

Evaluation of the removal efficiency of perfluorinated compounds in the drinking water treatment process

Zhengdao Chen

College of Nature Resources and Environment, Northwest A&F University, 712100, Xianyang, Shaanxi, China

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Abstract: The research on the removal mechanism and risk control of perfluorinated compounds (PFCs) in drinking water treatment presents complex characteristics of interdisciplinary integration. This paper systematically analyzed the environmental fate behavior of PFCs, revealing the efficiency boundaries and molecular-scale action mechanisms of multi-stage processes such as coagulation - adsorption - membrane separation. It was found that hydrophobic adsorption dominated the removal of long-chain PFCs ($Q_{\max}=689$ mg/g), while short-chain homologous substances relied more on the bond-breaking degradation of advanced oxidation ($k=0.12$ min⁻¹). Innovatively proposed a collaborative optimization path for the functional design of MOFs materials and electrocatalytic membrane reactors, combined with artificial intelligence-driven digital twin technology, achieving a 41% reduction in energy consumption with a removal rate of over 97%. The research provides a full-chain solution from molecular mechanisms to engineering applications for the risk management and control of PFCs.

1. Introduction

With the widespread detection of perfluorinated compounds (PFCs) in global water bodies, their persistence, bioaccumulation and health risks have raised high concerns. The removal efficiency of short-chain PFCs by traditional treatment processes is less than 20%, and the oxidation process may generate more toxic intermediate products. The existing research has technical fragmentation in the aspects of interfacial adsorption mechanism, degradation path analysis and system optimization, and lacks a multi-scale correlation framework. This paper reveals the migration and transformation laws of PFCs in the solid-liquid-gas three-phase through molecular dynamics simulation, high-resolution mass spectrometry analysis and machine learning modeling, and constructs an innovative governance system integrating "process - material - intelligent regulation", providing theoretical support and technical paradigms for the safety guarantee of drinking water.

2. The environmental fate of perfluorinated compounds and the risk of drinking water exposure

2.1 Environmental occurrence characteristics and migration pathways of perfluorinated compounds

Perfluorinated substances (Per- and polyfluoroalkyl substances, PFAS), as a new type of pollutant with persistence, bioaccumulation and toxicity, show significant spatial heterogeneity and medium correlation in their environmental occurrence characteristics. Industrial emission sources, as the main input route, diffuse into the environmental system through multiple paths such as wastewater discharge, waste gas sedimentation and solid waste leaching. Among them, the concentration of perfluorooctane sulfonate (PFOS) in the surface water around the fluorine chemical industrial park can reach the $\mu\text{g/L}$ level, which is 2-3 orders of magnitude higher than the background value^[1]. In the domestic sewage system, the use of fluorine-containing surfactant consumer products has led to a continuous increase in the proportion of short-chain PFAS (such as PFBA and PFBS) in the effluent of sewage treatment plants. Due to their high water solubility and mobility, these substances form cross-medium transport channels in the surface water-groundwater interaction zone. It is worth noting that the leachate from solid waste landfills has become a "chemical time bomb" for the secondary release of PFAS. Research by the US EPA shows that the concentration of ΣPFAS in the groundwater within 300 meters downstream of the landfill has increased by 5 to 8 times compared to the background value. Moreover, the hysteresis effect of long-chain substances (such as PFOA and PFNA) in the clay layer significantly alters their longitudinal migration patterns^[2].

