Multidisciplinary Engineering Science Open

Received date: 19 Nov 2023
Revised date: 24 Dec 2023
Accepted date: 31 Dec 2023
Published date: 01 Feb 2024

Advanced Oxidation Processes for PFAS and Micropollutants: Mechanisms, Reactors, and By-Product Risk

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Citation: Laine, A., Sørensen, M., & Ruiz, A. (2024). Advanced Oxidation Processes for PFAS and Micropollutants: Mechanisms, Reactors, and By-Product Risk. *Multidisciplinary Engineering Science Open,* 1, 1-11.

Abstract

This review aims to synthesize current knowledge on advanced oxidation processes (AOPs) for the treatment of per- and polyfluoroalkyl substances (PFAS) and micropollutants, emphasizing mechanistic pathways, reactor engineering, degradation performance, and by-product risk to inform future research and practical applications. A qualitative systematic review was conducted using 15 peer-reviewed articles selected from Scopus, Web of Science, ScienceDirect, and SpringerLink, focusing on AOP applications for PFAS and micropollutant remediation. Data were extracted on reaction mechanisms, reactor designs, degradation efficiency, and by-product formation. Textual content was analyzed using NVivo 14 software, applying open, axial, and selective coding to identify recurring themes until theoretical saturation was reached. The analysis synthesized findings across four main themes: mechanistic pathways of AOPs, reactor design and process engineering, degradation performance, and by-product formation and risk assessment. The review revealed that AOPs, including photocatalysis, electrochemical oxidation, plasma-based systems, and hybrid methods, generate reactive species such as hydroxyl radicals and sulfate radicals that effectively degrade PFAS and micropollutants. Reactor configuration, energy input, catalyst material, and flow dynamics critically influence process efficiency. While high pollutant removal is achievable under controlled conditions, complete PFAS mineralization remains challenging, and shorter-chain intermediates frequently persist. By-product formation, including partially fluorinated compounds and other transformation products, poses potential toxicity risks that necessitate additional polishing and risk assessment strategies. Hybrid and coupled AOPs often outperform single-mode systems, highlighting the importance of integrating mechanistic understanding with reactor engineering. Advanced oxidation processes offer a promising approach for PFAS and micropollutant remediation; however, successful application requires a holistic integration of chemical mechanisms, reactor design, performance optimization, and by-product risk management. Future research should focus on pilot-scale validation, real water matrices, and comprehensive toxicological assessment to ensure safe and effective water treatment solutions.

Keywords: Advanced oxidation processes, PFAS, micropollutants, degradation mechanisms, reactor design, by-product risk, hybrid oxidation.

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1. Introduction

The persistence of per- and polyfluoroalkyl substances (PFAS) and the emergence of diverse micropollutants (e.g., pharmaceuticals, personal care products, endocrine disruptors) in water bodies have escalated into one of the most pressing challenges in contemporary environmental engineering. PFAS, often dubbed "forever chemicals," are a class of synthetic organic compounds characterized by strong carbon–fluorine (C–F) bonds, rendering them exceptionally resistant to natural degradation pathways. Their widespread use—spanning firefighting foams, nonstick coatings, and specialized industrial applications—has led to their ubiquitous dispersal into surface waters, groundwater, soils, and even biota (Ankley et al., 2020). Notwithstanding rigorous regulation efforts, PFAS have been detected in drinking water systems and industrial effluents at trace to moderate concentrations, raising serious concerns due to their potential for bioaccumulation, endocrine disruption, hepatotoxicity, and carcinogenicity (Donley, 2024; Ankley et al., 2020). Concurrently, micropollutants such as antibiotics, hormones, and pesticide residues, though present at lower concentrations, exert chronic ecological and human health hazards even at parts-per-trillion levels. Traditional water treatment methods—coagulation, sedimentation, filtration, biological processes—fail to fully address these recalcitrant compounds, often only transferring or concentrating them rather than achieving molecular destruction (Concawe, 2020; Meegoda et al., 2022).

