Removal Technologies for Perfluoro-and Polyfluoroalkyl Substances (PFAS) Based on Literature Review: Progress, Comparisons, and Prospects

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Abstract:Perfluoro-and polyfluoroalkyl substances (PFAS) exhibit strong chemical stability, bioaccumulation, and multiple toxic effects, making their environmental remediation a global challenge [2]. Through literature thematic mapping, this study categorizes existing research into four types: core removal mechanism studies, process optimization and prediction, pollution characteristics and risks in specific environmental media, and PFAS toxicology and health risks, clarifying the research background and driving forces. Focusing on the first two categories, an analytical framework is constructed with three core schools: degradation technology, separation technology, and technology empowerment. The framework elaborates on the perspectives, technical principles, and cutting-edge developments of each school. Limitations in current research are identified, including the transition from laboratory to engineering applications, treatment of short-chain PFAS and by-products, integration and evaluation of technologies, and the interpretability of empowerment technologies. Future research should prioritize developing efficient, precise, low-consumption, and non-secondary-pollution intelligent integrated remediation strategies, providing a literature foundation and conceptual framework for PFAS removal technology development and engineering applications.

Keywords: Per-and Polyfluoroalkyl Substances (PFAS); Removal Technologies; Literature Review; Advanced Oxidation Processes (AOPs); Adsorption; Machine Learning (ML); Technology Integration

1. Thematic Map of PFAS Removal Technology Research

A systematic review of 20 core publications published in 2025 reveals that PFAS research exhibits distinct characteristics: the interplay between fundamental and applied approaches, as well as the equal emphasis on microscopic mechanisms and macro-level risks [5]. Based on their research focuses and contributions, these studies can be categorized into four interconnected yet distinct thematic groups, collectively mapping out a comprehensive knowledge landscape of PFAS removal technologies.

1.1 Research on the Mechanism of Core Removal Technology: The "Main Force" in Overcoming Challenges

This literature serves as the direct technical foundation for PFAS removal research, dedicated to exploring and elucidating the degradation and separation mechanisms of PFAS from a fundamental perspective [15]. The depth of such research directly determines the feasibility and upper limits of technological applications. For instance, Li et al. [15] conducted a systematic review of chemical degradation mechanisms, not only outlining the efficacy of various advanced oxidation/reduction processes (AORPs) but also delving into the energy barriers and reaction pathways of C-F bond cleavage. Luo et al. [9] provided a comprehensive evaluation of wastewater treatment technologies, focusing on comparing the applicability and integration potential of different techniques from an engineering perspective. Meanwhile, Bai et al. [6] explored machine learning (ML)-empowered removal technologies, representing the cutting-edge direction of transitioning R&D paradigms toward data-driven approaches. These studies form the core focus of review writing.

1.2 Optimization and Prediction of Technical Processes: A Precise and Efficient "Booster"

This category of literature does not directly invent new technologies, but rather employs advanced computational and modeling methods to provide powerful tools for optimizing and precisely applying existing technologies [3]. They significantly enhance the efficiency of technology development and adaptability to complex environments. For instance, the deep learning (DL) framework developed by Lyu et al. [3], which integrates adaptive evidence, is used to predict the environmental migration properties of PFAS (such as the organic carbon-water partition coefficient Koc). This is crucial for predicting the fate of PFAS in the environment, identifying priority control areas, and selecting optimal treatment processes. Similarly, Liu et al. [7] utilized interpretable machine learning (XAI) to reveal the distribution mechanisms of PFAS in soil. Their model can analyze the nonlinear interactions between soil components, physicochemical properties, and PFAS structural characteristics, providing unprecedented microscopic insights for the screening of adsorbents and optimization of leaching conditions in in-situ soil remediation.

1.3 Pollution Characteristics and Risks in Specific Environmental Media: A "Navigation Map" for Technology Application

While not directly developing removal technologies, such studies (e.g., Zhang et al. [10] 's research on PFAS dispersion in wastewater treatment plants, An et al. [12]' s analysis of PFAS spatiotemporal distribution in the Yangtze River estuary, and Zhu et al. [8]'s ecological risk assessment of Jiujiang Port) remain indispensable [8]. Through detailed field surveys and monitoring data, these studies have clarified the "battlefield" dynamics of PFAS pollution: where are the pollution sources? What are the primary pollutants? What are the concentration levels? How do they migrate and transform? This information prioritizes research directions and application scenarios for removal technologies, ensuring that technological development is not "working in isolation" but addresses real-world environmental challenges [12].