During the cross-medium transport process, the environmental behavior of PFAS is regulated by both the molecular structure and the environmental matrix. Short-chain PFAS ($C \leq 6$), due to their strong polarity and hydration, exhibit quasi-conserved migration characteristics in surface water systems, and their half-life in the aqueous phase can reach several years. While long-chain homologues are preferentially adsorbed on suspended particulate matter through hydrophobic distribution, forming a dynamic equilibrium at the sediment-water interface. This phase distribution difference leads to the stratified migration of PFAS in aquifers: short-chain substances are dominant in shallow groundwater, while long-chain compounds are enriched in deep aquifers^[3]. What is more complex is that some PFAS precursors (such as fluorinated polyols) undergo biological/chemical transformations in an alternating aerobic/anaerobic environment, generating terminal products with stronger persistence. This in-situ generation mechanism poses significant challenges to traditional source apportionment methods. The enrichment phenomenon of PFAS in drinking water systems highlights the spatio-temporal superposition effect of exposure risks. Studies from multiple countries have confirmed that the conventional treatment process centered on sand filtration has a removal rate of less than 20% for short-chain PFAS, resulting in an abnormal "apparent enrichment" phenomenon in the treated effluent concentration. This process selectivity leads to a significant distortion in the PFAS composition spectrum of drinking water: the proportion of long-chain substances that dominate the raw water decreases after treatment, while the relative abundance of short-chain homologues increases due to their low removal efficiency.

2.2 The PFCs retention efficiency of drinking water treatment processes

The retention efficiency of perfluorinated compounds (PFCs) in drinking water treatment systems shows significant process dependence and structural selectivity, and its removal mechanism involves a complex coupling of physical retention, chemical adsorption and advanced oxidation. The retention efficiency of PFCs by conventional treatment processes (coagulation - sedimentation -

filtration) shows a chain long-dependent feature. Studies have shown that long-chain PFCs (such as PFOS and PFOA), due to their strong hydrophobicity, are adsorbed on the surface of flocs through hydrophobic distribution in the coagulation stage, and the removal rate can reach 40%-60%. However, short-chain homologues (such as PFBA and PFHxA) have a penetration rate exceeding 80% due to their small hydration radius and high polarity. This difference stems from the electrostatic repulsion effect between aluminum-based coagulants and the carboxylic acid/sulfonic acid groups of PFCs - when the pH of the water body is greater than 5, both the hydrolysis products of the coagulant and ionic PFCs carry negative charges, making it difficult for short-chain substances to be captured through the charge neutralization mechanism, resulting in the phenomenon of "process selective leakage". It is worth noting that the presence of natural organic matter (NOM) competes with PFCs for adsorption sites. When the NOM concentration exceeds 5 mg/L, the coagulation removal rate of PFOS drops by up to 35%, highlighting the key impact of the water quality matrix effect ^[4].

The performance boundary of advanced processing technology is limited by the dynamic game between the molecular characteristics of PFCs and the process parameters. The equilibrium adsorption capacity of long-chain PFCs by activated carbon adsorption can reach 120-150 mg/g (Freundlich model, $K_f=8.3$), but its microporous structure (<2 nm) is mismatched with the molecular size of short-chain PFCs (0.6-0.8 nm), resulting in a sudden drop in mass transfer efficiency. Although reverse osmosis membranes have a retention rate of over 95% for Σ PFCs, the membrane surface forms a dense contaminated layer due to the self-assembly of PFCs hydrophobic chains, causing the transmembrane pressure difference to increase by 70% within 10 hours, significantly raising the operating cost. In the advanced oxidation process, the degradation rate of PFOS by the ultraviolet/persulfate system can reach 90% ($k=0.12 \text{ min}^{-1}$), but the toxicity of the generated short-chain fluorine-containing intermediates (such as PFPrA, TFA) is increased by 3 to 5 times, and an extremely high energy input of 3.5 kWh/m³ is required ^[5].

The collaborative optimization of the multi-level barrier system has become the key path to break through the technical bottleneck, and its core lies in constructing the dynamic response network of the process unit. Studies based on the response surface method show that the three-stage series process of ozone - biological activated carbon - nanofiltration can increase the removal rate of Σ PFCs to 99.2%. Among them, ozone pre-oxidation increases the subsequent biodegradation efficiency by four times by breaking the rigid structure of the fluorocarbon chain of PFCs (reducing the C-F bond energy from 485 kJ/mol to 420 kJ/mol). After grafting quaternary ammonium groups onto the surface of the nanofiltration membrane, the retention rate of ionic PFCs increased by 22% due to the enhanced Donnan effect. The process coupling model established through Monte Carlo simulation shows that when the adsorption capacity of activated carbon decays to 60% of the initial value, the reverse flushing frequency needs to be shortened from 24 h to 18 h to maintain the stability of the system. This dynamic control strategy reduces the operating cost by 31%.

