix-class-out validation, catalyst-family holdout, temporal holdout for online systems, and pilot confirmation under conditions not used during training. For operational decisions, uncertainty calibration is also necessary: a prediction of 85% removal is not equivalent to an 85% prediction interval. Ensemble methods, Gaussian-process surrogates, conformal prediction, Bayesian models, and calibrated residual models should be judged by whether they produce reliable intervals in the decision region, not merely by global R^2 .

Multi-objective optimization is more relevant to AOP deployment than single-objective maximization. In practice, operators do not maximize parent removal at any cost. They need to satisfy effluent limits while minimizing electricity, oxidant consumption, sludge or concentrate burden, byproduct formation, catalyst replacement, and operational complexity. Bayesian optimization, evolutionary multi-objective algorithms, reinforcement learning, and hybrid mechanistic-ML surrogates can help map Pareto fronts, but they require carefully bounded decision variables and explicit constraints [25,71,72,76,79,101]. An optimizer allowed to explore unrealistic pH, current density, oxidant dose, or residence time will generate recommendations that are numerically attractive and physically irrelevant [6,29,31]. Therefore, optimization should report both the Pareto set and the constraints that excluded unsafe or non-deployable regions.

Catalyst and electrode discovery is another high value but high-risk AI use case. Machine learning can accelerate exploration of metal oxides, perovskites, single-atom catalysts, MOFs, biochar, doped carbons, Ti_4O_7 , boron-doped diamond, mixed-metal oxides, and photo/electro-Fenton materials by connecting composition and characterization data with activity, selectivity, and stability [15,16,21,69,70,102]. However, catalyst discovery datasets are often small, non-standardized, and biased toward successful materials [27,66,84,98,103,104]. Reported activity can reflect different light fields, oxidant doses, catalyst separations, adsorption corrections, and analytical windows [85,86,88,105]. A credible AI discovery study should therefore include negative examples, uncertainty-aware acquisition, standardized benchmark tests, leaching and regeneration data, and validation on real matrix samples. Without those elements, an algorithm may rank materials by publication conditions rather than intrinsic suitability.

Mechanism inference is conceptually attractive because AOP datasets increasingly include EPR spectra, LC-MS/HRMS features, fluorescence excitation-emission matrices, online absorbance, current-potential histories, pH/ORP/DO time series, and toxicity endpoints. AI can cluster transformation pathways, predict suspect byproducts, identify

spectral signatures of DOM change, or link sensor patterns to drift in radical exposure. Yet inference must remain disciplined. A latent variable discovered by a neural network is not automatically a reactive species. It becomes mechanistic evidence only when it aligns with independent chemistry: probe kinetics, product formation, isotope patterns, or catalyst-state changes. This is where explainable AI has a legitimate role. Feature importance and local explanations can flag whether a model relies on chemically plausible variables, but explanation methods are diagnostic tools, not proof [18,20,23,24,26–28,73,92,100].

The most useful future models will likely be hybrid. Purely mechanistic models struggle with complex matrices and unmeasured disturbances; purely data-driven models struggle outside the training domain. Hybrid approaches can use mechanistic constraints for mass balance, radical exposure, non-negativity, monotonic ranges, or reactor transport, while ML corrects local kinetics, fouling, lamp ageing, sensor drift, or site-specific matrix effects. This architecture is more compatible with regulatory and operator trust because it can expose assumptions. It also provides a rational interface between laboratory datasets and digital twins. Table 3 summarizes the AI/ML task chain, the relevant feature sets, and validation gates.

A further point concerns data governance. The field will not obtain robust AI models by scraping heterogeneous papers without context. Curation must record the experimental unit, water source, analytical method, detection limits, blank corrections, adsorption controls, uncertainty, and censoring. Data should distinguish replicate measurements from independent experiments, and it should retain failed or low-performing cases. The strongest model papers will therefore look more like measurement-science papers than leaderboard exercises: they will define the data schema, document exclusions, expose code, quantify uncertainty, and include external validation. This may be less visually dramatic than a deep-learning architecture, but it is more likely to survive rigorous review.