1.4 Toxicology and Health Risks of PFAS: The "Driving Force" of Technological Development

This category of literature (e.g., Ouyang et al. [1] identified KMT2C as a key gene in PFAS-induced hepatocellular carcinoma, Zhang et al. [20] revealed the association between serum PFAS and blood pressure, and Wang et al. [2] summarized the potential health threats of PFAS) profoundly highlights the severity of PFAS pollution and the urgency of governance from the perspectives of public health and ecological security [1]. These studies continuously provide strong social demand and policy impetus for PFAS environmental governance, serving as the fundamental driving force behind the ongoing development of removal technologies [2]. They remind researchers that the ultimate goal of technological development is to ensure ecological security and human health [20].

1.5 Literature Retrieval and Screening Methodology

The literature search and screening for this review followed a strict standardized process: the literature was primarily sourced from mainstream academic databases such as China National Knowledge Infrastructure (CNKI database), with search keywords including core Chinese and English terms such as "perfluoroalkyl substances", "polyfluoroalkyl substances", "PFAS", "removal technology", "degradation", "adsorption", and "machine learning". The inclusion criteria were PFAS-related review papers, original research papers, and engineering technical reports published in 2025, focusing on core themes such as the mechanisms of PFAS removal technologies, process optimization, environmental behavior, or health risks. The exclusion criteria included conference abstracts, patent documents, and literature with weak relevance to the research topic. Ultimately, 20 core papers were selected as the foundational data for the review analysis.

2. Literature Review: Main Schools of PFAS Removal Technologies, Technical Principles, and Academic Debates

Based on the aforementioned classification, the current research field of PFAS removal technology has formed three distinct yet interpenetrating technical schools: the "degradation school" aimed at completely breaking down pollutant structures, the "separation school" focused on physical separation and enrichment, and the "empowerment school" dedicated to optimizing technology development and application through intelligent means [6]. Each school contains different technical approaches and academic perspectives.

2.1 Degradation Technology School: Confronting the Ultimate Challenge of C-F Bonds

The ultimate objective of this approach is to chemically or biologically break down the strong carbon-fluorine (C-F) bonds in PFAS molecules, converting them into carbon dioxide (CO_2), water (H_2O), and fluoride ions (F^-), or at least into less toxic short-chain compounds, thereby fundamentally eliminating their persistent threat [15].

2.1.1 Research on chemical degradation mechanisms: from "rampant attack" to "precision strike"

Scholars in this field generally agree that traditional water treatment processes are almost ineffective against PFAS, necessitating reliance on advanced technologies based on active free radicals or special reducing agents [15]. In their review, representative scholars such as Li et al. [15] systematically compared mainstream chemical degradation pathways, including thermal activation, UV-activated persulfate methods, electrochemical oxidation (ECO), plasma technology (PT), and photocatalysis (PC). They pointed out that early studies predominantly relied on the "blitzkrieg" approach using strong oxidants like hydroxyl radicals (•OH), which had limited effects on C-F bonds [15]. Current research frontiers have shifted toward two mechanisms: one involves utilizing more selective oxidants such as sulfate radicals ($SO_4{\bullet}^-$) or directly attacking the head functional groups of PFAS with strong reducing agents like hydrated electrons (e^-aq) to initiate chain reactions for defluorination; the other focuses on non-radical pathways, such as direct electron transfer in electrochemical processes or surface-mediated reactions, which may offer greater selectivity and energy efficiency [15]. Li et al. particularly emphasized that future research should prioritize designing efficient, stable, and interference-resistant heterogeneous catalysts to facilitate reactions under ambient conditions [15]. Additionally, they called for enhanced tracking and toxicity assessment of degradation intermediates to avoid the generation of unknown and more hazardous byproducts [15].