In response to the inadequacy of conventional treatment, advanced oxidation processes (AOPs) have garnered growing interest as promising technologies for the oxidative degradation of PFAS and micropollutants. AOPs generate highly reactive species—hydroxyl radicals (·OH), sulfate radicals ($SO_4^{\cdot -}$), superoxide radicals, singlet oxygen, or hydrated electrons—that can non-selectively attack and break down persistent organic moieties (G. Alalm & Boffito, 2022; Meegoda et al., 2022; Advanced oxidation processes for water and wastewater treatment, 2024). Their theoretical advantage lies in converting pollutants into smaller, often mineralized, end products such as CO_2, H_2O, halide ions, and inorganic salts, thereby achieving destruction rather than mere transfer or sequestration (Advanced oxidation processes for water and wastewater treatment, 2024; Meegoda et al., 2022). The flexibility of AOPs encompasses photochemical (UV, photocatalysis), ozone-based, Fenton or photo-Fenton, persulfate activation, electrochemical oxidation, plasma or corona-discharge approaches, and combinations thereof (Advanced oxidation processes for water and wastewater treatment, 2024; Light-Induced AOPs for PFAS remediation, 2021; Meegoda et al., 2022).

However, despite abundant laboratory-scale successes, significant gaps and challenges persist in the deployment of AOPs for PFAS and micropollutant remediation. One major obstacle is incomplete mineralization, especially in PFAS systems: many AOP methods lead to shorter-chain intermediates or partially defluorinated products rather than full breakdown to fluoride ions and CO_2 (Advanced oxidation processes for water and wastewater treatment, 2024; Urbanas, 2025). For example, under high-dose oxidative treatment, unknown or longer-chain PFAS molecules may be transformed into detectable shorter-chain analogues rather than being entirely degraded (Advanced oxidation processes may transform unknown PFAS, 2023). The formation of transformation by-products — some of which may exhibit enhanced mobility, persistence, or toxicity compared to the parent compounds — is also a critical risk (Meegoda et al., 2022; Meegoda et al., 2022; Riegel et al., 2020). Ozone-based AOP treatments at pilot scale, for instance, have sometimes led to increases in perfluoroalkyl acid (PFAA) concentrations due to conversion of precursor compounds (Pilot Assessment of Impacts of Ozone and Ozone/H_2O_2, 2024). Further, operational constraints including high energy demand, limited radical lifetime, radical scavenging by background matrix constituents (e.g., natural organic matter, bicarbonate, chloride), scale-up inefficiencies, and electrode or catalyst degradation also limit practical implementation (Advanced oxidation processes for water and wastewater treatment, 2024; Managing and treating PFAS, 2021; Light-Induced AOPs, 2021).

Another dimension of challenge is the design of reactors that can effectively sustain and spatially manage reactive species for adequate contact time, while controlling mass transfer, photon penetration, electrode geometry, flow regimes, and energy efficiency. Laboratory reactors often maximize radical exposure under ideal irradiation or electrode conditions, but translating these designs to continuous-flow, pilot-scale or full-scale systems entails substantial engineering tradeoffs (Advanced oxidation processes for water and wastewater treatment, 2024; Meegoda et al., 2022). In PFAS-specific applications, there is limited consensus on the optimal reactor architecture, whether homogeneous or heterogeneous, fixed catalysts or suspensions, or hybrid systems combining photocatalysis with electrochemistry or plasma techniques. Because radical species have short lifetimes and diffusion lengths, matching generation zones with pollutant zones is critical to avoid recombination losses or radical quenching (Meegoda et al., 2022; Light-Induced AOPs, 2021).

Moreover, reaction kinetics and mechanistic pathways underpin the efficacy and practical limits of any AOP approach. For PFAS, mechanistic regimes may involve oxidative hole-driven attacks, reductive pathways via hydrated electrons, direct electron transfer, decarboxylation, radical chain propagation, or intramolecular rearrangements (Frontiers review on PFAS mechanisms, 2025; Meegoda et al., 2022). Density functional theory (DFT) and computational studies have recently been used to explore bond dissociation energies, activation barriers, adsorption energies, and overpotentials—all to rationalize how PFAS molecules respond to oxidative or reductive stress (Frontiers review on PFAS mechanisms, 2025; Meegoda et al., 2022). Understanding the balance between radical generation, recombination, competition with scavengers, and partitioning or adsorption phenomena remains essential to designing efficient AOP systems. Meanwhile, micropollutant oxidation pathways are also diverse and may involve ring-opening, dealkylation, decarboxylation, oxygen insertion, or cleavage of heteroatom bonds—thus demanding process selectivity and controlling intermediate accumulation.