AI/ML should be used to sharpen decision boundaries. The practical output should be an operating envelope: for this water class, target set, and reactor geometry, the process is expected to satisfy removal and toxicity constraints at a given energy range, while by-products remain below specified thresholds and catalyst, or electrode lifetime remains acceptable. For operational models, the envelope should also specify when uncertainty, sensor drift, or influent composition requires fallback operation rather than autonomous control. If the model cannot support that envelope, the appropriate conclusion is not that more layers are needed. It is that the evidence is insufficient for deployment-oriented claims (Figure 3).

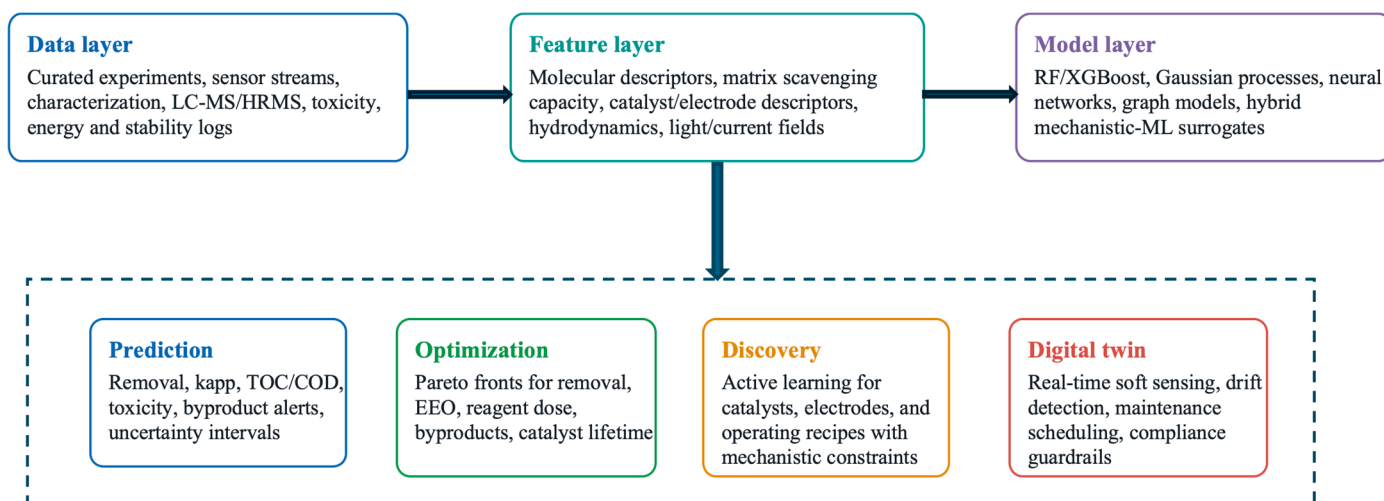


Figure 3. AI/ML task chain for AOP prediction, optimization, discovery, mechanism inference, and digital operation. The intended output is a feasible operating envelope with uncertainty and guard-rails, not a single high-removal condition.

Table 3. AI/ML task chain for AOP studies, with feature classes, decision outputs, and validation gates.

AI/ML Task	Core Features	Decision Output	Validation Gate
Performance prediction	Pollutant descriptors, matrix chemistry, oxidant/light/current inputs, catalyst/electrode descriptors, reactor mode.	Removal, kinetics, TOC/COD, toxicity or by-product alerts with uncertainty.	Pollutant-family and matrix-class holdouts; uncertainty calibration [14–18,20,23–25,59,100].
Multi-objective optimization	Operating variables, constraints, energy, byproduct indicators, stability and maintenance proxies.	Pareto envelope rather than a single optimum.	Physical feasibility screen and pilot confirmation of selected Pareto points [6,25,29,31,71,72,76,79,101].
Catalyst/electrode discovery	Composition, synthesis descriptors, XPS/XRD/SEM/BET/spectra, activity, selectivity, leaching, regeneration.	Ranked candidates and active-learning experiments.	Negative examples, benchmark matrices, external material-family validation [15,16,21,66,69,70,84–86,88,102–105].
Mechanism inference	EPR/probe signals, HRMS features, spectra, product networks, radical-exposure estimates, kinetic profiles.	Hypothesis generation and evidence prioritization.	Agreement with independent product, isotope, probe, or kinetic evidence [34,82,83,87,89–93,95–97].
Soft sensing and digital twins	Online pH, conductivity, UV, ORP, DO, flow, lamp/current/ozone data, lab anchors, maintenance logs.	Real-time state estimation, drift alarms, control recommendations, maintenance scheduling.	Temporal holdout, sensor-drift tests, operator-relevant error bands [22,47,65,67,68,74,77–80,106–109].
Removal-recovery coupling	Metal speciation, nutrient forms, complexing ligands, recovery purity, residual organics, energy and chemical use.	Joint purification and recovery envelope.	Selectivity, product purity, residual toxicity, and lifecycle-relevant accounting [84,110–115].