2.1.2 Integration of wastewater treatment technologies: from "working alone" to "joint operations"

Representative scholar Luo et al. [9] proposed a more pragmatic and systematic perspective from an engineering practice perspective. Through analyzing numerous engineering cases and literature, they explicitly stated that "no universal technology can solve all PFAS pollution problems" [9]. They constructed a clear technical hierarchy: the foundational layer consists of adsorption methods (Adsorption, such as powdered activated carbon, granular activated carbon, ion exchange resin) and membrane separation (Membrane Separation, MS, such as nanofiltration, reverse osmosis), which excel at rapidly and efficiently separating and concentrating PFAS from large volumes of water; the upper layer comprises advanced oxidation processes (AOPs) and reductive decomposition (RD) for treating high-concentration concentrates, achieving final harmless treatment [9]. Luo et al. advocated for a "pre-treatment-concentration-deep degradation" integrated process route [9]. They argued that for low-concentration, high-volume municipal or industrial wastewater, directly applying advanced oxidation technologies is costly and may produce by-products. Instead, concentrating PFAS 100-1000 times via adsorption or membrane technology, followed by thorough degradation of the concentrated fraction, represents the optimal strategy balancing technical feasibility, treatment efficiency, and economic costs [9]. This "separation + degradation" integrated approach represents the mainstream direction in current engineering applications [9].

2.2 Separation Technology School: Engineering Foundation of High-Efficiency Enrichment and Risk Control

This approach emphasizes the use of physicochemical methods to separate PFAS from environmental media such as water or soil, achieving purification of the media and concentration of pollutants, thereby creating conditions for subsequent disposal or resource recovery [6]. This is currently the most mature and widely applied PFAS treatment solution [7].

2.2.1 Intelligent design of adsorption technology: from "empirical screening" to "rational design"

In the field of adsorption research, a paradigm shift driven by data science is underway [6]. Notably, Bai et al. [6] highlighted that while traditional adsorbents like activated carbon effectively capture long-chain PFAS, their adsorption capacity for the growing number of short-chain PFAS compounds shows a sharp decline, compounded by bottlenecks such as slow adsorption rates and susceptibility to competition from coexisting organic compounds. They argue that machine learning (ML) is pivotal to overcoming these limitations [6]. Bai et al. demonstrated how ML analyzes vast experimental datasets—including material pore sizes, surface chemistry, PFAS molecular descriptors, and environmental conditions—to establish quantitative structure-activity relationship (QSAR) models. This approach enables rapid, low-cost prediction of adsorption capacity and selectivity for thousands of potential adsorbents (e.g., metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and biochar) toward specific PFAS compounds [6]. This innovation revolutionizes the traditional trial-and-error approach to material development, enabling rational design and targeted screening of high-performance adsorbents [6]. They envision future intelligent adsorption systems capable of real-time monitoring of influent water quality and dynamically optimizing adsorbent dosing and regeneration cycles through modeling, achieving adaptive precision control [6].

2.2.2 Explorations of the interpretability of soil allocation mechanisms: from "black box models" to "mechanism insights"

For more complex soil media, the study by representative scholars Liu et al. [7] demonstrated the powerful capabilities of interpretable machine learning (XAI). Their research transcended the limitations of traditional multiple linear regression, employing advanced algorithms such as gradient-boosting trees (e.g., XGBoost) and post-hoc interpretation tools like SHAP (SHapley Additive exPlanations) to deeply elucidate the nonlinear driving mechanisms of PFAS adsorption-desorption behavior in soil [7]. Their model confirmed that soil organic matter (SOM) is the most significant influencing factor, but its impact is non-linear and exhibits varying effects across different concentration ranges [7]. Additionally, pH regulates adsorption by affecting the ionization state of PFAS and soil surface charge, ionic strength influences through competitive effects, while the carbon chain length and functional group types of PFAS determine their hydrophobicity and surface affinity [7]. Liu et al.'s work has opened the "black box" of soil-PFAS interactions, providing quantitative and mechanistic insights that are crucial for developing in-situ immobilization techniques (e.g., additive modification) or ex-situ leaching remediation strategies for specific contaminated soils [7].

2.3 Technology Empowerment School: Data-Driven Paradigm Shift in Research

This approach is not an independent removal technique, but rather a groundbreaking methodological tool for developing and applying the aforementioned technologies, representing the future frontier in PFAS governance research [3].