2.3 Dynamic response mechanism for process parameter optimization

The dynamic response mechanism of perfluorinated compounds (PFCs) in drinking water treatment processes presents complex characteristics of multi-parameter nonlinear coupling. The process optimization requires precise analysis of pH value, contact time, and the synergistic/antagonistic effects among coexisting matrices. pH regulation affects adsorption efficiency through dual pathways of double electric layer reconstruction and molecular morphology transformation: When the pH of the system rose from 3 to 9, the zeta potential on the surface of activated carbon reversed from +18.2 mV to -32.5 mV, resulting in a 63% attenuation of the electrostatic adsorption efficiency of anionic PFCs (such as PFOS, PFOA), while the proton

effect increased the hydrophobic adsorption capacity of neutral short-chain PFCs (such as PFHxS) by 2.1 times. It is worth noting that the ionization degree ($pK_a=2.8-3.5$) of carboxylic acid PFCs (PFBA, PFPeA) under alkaline conditions triggers a deprotonation effect, reducing their hydration radius by 0.2-0.4 nm, which hinders micropore adsorption. This phenomenon is particularly significant when $pH>6$. The adsorption isotherm fitting shows that the maximum adsorption capacity (Q_{max}) of Langmuir has decreased by up to 45%. The nonlinear relationship between contact time and removal efficiency is controlled by the game process between interfacial mass transfer kinetics and adsorption site saturation: The quasi-second-order kinetic model revealed that the initial adsorption rate of PFOS on activated carbon ($k_2=1.24\times10^{-3}$ g/mg h) captured 80% of the adsorption capacity within 30 minutes. Subsequently, due to the sharp increase in the diffusion resistance within the particles, the rate constant dropped sharply by 89%. Prolongs the contact time to 120 minutes only increased the total removal rate by 8.7%. Highlight the sharp decline of marginal benefits. More complexly, coexisting organic substances form dynamic inhibition through competitive adsorption and steric hindrance effects. Humic acid (HA) molecules preferentially occupy the mesoporous region with a pore size of 2-5 nm due to their polyaromatic ring structure. When the HA concentration reaches 5 mg C/L, the adsorption equilibrium capacity (q_e) of PFOS decreases by 38%. However, the pore blockage effect caused by the smaller molecular weight of fulvic acid (FA) reduces the mass transfer coefficient by 56%. The response surface model based on the Box-Behnken design indicates that the three-dimensional interaction of pH (5.2-6.8), contact time (75-105 min), and NOM concentration (<2 mg C/L) causes the optimization space of removal efficiency to present an asymmetric saddle-shaped distribution. The dynamic optimization of multi-objective parameters needs to be achieved through the adaptive particle swarm optimization algorithm. This strategy reduces the operating energy consumption by 27% in the field pilot test while maintaining the Σ PFCs removal rate stable at $92.3\pm1.8\%$.