5. Reactor Translation, Digital Operation, and Circular Coupling

Photoreactor scale-up illustrates why reactor physics must be connected to AI/ML. The same UV dose can have different consequences depending on optical path length, lamp spectrum, absorbance by DOM or nitrate, sleeve fouling, mixing, and residence-time distribution. A model trained on nominal lamp power may fail if it lacks fluence or absorbance descriptors. Likewise, photocatalytic performance depends on whether particles are suspended or immobilized, whether mass transfer or photon delivery limits the rate, and how catalyst surfaces age. These variables are engineering descriptors, not secondary details.

Electrochemical AOPs expose a different set of scale-up constraints. Current density, anode material, cathode reaction, electrolyte conductivity, chloride concentration, mass transfer, electrode gap, gas evolution, and flow-through architecture jointly determine oxidant generation and energy use. At small scale, high removal may be obtained under conditions that are uneconomic or byproduct-prone at larger scale. Pilot continuous-reactor studies and reviews of electrode stability therefore deserve more weight than batch demonstrations when assessing deployability [4,64,65,67,68,97]. Bibliometric or trend

analyses of EAOPs are useful for mapping growth, but they do not substitute for stability and byproduct evidence [56,116].

Hybrid treatment trains may be more realistic than stand-alone AOPs. AOPs can serve as pretreatment to increase biodegradability, as polishing after biological treatment, as a concentrate treatment step after membranes, or as a targeted process for high-risk trace contaminants. Coupling with biological systems can reduce the need for complete mineralization by using oxidation to convert recalcitrant organics into biodegradable intermediates. Coupling with algae-bacteria or other biological resource systems broadens the sustainability conversation but also makes causal attribution more complex [60,75,99,106,108,117]. A review should therefore specify the role of AOP in the train rather than evaluating it in isolation [118,119].

Digital operation should be framed as decision support before autonomous control. Many sensors relevant to wastewater are indirect, noisy, or maintenance-intensive. UV absorbance may correlate with DOM but not with a specific toxicant. ORP may respond to multiple redox couples. Conductivity may indicate salinity but not halide speciation. A digital twin that ignores such limitations will produce false precision. Strong digital-twin studies should report sensor calibration, data reconciliation, missing-data handling, drift alarms, fallback control rules, and the consequences of wrong predictions. These elements are editorially important because water treatment is a safety-critical application, even when the process is used for industrial rather than drinking-water streams.

Circular coupling requires equally careful accounting. Recovering metals or nutrients while degrading organics is attractive, but the coupled system must be evaluated by mass balance and product quality. A metal captured in sludge is not the same as a reusable recovered product. Hydrogen generation is not a benefit if the energy input and separation burden exceed its value. Nutrient recovery must consider competing recovery routes and downstream use. AI/ML can help explore these coupled objective spaces, but only if the objectives are measured rather than asserted [84,110–115].

The scale-up problem is not solved by optimizing chemistry alone. Photochemical AOPs must translate photon absorption, optical path length, turbidity, lamp ageing, sleeve fouling, and hydrodynamic residence-time distribution into radical exposure. Electrochemical AOPs must manage current distribution, mass-transfer limitations, gas evolution, electrode spacing, conductivity, passivation, active-area utilization, and service life. Catalytic and photocatalytic systems must address immobilization, pressure drop, catalyst recovery, leaching, fouling, and regeneration. Continuous reactors must preserve treatment performance under variable loading rather than under a single batch curve [5,44,56,65,67,68,76,77,108,109,120–123].