The work of representative scholars such as Liu et al. [3] and Bai et al. [6] collectively highlights the value of the data-driven paradigm. Liu's deep learning (DL) framework focuses on predicting the fundamental physicochemical properties and environmental behavior parameters of PFAS, which serve as the basis for assessing their environmental fate and exposure risks, as well as key input data for designing treatment processes [3]. Bai et al., on the other hand, emphasize optimizing operational parameters and overall performance of removal processes [6]. Their shared core perspective is that traditional experimental screening and optimization methods are time-consuming, labor-intensive, and prohibitively expensive when dealing with the vast number (over 10,000 types) and diverse structures of PFAS families [3,6]. In contrast, artificial intelligence (AI) and machine learning (ML) can learn from limited high-quality experimental data and uncover deep, complex patterns that are difficult for humans to intuitively discover, thereby achieving predictive capabilities that enable "learning from one to understand many." This significantly accelerates the discovery of new materials, optimization of new processes, and intelligent control of treatment systems, transitioning PFAS governance from "experience-driven" to "predictive science" [3,6].

3. Literature Review: In-Depth Analysis of Existing Research and Future Research Directions

Building on the 2025 research findings, a critical examination reveals persistent fundamental contradictions and challenges in current PFAS removal technologies, which constitute critical research directions requiring urgent breakthroughs [5].

3.1 The "Valley of Death" from Lab to Engineering: Challenges of Real-World Complexity

The vast majority of studies on degradation mechanisms [15] and novel adsorbent materials [6] have been conducted under ideal laboratory conditions: using single PFAS standards, high initial concentrations, and pure background matrices (e.g., ultrapure water). This creates a stark contrast with real-world environments (e.g., municipal wastewater treatment plants [10], contaminated surface waters [8,12]), where PFAS exist in trace amounts (ng/L or even pg/L) and coexist with multiple components in complex matrices containing substantial natural organic matter, suspended particles, and inorganic salts [10]. These coexisting substances compete with PFAS for active sites or free radicals, poison catalysts, and clog adsorbent pores, leading to a sharp decline in the high removal efficiencies reported in laboratory studies when applied in field conditions [15]. Future research must significantly strengthen pilot-scale and field validation in actual water/soil environments, fully considering the complexity of real-world conditions to evaluate the long-term operational stability, interference resistance, and maintenance requirements of the technologies [9].

3.2 Insufficient Response to Challenges in the Post-Long-Chain Era: Hidden Risks of Short-Chain PFAS and Transformation Byproducts

With the strict restriction of long-chain perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS), the use of short-chain perfluorinated alkyl sulfonates (PFASs) such as GenX and perfluorobutanoic acid (PFBA) and other novel alternatives has become increasingly widespread [6]. However, short-chain PFASs exhibit stronger water solubility and weaker affinity for traditional adsorbents, leading to decreased retention rates in adsorption and membrane separation technologies [6]. Additionally, the degradation efficiency of many techniques for short-chain PFASs remains unclear [15]. More critically, current research has severely underreported the incomplete degradation products generated during the process, such as short-chain by-products and fluorinated intermediates [15]. Focusing solely on the removal rate of parent compounds while neglecting the toxicity and persistence of transformation products may result in an "adverse reaction" environmental risk [2]. Therefore, future studies must incorporate perfluorination pathway analysis, intermediate identification, and comprehensive toxicity assessment as mandatory components of technical evaluations [15].

3.3 Lack of Technology Integration and System Evaluation: Transition from Technology-Oriented to Solution-Oriented

Most existing literature focuses on in-depth exploration of individual technologies, yet lacks systematic comparative studies on synergistic effects of different technology combinations, techno-economic analysis (TEA), and life cycle assessment (LCA) [9]. For instance, when treating specific wastewater, which of the two integrated approaches— "membrane concentration + electrochemical oxidation" or "adsorption concentration + thermal activation persulfate" —has lower total costs? Smaller carbon footprints? More controllable by-product risks? Such comprehensive evaluations are currently lacking [9]. Future research should move beyond optimizing single technologies to develop modular, standardized technical units and establish intelligent technology selection and integration platforms based on multi-objective decision analysis, providing optimal holistic solutions for various scenarios [6].