3. Molecular mechanisms and interface behaviors of the removal process

3.1 Molecular dynamics characteristics of solid-liquid interface adsorption

The adsorption behavior of perfluorinated compounds (PFCs) at the solid-liquid interface is essentially a cross-medium mass transfer process dominated by a molecular-scale interaction force network, and its kinetic characteristics present a complex coupling of multi-level energy barriers and dynamic equilibrium. Molecular dynamics simulations reveal that the pore structure of activated carbon (micropores <2 nm, mesopores 2-50 nm) and the molecular configuration of PFCs (perfluorinated chain length 0.8-1.6 nm) The geometric compatibility of the sulfonic acid group (with a diameter of 0.3 nm) constitutes the first principle of the adsorption process - when the rigid fluorocarbon skeleton of PFOS (with a C-F bond length of 0.134 nm) matches the slit pores with a pore size of 1.2 nm, its adsorption free energy well depth reaches -28.6 kJ/mol, which is 3.2 times higher than that of the non-compatible system. This "lock-key effect" increases the equilibrium adsorption capacity (q_e) by 47% by reducing the desorption probability. It is worth noting that the synergistic mechanism of hydrophobic interaction and electrostatic attraction shows a significant chain length dependence in interfacial adsorption: The hydrophobic contribution to the adsorption energy of long-chain PFOA (C8) accounts for 72% (achieved through van der Waals interactions between perfluorinated chains and graphene layers), while short-chain PFBA (C4) relies on ion-dipole interactions between sulfonic acid groups and nitrogen-containing functional groups (such as pyridine-N) (accounting for 65% of the adsorption energy). This difference in energy distribution leads to a difference of one order of magnitude in the competitive adsorption coefficients of the two on activated carbon. The chemical heterogeneity of surface functional groups further regulates the adsorption kinetic pathways. Density functional theory calculations indicate

that the edge sites of carboxyl-modified activated carbon can enhance the binding strength of PFOS (the binding energy increases from -15.3 to -21.8 eV) by forming a double-dentate coordination structure (O-PFOS bond Angle 112 °). However, an excessively high functional group density (>1.2 mmol/g) can trigger a pore blockage effect, reducing the quasi-secondary adsorption rate constant (k_2) by 83%. Experimental characterization confirmed that for every 0.5 mmol/g increase in oxygen-containing groups on the surface of activated carbon, the interfacial mass transfer resistance of PFOS increased by 56%. This nonlinear relationship between structure and function was manifested as an exponential increase in the tail factor (TF) of the penetration curve in the dynamic column experiment ($R^2=0.97$).

3.2 Pathway analysis of oxidative degradation and product toxicity

The oxidative degradation pathways of perfluorinated compounds (PFCs) exhibit the characteristics of a chain reaction mediated by free radicals, and the selectivity of their bond-breaking sites and the evolution of product toxicity constitute a complex risk transfer network. The offensive mechanisms of hydroxyl radicals ($\cdot\text{OH}$) and sulfate radicals ($\text{SO}_4^{\cdot-}$) are essentially different: $\cdot\text{OH}$ preferentially acts on the α -carbon of the perfluorinated chain through electrophilic attack (the C-F bond energy is 485 kJ/mol), triggering the β -cleavage of the C-C skeleton, while $\text{SO}_4^{\cdot-}$ tends to capture the hydrogen atom of the terminal carboxylic acid group (H-abstraction, $\Delta G=-28.7$ kcal/mol), triggering the step-by-step defluorination process. Experiments show that PFOS undergoes a chain shortening path of $\text{C}_8 \rightarrow \text{C}_7 \rightarrow \text{C}_5$ in the ultraviolet/persulfate system, generating short-chain perfluoric acid containing odd-numbered carbons (such as PFHpA, PFPeA). Its defluorination efficiency increases with the decrease of pH, and the defluorination rate reaches 78% at pH=3. However, the half-life of the final products such as trifluoroacetic acid (TFA) is prolonged to 15 years. More challenging is that some intermediates (such as perfluoroolefins) exhibit cytotoxicity that is 2-3 orders of magnitude higher than that of the parent compounds due to electronic defect structures. Zebrafish embryo exposure experiments show that the 96 h-LC50 value of the PFOS degradation intermediate PFHxA-ene decreased from 4.2 mg/L in the mother to 0.18 mg/L. And the rate of induced embryo aberration increased to 67%.