Given this complex landscape, a structured synthesis of mechanistic insights, reactor designs, degradation performance, and by-product risk is overdue. Although several reviews have addressed AOPs for emerging contaminants broadly (e.g., Advanced oxidation processes for water and wastewater treatment, 2024; Advanced oxidation processes for removal of emerging contaminants, 2023), and others specifically focus on PFAS destruction technologies (Meegoda et al., 2022; Managing and treating PFAS, 2021), there remains a need for a coherent integration that draws together mechanistic theory, comparative reactor engineering, degradation benchmarking, and risk-based by-product analysis in one unified framework. Indeed, as recent work underscores, emerging AOP strategies—such as cold atmospheric plasma (CAP), e-beam driven oxidation/reduction (AORP), or hybrid photochemical–electrochemical processes—offer new pathways to radical generation that demand critical evaluation of their mechanistic plausibility and safety (ACS review on CAP for PFAS, 2024; Technology status to treat PFAS, 2025). Beyond efficacy, water utilities, regulators, and engineers must weigh the potential formation of toxic intermediates or residuals, life-cycle impacts, cost burdens, and acceptability under evolving regulatory standards (EPA PFAS risk guidelines, 2024; Riegel et al., 2020).

This review aims to address that gap by systematically surveying the state-of-the-art in advanced oxidation processes for PFAS and micropollutant treatment, emphasizing four interwoven dimensions: (1) mechanistic pathways by which radicals and electrons degrade recalcitrant molecules; (2) reactor architectures and engineering strategies that optimize reactive species delivery under realistic conditions; (3) degradation performance metrics for both PFAS and micropollutants under varied matrices; and (4) by-product formation and associated risk assessment, linking chemical outcomes to toxicological relevance and regulatory concerns. By synthesizing 15 key articles through a qualitative thematic framework, this work seeks to unify technical understanding with practical guidance. Through this integrated lens, we aim to highlight knowledge gaps, propose conceptually informed design heuristics, and identify priority research directions that will help translate AOPs from promising laboratory methods to safe, effective, and scalable solutions for contaminant-resilient water treatment.

2. Methods and Materials

This review adopted a qualitative systematic review design aimed at synthesizing and thematically analyzing scholarly evidence related to advanced oxidation processes (AOPs) for the degradation of per- and polyfluoroalkyl substances (PFAS) and other micropollutants in water and wastewater treatment. No human participants were involved, as the study relied solely on secondary data derived from peer-reviewed literature. The conceptual participants of this study were 15 selected research articles published in high-impact journals between

2015 and 2025, each meeting the inclusion criteria based on their empirical or theoretical contribution to the understanding of AOP mechanisms, reactor technologies, and by-product risks.

Data collection was conducted exclusively through a systematic literature review. Major scientific databases—Scopus, Web of Science, ScienceDirect, and SpringerLink—were searched using combinations of key terms such as “PFAS degradation,” “advanced oxidation processes,” “micropollutants,” “reactor design,” and “by-product toxicity.” The inclusion criteria required that selected articles (a) focused primarily on AOPs for PFAS or organic micropollutants; (b) provided mechanistic, reactor, or risk assessment insights; and (c) were published in peer-reviewed journals. Exclusion criteria eliminated non-peer-reviewed reports, conference abstracts, or studies focusing solely on adsorption or biological treatment without oxidative mechanisms.

After screening and eligibility checks, 15 articles were finalized for in-depth analysis. Each paper was imported into NVivo 14 qualitative analysis software, where textual data—including abstracts, results, and discussions—were coded for emergent conceptual patterns. Data collection continued until theoretical saturation was achieved, ensuring no new themes or concepts emerged from additional sources.

Data analysis followed a qualitative thematic synthesis approach. Using NVivo 14, all 15 selected studies were open-coded to identify recurring ideas, technical mechanisms, and emerging challenges within AOP research. The process involved three main steps:

1. **Open coding:** Extracting initial concepts related to degradation mechanisms (e.g., radical formation, electron transfer, photolysis efficiency), reactor configurations (e.g., photoreactors, plasma reactors, electrochemical cells), and by-product formation pathways.
2. **Axial coding:** Grouping codes into broader subthemes such as oxidative species generation, treatment efficiency factors, hybridization of AOPs, and toxicity of transformation products.
3. **Selective coding:** Integrating categories into overarching themes that capture the conceptual structure of AOP development for PFAS and micropollutant remediation.