Soft sensors and digital twins are credible only when framed as decision support before autonomous control. Soft sensors can infer unmeasured water-quality variables from online pH, conductivity, UV absorbance, ORP, dissolved oxygen, flow, temperature, current, lamp power, ozone dose, and historical laboratory measurements [22,47,74,78,80,81]. Digital twins can integrate these estimates with mechanistic or empirical reactor models to simulate dose changes, lamp-cleaning intervals, electrode replacement, bypass strategies, maintenance schedules, byproduct risk, and energy use [30]. Their value is not perfect replication of every reaction. Their value is a controlled decision environment with explicit uncertainty and fallback rules.

The current evidence base for real-time AI/ML control of AOPs remains limited. Pilot and continuous-reactor AOP studies provide important engineering evidence [65,67,68,77,121–123], and soft-sensor studies show that data-driven monitoring can support wastewater operation [22,47,74,78,80,81]. However, fully integrated AI-controlled AOP pilots that simultaneously demonstrate contaminant removal, byproduct safety, calibrated uncertainty, and operator-relevant control are still rare. This review therefore

treats adaptive and controllable AOPs as a research direction, not as an established deployment outcome.

Resource recovery expands the decision space further. Electrochemical oxidation and reduction can be coupled for heavy-metal removal or recovery, hydrogen and energy recovery have been proposed in electrochemical wastewater contexts, and nutrient recovery increasingly frames wastewater as a resource stream rather than a disposal burden [110–115]. AOPs can also improve biodegradability before downstream biological treatment or liberate complexed metals before separation [84]. The risk is conceptual dilution: if the review claims circularity, it must specify what is recovered, at what purity, with what energy and chemical burden, and whether oxidation byproducts or secondary wastes compromise the claimed benefit. AI/ML can optimize such coupled systems only if the objective functions include recovery quality, selectivity, residual toxicity, and life-cycle-relevant costs.

The engineering translation standard should therefore be conservative. AOP readiness is not demonstrated by one optimized batch experiment, one high-accuracy model, or one schematic digital twin. It is demonstrated by a connected evidence package: characterized influent variability, mechanism and byproduct evidence appropriate to the claim, a validated predictive or control-support model with uncertainty, continuous-flow operation, and a decision analysis showing that the process satisfies removal, safety, energy, and lifetime constraints under plausible disturbances. Figure 1 places these elements in a single architecture.

6. Research Agenda and Review-Level Failure Modes

Future AI/ML-enabled AOP studies should be evaluated through decision gates rather than through technology accumulation. Gate 1 asks whether the water matrix and target contaminants are defined. Gate 2 asks whether parent removal corresponds to risk reduction. Gate 3 asks whether the mechanism is supported by evidence strong enough for the claim. Gate 4 asks whether the AI/ML model passes an external validation relevant to its intended use. Gate 5 asks whether the operating envelope survives energy, byproduct, stability, and maintenance constraints. Gate 6 asks whether continuous or pilot-scale evidence exists.

Not every study must pass every gate. Early mechanistic work may legitimately stop at Gate 3. Catalyst-discovery papers may focus on Gate 4 for material selection. Pilot-engineering papers may emphasize Gates 5 and 6. The failure occurs when authors claim a later gate without providing its evidence. This distinction also clarifies where supplementary materials are useful: literature maps, data schemas, benchmark definitions, uncertainty protocols, and validation checklists can carry technical detail without overloading the narrative.

Several common failure modes follow from this framework. First, real wastewater is sometimes used as a token validation sample rather than as the target distribution. Studies should either restrict their claims to the matrix tested or deliberately sample a matrix space wide enough to support generalization. Second, mechanistic claims are sometimes assigned as binary labels even when the evidence is limited to scavenger inhibition. Such labels should be stored with evidence scores and uncertainty rather than treated as ground truth.