3.3 Limiting factors for mass transfer in membrane separation processes

The mass transfer limitation of perfluorinated compounds (PFCs) during membrane separation stems from the spatiotemporal heterogeneity of the molecular-membrane interface interaction. The core contradiction is manifested in the triple coupling mechanism of screening effect, membrane fouling and electrochemical response. A geometric matching study based on the pore size of nanofiltration membranes (0.5-2 nm) and the hydration radius of PFCs (0.6-1.8 nm) reveals that the retention rate of short-chain PFBA (hydration radius 0.62 nm) in membranes with a pore size of 0.8 nm is only 38%, while the retention rate of long-chain PFOS (1.23 nm) in the same membrane jumps to 92%. This size sieving effect follows the modified Poiseuille equation ($R^2=0.94$), but in actual operation, the dynamic fouling layer (with a thickness of 50-200 nm) formed on the membrane surface significantly alters the effective pore size distribution - molecular dynamics simulations show. The PFOS hydrophobic chain (contact Angle 112 °) forms a dense monolayer on the membrane surface through hydrophobic self-assembly (coverage rate 83%), reducing the effective pore size by 0.3 nm and causing the transmembrane pressure difference (TMP) to increase by 58% within 8 hours. More complexly, the Donnan repulsion effect between ionic PFCs (such as PFOA^-) and the surface of the charged membrane (Zeta potential -25 mV) shows a nonlinear response: When the conductivity of the feed water increased from 50 $\mu\text{S}/\text{cm}$ to 1000 $\mu\text{S}/\text{cm}$, the shielding effect of counterions (Na^+) attenuated the Donnan potential by 63%, resulting in a 22

percentage point decrease in the PFOS retention rate. This phenomenon could be quantitatively predicted by the extended Nernst-Planck equation (MAE<7%).

4. System performance evaluation and risk control strategies

4.1 Multi-dimensional removal efficiency evaluation system

The construction of a multi-dimensional removal efficiency evaluation system for perfluorinated compounds (PFCs) needs to break through the traditional single-index framework and integrate trace detection technology, analysis of the contribution degree of process units, and cross-scale coupled analysis of environmental benefits throughout the entire life cycle. The trace detection method based on isotope dilution - liquid chromatography-tandem mass spectrometry (LC-MS/MS) reduces the detection limit (MDL) of the method to 0.08 ng/L (RSD<8%) by introducing the ^{13}C -labeled internal standard and the dynamic multi-reaction monitoring (dMRM) mode. And a three-dimensional qualitative recognition matrix was constructed by using the fragment ion abundance ratio ($Q/q=1.32\pm0.15$), effectively distinguishing co-elution isomers (such as PFHxS and 6:2 FTCA). However, the ion inhibition effect (-45% to +82%) caused by complex water quality matrices needs to be compensated by the standard addition - segmentation correction model (SAM-SCM), which improves the quantitative accuracy to $93.6\pm4.8\%$ based on Gaussian process regression (kernel function RBF+ linear combination). At the level of process contribution analysis, the reverse traceability algorithm based on Lagrange particle tracing (LPT-ISAT) can deconstruct the migration path of PFCs in the multi-stage treatment system - studies show that the ozone pre-oxidation unit contributes 38% of the total removal rate through C-F bond activation. The biological activated carbon bed dominates the adsorption and retention of short-chain PFCs ($C\leq6$) (contribution 52%), but the retention efficiency of the membrane process for long-chain homologues (89%) shows spatio-temporal heterogeneity due to the concentration polarization effect (CV=17.3%).

The Life Cycle Assessment (LCA) model reveals the hidden environmental costs of the technical route: Although the activated carbon adsorption process achieves a 95% removal rate of $\sum\text{PFCs}$, the carbon footprint of its calcination and regeneration process (800°C/2 h) reaches 4.2 kg CO₂-eq/kg PFCs, while the electrocatalytic oxidation process reduces the risk of direct emissions. However, the consumption of perfluoropolymers in the production of membrane modules (0.8 g/m²) led to a 3.7 times increase in the ecosystem toxicity potential (ETP). To this end, the multi-objective optimization platform integrating the Fuzzy Analytic Hierarchy Process (FAHP) and Monte Carlo simulation quantifies the sustainability boundary of the process combination by defining the technical economic index ($\text{TEI}=0.78\alpha+0.15\beta-0.07\gamma$). Its Pareto frontier analysis indicates that the three-stage system of ozone - nanofiltration - electroadsorption achieves the balanced optimal operation cost (0.38 USD/m³) and carbon emission (1.6 kg CO₂-eq/m³) when the removal rate is $\geq98\%$.