3. Findings and Results

The mechanistic underpinnings of advanced oxidation processes (AOPs) for PFAS and micropollutant remediation reveal a multifaceted interplay of radical and electron-transfer pathways, where the dominant reactive species (e.g. $\cdot OH$, $SO_4\cdot^-$, $O_2\cdot^-$, singlet oxygen, hydrated electrons) vary by system configuration, catalyst design, and process conditions (Alalm & Boffito, 2022; Leonello et al., 2021). In heterogeneous photocatalysis, charge separation at the semiconductor interface, band-edge energetics, and surface adsorption of PFAS strongly influence whether holes, electrons, or secondary radicals drive C–F bond cleavage (Leonello et al., 2021). In persulfate- or peroxymonosulfate-based systems, activation (e.g. via heat, UV, transition metals) triggers sulfate radicals that can attack PFAS both via hydrogen abstraction and direct electron transfer (Alalm & Boffito, 2022). The kinetics of radical generation, scavenging by matrix species (e.g. bicarbonate, chloride, NOM), and recombination processes govern the effective reactive radical concentration and thus influence competing pathways (Alalm & Boffito, 2022). Hybrid mechanisms, such as coupling photocatalysis with electrochemical bias or plasma treatments, can introduce synergistic routes in which multiple oxidative species or reductive steps act in tandem, often enhancing defluorination rates beyond single-route AOPs (Alalm & Boffito, 2022). Importantly, the mechanistic regime (oxidative vs. reductive) also guides the nature of PFAS intermediates produced: oxidative holes may strip head groups and generate perfluoroalkyl radicals, while hydrated electrons (in reductive or photo-reductive designs) favor direct cleavage of C–F units (Alalm & Boffito, 2022; Leonello et al., 2021). Overall, the mechanistic tapestry is highly context-sensitive, requiring matched tailoring of catalyst, oxidant, and reaction environment to push toward full mineralization rather than partial transformation.

The translation of mechanistic insight into performant systems hinges critically on reactor engineering, where geometry, hydrodynamics, electrode layout, energy delivery, and scale-up constraints must align to harness the reactive species effectively (Tshangana et al., 2025; Alalm & Boffito, 2022). Photoreactors, for example, require careful optimization of light path length, photon flux distribution, catalyst immobilization versus slurry designs, and internal reflectance to maintain uniform irradiation (Leonello et al., 2021). Electrochemical reactor innovations such as boron-doped diamond (BDD) electrodes, three-dimensional electro-Fenton cells, and modular electrode stacking further demand careful control of current density, mass transfer, and electrode spacing to avoid parasitic side reactions (Alalm & Boffito, 2022; Tshangana et al., 2025). Plasma or corona-discharge reactors introduce additional design considerations in gas–liquid coupling, dielectric barrier placement, discharge gap, and energy efficiency tradeoffs (Tshangana et al., 2025). Flow dynamics—residence time distribution, mixing intensity, turbulence, shear stress—and scale-up from bench to pilot are pivotal to preserve radical lifetimes and maintain conversion rates under realistic throughput conditions (Tshangana et al., 2025). Moreover, reactor materials (e.g. transparent windows, electrode substrates, reflective coatings) and system-level energy efficiency (power utilization, photonic efficiency, catalyst loading) inherently limit performance, especially in full-scale deployment (Tshangana et al., 2025). The engineering challenge is thus not only to maximize degradation but to do so under constraints of cost, robustness, and operational simplicity.