Model validation should be matched to the decision. Random splits may test interpolation within a dataset, but they do not establish transfer across pollutant families, catalyst families, reactor geometries, water sources, or time. Stronger validation should use pollutant-family holdouts, matrix-class holdouts, catalyst-family holdouts, temporal holdouts for online systems, and pilot confirmation when the intended output is

operational. The most useful model metric is not global R^2 alone, but reliable uncertainty in the decision region.

Benchmark systems are needed but should be used carefully. A useful benchmark package would include at least one low-DOM municipal effluent surrogate, one high-alkalinity/chloride matrix, one high-COD industrial surrogate, and one real wastewater challenge sample with blinded composition. It should specify target contaminants, analytical methods, toxicity assays, energy accounting, byproduct panels, and reference reactors. Such benchmarks would not replace site-specific trials. They would enable cumulative learning and model comparison across laboratories [1,9,33,36,38,39,61,92].

AI/ML novelty should be defined by improved inference rather than by architecture complexity. A neural network applied to underreported removal data does not by itself justify a strong deployment claim. Novelty is stronger when the study provides richer descriptors, transparent data provenance, stronger evidence labels, external validation, calibrated uncertainty, mechanistic constraints, or decision outputs that conventional experiments alone could not provide.

For primary AOP studies, a minimum deployment-oriented package should include: (i) explicit matrix characterization; (ii) at least one realistic water matrix and one controlled synthetic comparator; (iii) parent removal plus TOC/COD or biodegradability; (iv) byproduct and toxicity screening appropriate to halide and precursor chemistry; (v) energy and reagent accounting; (vi) stability or regeneration data for catalysts/electrodes; (vii) uncertainty for experimental and model outputs; and (viii) validation that tests extrapolation rather than interpolation.

For AI/ML studies, the minimum additional package should include code or model details, data provenance, feature definitions, replicate structure, missing-data handling, train/test split logic, external validation, uncertainty calibration, and a check that recommended conditions are chemically and operationally plausible. Negative examples, censored measurements, and failed operating windows should be retained because they define the boundaries of deployability.

For digital operation, the field should report sensor calibration, drift diagnostics, data reconciliation, temporal holdouts, alarm thresholds, fallback control rules, and operator-relevant error bands. A digital twin or soft sensor should not be assessed only by average prediction error. It should be assessed by whether it prevents unsafe dosing, recognizes out-of-domain influent conditions, and maintains removal, byproduct, and energy constraints under disturbances.

These requirements may narrow the apparent novelty of some studies. That is appropriate. A narrower claim that survives evidence-based scrutiny is stronger than a broad claim supported by removal curves and high R^2 . The route to more credible AI/ML-enabled AOP research is not to expand the catalogue of AOP variants. It is to show, with disciplined evidence, how a specific class of AOPs can be selected, operated, monitored, and constrained under real-matrix conditions.

7. Conclusions

AI/ML-enabled AOPs can become a serious platform for real wastewater treatment only if the field shifts from demonstration to inference. The strongest future studies will not merely report higher removal or more accurate prediction. They will define the water matrix, quantify oxidant and byproduct chemistry, expose multi-objective trade-offs, validate models outside their comfort zone, and show how resulting decisions translate into continuous-flow operation. Under that standard, AI/ML is a useful layer in a broader evidence chain rather than a substitute for mechanistic and engineering proof.

This review argues for a conservative but constructive roadmap. AOP research should standardize matrix and performance reporting, grade mechanistic evidence, treat

toxicity and byproducts as primary endpoints, build interoperable datasets, and use AI/ML to map feasible operating envelopes rather than isolated optima. Digital twins and soft sensors should currently be evaluated as decision-support tools unless real-time pilot evidence demonstrates safe autonomous operation. Removal-recovery coupling should be judged by selectivity, purity, energy, and residual risk. If these standards are met, AI/ML can help AOPs move from empirically tuned laboratory systems toward adaptive, auditable, and deployable treatment units. If they are not met, the literature will continue to accumulate plausible but weakly generalizable case studies.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/catal16070596/s1>, Table S1: Literature matrix; Table S2: Search strategy; Table S3: Selection criteria.

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