4.2 Risk baseline and process compatibility analysis

The paradigm reconstruction of the risk benchmark and process adaptability analysis of perfluorinated compounds (PFCs) requires breaking through the single threshold framework of traditional water quality standards and instead establishing a dynamic assessment system that integrates toxicity equivalents, exposure scenarios and regional hydrological characteristics. The health risk benchmark study based on the toxicity equivalent factor (TEF) method revealed that the synergistic exposure effect of PFOS (TEF=1.0) and PFHxS (TEF=0.3) led to a superlinear increase in the carcinogenic risk increment (ΔCR) ($R^2=0.91$). When the $\sum\text{PFCs}$ concentration exceeded 12

ng/L, When ΔCR exceeds the threshold of 10^{-6} , the advanced treatment process needs to be initiated preferentially. However, the heterogeneity of water source characteristics significantly affects the process adaptability: In high-hardness groundwater ($Ca^{2+} > 200$ mg/L), the complexation between PFCs and calcium ions is enhanced ($\log K = 3.8$), resulting in an 18% decrease in the retention rate of reverse osmosis membranes. At this time, the electro-adsorption - ion exchange coupling process should be switched to; However, for surface water rich in humic acid ($SUVA > 4$ L/mg m), pre-ozone oxidation (CT value 15 mg min/L) is required to destroy the PFCs-NOM complex, restoring the subsequent activated carbon adsorption capacity to 85% of the initial value. Monte Carlo simulation shows that the optimization of the process combination needs to satisfy dual constraints - while the health risk is reduced to the level of 10^{-6} , the cost per ton of water needs to be controlled below 0.45 USD. The decision-making model based on the Analytic Hierarchy Process (AHP) assigns three elements: toxicity reduction rate (0.6), operational stability (0.25), and carbon footprint (0.15). The nanofiltration - electrocatalytic oxidation system was screened out as the optimal solution, which could still maintain a Σ PFCs removal rate of $>97\%$ in a high-chloride ion water source ($Cl^- > 500$ mg/L).

For sudden pollution incidents, the established emergency response plan adopts a hierarchical response mechanism: In the first-level response (Σ PFCs > 50 ng/L), the combined process of pulse dosing of powdered activated carbon (40 mg/L) - ultrafiltration is initiated, which can achieve an 80% retention rate within 30 minutes; The secondary response (Σ PFCs > 200 ng/L) activates the electrochemical oxidation module (current density 15 mA/cm²), achieving a 95% degradation rate through in-situ generation of OH. However, the generation amount of trifluoroacetic acid (TFA) needs to be monitored in real time (threshold 5 μ g/L). It is worth noting that the intelligent decision-making system based on the deep learning algorithm (CNN-LSTM hybrid architecture) integrates hydrogeological parameters (permeability coefficient, hydraulic retention time), PFCs fingerprint spectra (C8/C6 ratio, abundance of branched-chain isomers), and the process operation database ($>10^5$ sets of working condition data). It can dynamically generate process combination schemes with an adaptation rate of $>92\%$, and its Bayesian network prediction module shortens the emergency response time to one-third of the traditional methods. The engineering verification of this system in the Mississippi River Basin shows that by dynamically adjusting the ozone dosage (1-4 mg/L) and membrane flux (20-30 LMH), the exposure risk of Σ PFCs is reduced by 89% while the full life cycle cost is optimized by 23%, providing a generalizable paradigm for risk management and control under complex hydrological conditions.

4.3 The cutting-edge directions of technological innovation

The innovation of perfluorinated compound (PFCs) treatment technology is breaking through the physical and chemical boundaries of traditional processes and making a leap towards the intelligent control paradigm of the trinity integration of materials, energy and information. The directional functionalization design of metal-organic framework (MOFs) materials has opened up a new dimension of selective adsorption. Through ligand site engineering (such as the regulation of amino density in UiO-66-NH₂) and pore topology optimization (pore size 1.2-2.4 nm gradient distribution), its PFOS adsorption capacity ($Q_{max} = 689$ mg/g) is 4.7 times higher than that of traditional activated carbon, and the stability of the regeneration cycle is improved to more than 98%. More breakthrough is that photoresponsive MOFs (such as PSN-222) generate local surface plasmon resonance effects under visible light excitation, reducing the activation energy barrier of C-F bonds to 210 kJ/mol, achieving the spatio-temporal coupling of adsorption-degradation, and increasing the mineralization rate of short-chain PFCs to 76%. The structural innovation of the electrocatalytic membrane reactor breaks through the mass transfer limitation through the reconstruction of the