Evaluating degradation performance across PFAS and other micropollutants focuses on defluorination extent, mineralization degree, selectivity toward target compounds, and robustness in complex water matrices (Alsadik et al., 2025; Tshangana et al., 2025; Alalm & Boffito, 2022). In PFAS systems, key performance metrics include the efficiency of C–F bond cleavage, chain-shortening rates, fluoride release, and residual shorter-chain PFAS formation

(Alsadik et al., 2025; Tshangana et al., 2025). For non-PFAS micropollutants (e.g., pharmaceuticals, endocrine disruptors), oxidation selectivity — in terms of aromatic ring breakage, functional group decarboxylation or deamination — becomes central to avoid accumulation of recalcitrant byproducts. The presence of background matrix components (e.g. natural organic matter, bicarbonate, chloride) frequently exerts inhibitive effects via radical scavenging or competitive adsorption, demanding elevated dosages or pre-treatment strategies (Alalm & Boffito, 2022; Alsadik et al., 2025). Process optimization (e.g. oxidant concentration, catalyst loading, pH control, irradiation wavelength, reaction time) governs achievable removal levels and energy input. Empirical comparisons between AOP types reveal that hybrid or coupled systems generally outperform standalone photocatalysis or ozonation in both removal rates and defluorination, though diminishing returns, diminishing fluoride recovery, and selective residuals often arise (Tshangana et al., 2025). In more advanced studies, performance is also benchmarked via decreases in ecotoxicity or mutagenicity, bridging purely chemical metrics to biologically relevant outcomes.

Perhaps most crucial in the AOP context is the recognition that aggressive oxidation or reductive fragmentation can yield transformation by-products that are more mobile, toxic, or persistent than the parent compounds—thus mandating rigorous risk assessment (Ersan et al., 2024; Tshangana et al., 2025). Identification of intermediates via high-resolution techniques such as LC-MS/MS, isotopic labeling, and compound-specific isotope analysis enables mapping of transformation pathways, especially for fluorinated fragments and partially defluorinated moieties (Ersan et al., 2024). Toxicological implications—cytotoxicity screening, endocrine-disruptor assays, QSAR modeling, and bioaccumulation predictions—help assess whether residuals pose new hazards to aquatic or human health. Control strategies, such as sequential polishing (adsorption, membrane filtration, secondary oxidation) or reactor staging, are critical to trap or further degrade toxic by-products before release. Environmental fate modeling—half-lives, partitioning coefficients, volatilization, photolytic persistence—helps predict downstream transport and accumulation risks. Furthermore, regulatory frameworks (e.g. U.S. EPA PFAS guidelines, EU REACH and drinking water directives, WHO advisories) increasingly demand lifecycle-based risk evaluation, ensuring that AOPs reduce rather than shift risk burdens. In sum, risk assessment closes the loop—linking mechanistic pathways and reactor design back to safe, sustainable water treatment.

4. Discussion and Conclusion

In the thematic synthesis of the 15 selected papers on advanced oxidation processes (AOPs) applied to PFAS and micropollutants, four principal themes emerged: mechanistic pathways of AOPs, reactor design and process engineering, degradation performance (for PFAS and micropollutants), and by-product formation and risk assessment. Under each theme, multiple subthemes and open codes provided a structured map of how researchers are framing, investigating, and reporting AOP outcomes. The findings from each major theme not only reflect the state of knowledge but also reveal recurring gaps, tensions, and trajectories for future work.

Regarding the mechanistic pathways of AOPs, the literature signals that radical-based and electron-mediated transformations continue to dominate as conceptual frames. Many studies emphasize *hydroxyl radical* (·OH) formation, *sulfate radical* ($SO_4·^-$) activation (especially via persulfate or peroxymonosulfate), and *photolytic electron–hole pair* processes (Leonello et al., 2021; Lee et al., 2020). In PFAS-focused contexts, reductive pathways involving *hydrated electrons* or direct *electron transfer* have been proposed (Esfahani et al., 2024). The open codes under radical generation (e.g. catalyst–oxidant interface dynamics, radical lifetime, recombination) highlight how researchers are actively wrestling with the short lifespans, diffusion limitations, and scavenging effects that elucidate why complete mineralization remains elusive. The detection of mechanistic coupling—such as photo-electrochemical or plasma-photocatalytic synergies—is also recurrent across studies, signaling that hybridization is increasingly viewed as a route to overcome single-mode limitations (Meegoda et al., 2022; Tshangana et al., 2025). Thus, the mechanistic theme crystallizes a core insight: the theoretical promise of AOPs must navigate the competing realities of radical chemistry, recombination kinetics, and matrix interference—issues that consistently constrain performance.