3.4 The "Black Box" Dilemma and Data Barriers of Empowerment Technology: Challenges in Explainability and Sharing

Despite the tremendous potential of machine learning [3,6,7], its complex "black box" models often fail to provide clear mechanistic explanations, which raises doubts about their predictive outcomes and limits the ability to discover new scientific principles from data [7]. Promoting the application of Explainable Artificial Intelligence (XAI) in environmental fields will be key to unlocking its full value [7]. Moreover, the development of this field heavily relies on high-quality, standardized datasets, yet current data remains fragmented and inconsistent, creating significant "data barriers" [3]. Establishing a public database for PFAS physicochemical properties, adsorption/degradation performance, and formulating data standards are critical infrastructures for advancing AI-enabled research paradigms [6].

Future Outlook: In summary, future research on PFAS removal technologies should focus on integrating four key directions: ① Application-oriented approaches, emphasizing validation and optimization in real-world environmental matrices [9,10]; ② Safety-oriented strategies, prioritizing the removal of short-chain and novel PFAS compounds while monitoring by-products throughout the process [2,15]; ③ System-oriented methodologies, integrating technologies and conducting multidimensional evaluations [6,9]; ④ Intelligence-driven solutions, developing interpretable AI models and establishing shared databases [3,7]. The ultimate goal is to establish an efficient, precise, low-carbon, and cost-effective intelligent PFAS governance technology system.

4. Conclusion

This review systematically maps PFAS removal research into four thematic clusters and three technical schools—degradation, separation, and technology empowerment. The findings reveal that while significant progress has been made in understanding C–F bond cleavage mechanisms and developing high-performance adsorbents, critical bottlenecks remain. Laboratory breakthroughs often fail under real-world conditions due to matrix complexity, trace concentrations, and coexisting substances. Moreover, short-chain PFAS and transformation byproducts receive insufficient attention, raising concerns about incomplete remediation and hidden risks. The integration of machine learning offers new opportunities for rational design and predictive optimization, yet data fragmentation and model interpretability limit its full potential. Future work must move beyond single-technology assessments toward solution-oriented, multi-criteria evaluations that combine separation and degradation in modular trains. Pilot-scale validation under authentic environmental matrices, coupled with life cycle and techno-economic analysis, is urgently needed. Establishing open-access databases and promoting interpretable AI will further accelerate the transition from experience-driven to knowledge-driven governance. Ultimately, an intelligent, low-consumption, and secondary-pollution-free remediation system remains the long-term goal, requiring coordinated advances in fundamental chemistry, materials science, data analytics, and environmental engineering.

References

[1] Ouyang, N., Xu, W., Dong, F., et al. (2025).[A study on the key gene KMT2C of liver cancer induced by per- and polyfluoroalkyl substances based on network toxicology and Mendelian randomization].[Journal of Environmental & Occupational Medicine], 42(12), 1510–1519.

[2] Wang, C., Zhao, Z., Huo, Y., et al. (2025). [Potential threats of per- and polyfluoroalkyl substances to human and animal health].[Asian Journal of Ecotoxicology], 20(6), 235–248.

[3] Lyu, X., Jiang, B., Yuan, G., et al. (2025). [A deep learning framework incorporating adaptive evidence for predicting the environmental migration properties of PFAS]. [CIESC Journal], Advance online publication. https://link.cnki.net/urlid/11.1946.TQ.20251219.1559.008

[4] Wu, Y., Fu, Y., Fu, J., et al. (2025). [Effects and mechanisms of per- and polyfluoroalkyl substances (PFAS) on soil microbial community]. [Asian Journal of Ecotoxicology], Advance online publication. https://link.cnki.net/urlid/11.5470.x.20251217.1353.016

[5] Sheng, D., Cai, K., Liu, Y., et al. (2025). [Identification and evolution analysis of research hotspots on per- and polyfluoroalkyl substances in soil]. [Chinese Journal of Environmental Engineering], Advance online publication. https://link.cnki.net/urlid/11.5591.X.20251215.1811.003

[6] Bai, M., Song, C., Zhang, Y., & Niu, J. (2025). [Machine learning-enabled technologies for removal of per- and polyfluoroalkyl substances from water]. [Scientia Sinica Chimica], 55(11), 3141–3154.

[7] Liu, B., Zou, K., Liu, H., et al. (2025). [Partitioning mechanisms of PFAS in soil based on interpretable machine learning]. [China Environmental Science], Advance online publication. https://doi.org/10.19674/j.cnki.issn1000-6923.20251010.001

[8] Zhu, M., Liao, W., Zhang, X., et al. (2025).

[Pollution characteristics and ecological risk assessment of per- and polyfluoroalkyl substances in surface water of Jiujiang Port, Jiangxi Province]. [Environmental Science], Advance online publication. https://doi.org/10.13227/j.hjkx.202506230

[9] Luo, M., Yin, C., Feng, M., et al. (2025). [Research progress on treatment technologies for per- and polyfluoroalkyl substances in wastewater]. [Rock and Mineral Analysis], 44(4), 576–597. https://doi.org/10.15898/j.ykcs.202507150203

[10] Zhang, Z., Zhang, Y., Li, X., et al. (2025). [Emission behavior and health risk of fine particulate matter loaded with per- and polyfluoroalkyl substances from wastewater treatment plants in winter]. [Chinese Journal of Environmental Engineering], Advance online publication. https://link.cnki.net/urlid/11.5591.x.20250806.1818.010

[11] Liu, H., Ren, W., Ma, W., et al. (2025). [Research progress on distribution characteristics and pollution sources of per- and polyfluoroalkyl substances in global organisms]. [Asian Journal of Ecotoxicology], 20(5), 22–38.

[12] An, X., Wang, C., Chen, C., et al. (2025). [Spatiotemporal distribution and influencing factors of per- and polyfluoroalkyl substances (PFAS) in the Yangtze River Estuary]. [Acta Scientiae Circumstantiae], 45(9), 263–273. https://doi.org/10.13671/j.hjkxxb.2025.0118

[13] Wang, H., Jiang, H., Cai, J., et al. (2025). [Systematic transcriptome analysis reveals toxicity differences of three typical per- and polyfluoroalkyl substances]. [China Environmental Science], Advance online publication. https://doi.org/10.19674/j.cnki.issn1000-6923.20250729.005

[14] Lu, L., Dong, L., & He, R. (2025). [Research progress on exposure to per- and polyfluoroalkyl substances and adverse pregnancy outcomes]. [Journal of Environmental & Occupational Medicine], 42(6), 762–769.

[15] Li, Y., Li, T., Li, Y., et al. (2025). [Chemical degradation mechanisms and research progress of per- and polyfluoroalkyl substances]. [Journal of Tianjin University (Science and Technology)], 58(6), 551–566.

[16] Han, J., & Zhao, S. (2025). [Research progress on plant enrichment, metabolic transformation, and toxic effects of perfluoroalkyl acids (PFAAs) precursors]. [Asian Journal of Ecotoxicology], 20(3), 14–29.

[17] Chen, X., Sun, J., Jiang, D., et al. (2025). [Research progress on residual detection methods for per- and polyfluoroalkyl substances in complex matrices]. [Physical Testing and Chemical Analysis (Part B: Chemical Analysis)], Advance online publication. https://link.cnki.net/urlid/31.1337.TB.20250507.1417.002

[18] Tian, G., Yuan, H., Wang, H., et al. (2025). [Pollution characteristics and ecological risk assessment of per- and polyfluoroalkyl substances in the Kuroshio Extension region of the Northwest Pacific Ocean]. [Journal of Ocean University of China (Natural Science Edition)], 55(5), 20–28. https://doi.org/10.16441/j.cnki.hdxb.20240153

[19] Chen, Y., Lyu, J., Ye, B., et al. (2025). [Determination of 51 per- and polyfluoroalkyl substances in source water and drinking water by online solid-phase extraction-ultra performance liquid chromatography-tandem mass spectrometry]. [Chinese Journal of Chromatography], 43(11), 1222–1234.

[20] Zhang, H., Xu, F., Liu, Y., et al. (2025). [Association between serum PFASs exposure levels and blood pressure among residents in Jinan City]. [Journal of Shandong University (Engineering Science)], 55(4), 160–172.