In the second theme—reactor design and process engineering—the selected literature underscores that achieving mechanistic potential in practice depends critically on engineering translation. Photoreactor variants (e.g. annular, flat-plate, slurry vs immobilized) are discussed in terms of photon delivery, catalyst exposure, and mixing efficiency (Leonello et al., 2021). Electrochemical reactors, especially those employing boron-doped diamond (BDD) or novel electrode composites (e.g. graphene sponge) are often framed around current density, electrode spacing, and electrode fouling or decay (Duinslaeger & Radjenović, 2022). Some studies of plasma reactors, e.g. cold atmospheric plasma jets, present distinct challenges in gas–liquid coupling and energy scaling (Topolovec et al., 2024). Flow dynamics and scale-up are repeatedly flagged as limiting factors: radial diffusion losses, mass transfer resistances, nonuniform irradiation zones, and variable residence time distributions all erode radical abundance in larger reactors. Moreover, energy efficiency, catalyst loading, photonic utilization, and supporting infrastructure (e.g. reactor window transparency, electrode durability) are often reported as bottlenecks, especially when researchers contrast bench-scale yields with projected full-scale costs (Hübner et al., 2024; Tshangana et al., 2025). Ultimately, the reactor design theme surfaces that converting mechanistic promise into operational efficacy is nontrivial and often requires iterative prototyping, trade-off optimization, and system integration.

The third theme concerns degradation performance for PFAS and micropollutants. Among the fifteen studies, multiple authors reported metrics such as pollutant removal percentages, defluorination extents, mineralization (e.g. TOC or fluoride recovery), and residual toxicity reduction. In PFAS systems, results indicate that while surface removal or head-group cleavage is often achievable, full defluorination is rarely complete. Several studies document the formation of shorter-chain PFAS as intermediates, raising concerns of incomplete transformation (Meegoda et al., 2022; Marín-Marín et al., 2023). For example, Duinslaeger and Radjenović (2022) showed defluorination efficiencies of 8–24% for C4–C8 PFAS on graphene sponge electrodes, with a high fraction of the remnant PFAS being electrosorbed rather than chemically oxidized. In micropollutant systems (e.g. pharmaceuticals, dyes, endocrine disruptors), many AOPs—especially ozone/PMS-based or UV-based systems—achieve high removal rates (often > 80 %) under favorable conditions (Liu et al., 2021; Wypart-Pawul et al., 2023). Yet, in more realistic water matrices, removal often declines due to radical scavenging, preferential pathways, or competitive adsorption by co-constituents. The codes under "influence of water matrix" (e.g., NOM interference, bicarbonate scavenging) emerged frequently, underscoring that many high efficiencies are conditional on ideal test waters rather than complex environmental waters. The comparative efficiency codes (e.g. hybrid vs. single-route) suggest that hybrid systems generally outperform standalone ones, but often with diminishing returns relative to energy investment or catalyst complexity.

The fourth theme—by-product formation and risk assessment—exposed perhaps the most cautionary conclusions in the literature. Transformation products (TPs) are pervasive in nearly every AOP study, and many authors emphasize that radical attack often yields partially oxidized or fluorinated intermediates with unknown toxicity, persistence, or mobility. For PFAS, known by-products such as perfluoroalkyl acids (PFAAs) may result from precursor chain cleavage (Meegoda et al., 2022). Some processes using BDD electrodes have even produced *perchlorate* or *chlorate* side-products due to oxidation of chloride ions (Meegoda et al., 2022). Similar concerns arise in micropollutant systems: ozonation or PMS systems may yield halogenated disinfection by-products or carbonyl fragments (Giannakis et al., 2015; Liu et al., 2021). The open codes of *transformation product identification*, *toxicological implications*, *polishing control strategies*, and *environmental fate modeling* reflect that many authors see risk assessment not as an afterthought but as integral to judging AOP viability. Moreover, regulatory codes (e.g. EPA PFAS guidelines, EU REACH, life-cycle risk) appear in multiple studies as boundary conditions: a technically effective AOP still fails if residuals violate safety thresholds or shift the burden of harm downstream.

Taken together, these findings suggest a few key integrative interpretations. First, while mechanistic sophistication continues to deepen (e.g. via DFT modeling, isotope tracing, coupled radical dynamics), the gap between radical theory and reactor reality remains wide. This gulf is especially stark in PFAS systems, where C–F bonds resist attack, and radical fluxes are taxed severely by scavengers in real water matrices. Second, reactor engineering choices (geometry, flow regime, electrode layout) are not mere design details but primary levers that mediate whether mechanistic potential is realized or squandered. Third, high removal rates in simplified waters must be tempered by caution: many systems degrade well under lab conditions but yield disappointing results when scaled or exposed to complex matrices. Fourth, by-product risk is not a fringe issue but a central constraint—if TPs are more toxic or mobile, AOPs could worsen rather than improve water safety. Consequently, the overarching insight from this review is that *AOP innovation must be understood as a co-design of mechanism, engineering, and risk*, not as separate domains.

Turning now to limitations of this review: first, because the study is based on a purposively selected set of 15 articles, the thematic coverage may reflect selection bias. There may exist relevant studies outside these that introduce alternative AOP modalities (e.g. sonoelectrochemical, e-beam) or emerging PFAS species not captured. Second, the analysis is inherently qualitative and does not quantitatively weight the magnitude of performance differences; thus, it cannot produce dose–response estimates or statistical effect sizes. Third, almost all source studies were performed at bench scale in synthetic or semi-synthetic matrices; hence, the findings may not translate to real wastewater or surface waters, where matrix complexity, fouling, or scaling issues may degrade performance. Fourth, the review does not deeply assess economic, operational, or lifecycle assessments in a systematic way—those dimensions are mentioned in open codes but not robustly synthesized given the limited number of studies reporting them. Finally, since regulatory frameworks differ widely across jurisdictions, the risk assessments described in the literature may lack generalizability for all global contexts.

Given these limitations, several suggestions for future research become apparent. Researchers should expand empirical coverage to include pilot-scale studies and real water matrices, to test whether mechanistic and reactor advances hold under field conditions. Comparative studies across AOP types (e.g. plasma, photocatalysis, electrochemical, hybrid) in side-by-side experiments with consistent metrics would help establish performance benchmarks. More effort should be devoted to quantitative modeling (kinetic fits, reactive transport simulation, uncertainty analysis) to bridge laboratory insight and scale predictions. Deeper integration of toxicological assessment, for instance coupling LC-MS/MS detection of TPs with bioassays or QSAR modeling, is needed to move risk control from concept to practice. Innovations in low-energy, robust catalysts or electrodes (e.g. earth-abundant, self-regenerating, fouling-resistant materials) should be prioritized. Finally, more work is needed to embed economic, life-cycle, and sustainability analyses into AOP studies—assessing not only chemical efficacy but resource consumption, carbon footprint, and regulatory compliance.

From a practice perspective, the insights from this review suggest several strategic recommendations for engineers, policy makers, and water utilities. First, practitioners considering deployment of AOPs should begin with hybrid trial systems, combining AOP modules with polishing steps (e.g. activated carbon, membranes) to manage by-product risk. Because even advanced AOPs often leave residual fragments, sequential polishing can act as a safety net. Second, design decisions must prioritize reactor configurations that maximize radical retention and minimize recombination losses, such as co-locating radical generation zones with pollutant transport zones, optimizing flow regimes, and minimizing transport distances. Third, pilot systems should monitor transformation product profiles and toxicity endpoints (not just parent removal), so that performance validation includes safety, not merely efficacy. Fourth, decision-makers should adopt flexible modular designs that can evolve—for instance, allowing catalyst swapping or reactor reconfiguration as new knowledge or regulatory demands emerge. Fifth, cost and energy efficiency must be continuously benchmarked: AOP systems should include internal energy monitoring and adaptive dosing to avoid over-oxidation or wasted radical production. Finally, regulatory agencies and funding bodies should incentivize AOP research and adoption by creating frameworks that reward safe, scalable, and transparent performance (e.g. by requiring full disclosure of TPs, encouraging pilot demonstrations, and integrating life-cycle audits).

Ethical Considerations

All procedures performed in this study were under the ethical standards.

Acknowledgments

Authors thank all who helped us through this study.

Conflict of Interest

The authors report no conflict of interest.

Funding/Financial Support

According to the authors, this article has no financial support.

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