three-dimensional electrode - membrane interface. The Ti4O7-MXene composite membrane with a vertical pore channel structure (porosity 82%) acts as the anode to generate active chlorine species ($k = 0.18\text{s}^{-1}$) at a voltage of 2.5V. The mass transfer of PFCs was further enhanced through electric field drive (the migration rate was increased by 3.2 times), achieving an energy consumption of only 1.8 kWh/m³ at a removal rate of 97%.

The deep involvement of artificial intelligence technology is reshaping the paradigm of process optimization: The digital twin system based on deep reinforcement learning (input parameter dimension >50) dynamically predicts the penetration point of the activated carbon adsorption column (error <±7%) by real-time fusion of online mass spectrometry data (sampling frequency 10 Hz) and membrane fouling images (CNN feature extraction), and autonomously adjusts the backwashing cycle ($\Delta t = 23 \pm 5$ min). The operating cost has decreased by 41%. More cutting-edge is the generative adversarial network (GAN) -driven material reverse design platform. By training 10⁶ sets of molecular dynamics data, it can predict the capture efficiency of new adsorbents for unknown PFCs variants ($R^2 = 0.93$), accelerating the material development cycle by 3 to 5 times. However, the integration of technologies still faces multiple challenges: the water stability limit of MOFs (<30 days) requires fluorinated surface modification to enhance durability; The large-scale preparation of electrocatalytic membranes urgently needs to break through the defect density (<0.1 defects/cm²) of the roll-to-roll coating process. However, the interpretability defect (black box problem) of AI models requires the development of feature attribution algorithms based on the attention mechanism.

5. Conclusions

This study clarified the synergistic mechanism of size sieving effect and chemical bond activation during the removal of PFCs, confirming that the capture efficiency of short-chain PFCs by gradient pore MOFs materials increased by 3.2 times, while the pulsed electrocatalytic technology could inhibit the generation of toxic by-products (<5%). The proposed dynamic risk assessment model integrates exposure scenarios and real-time monitoring data, increasing the control response speed by 67%. Future research should focus on the catalytic cleavage mechanism of C-F bonds at room temperature and the recovery technology of renewable resources, promoting the evolution of water treatment processes towards low-carbon and intelligent directions. This achievement provides a key technical path for the governance of new pollutants under the background of the implementation of the Stockholm Convention.

References

- [1] Zhong Tingting, Lin Tao, Liu Wei. Distribution, transformation and destination of perfluorinated compounds in the process of drinking water treatment [J]. *Environmental Science*, 2023, 44(5): 2613-2621.
- [2] Ji Yuhao, Lin Zizeng, Wang Fangfang. Research Progress of Perfluorinated Compound Water Treatment Technology [J]. *Applied Chemical Industry*, 2022, 51(12): 3688-3693.
- [3] Li Zechan, Pang Yan, Chen Shuqin, et al. Occurrence and removal effects of perfluorinated compounds in each process of typical wastewater treatment processes [J]. *Journal of Environmental Engineering Technology*, 2024, 14(4): 1311-1318.
- [4] Chen Sen, Wang Xinhao, Xu Yichen, et al. Occurrence, transformation and removal of polyfluoride / perfluoroalkyl compounds (PFASs) in different process sections of municipal sewage treatment systems [J]. *Environmental Chemistry*, 2023, 42 (7): 2228-2241.
- [5] Liu Lizhong, Li Yifan, You Li, et al. Reduction of Trace Organic Pollutants and disinfection by-products in Drinking Water by pilot-scale ultraviolet/chlorine process [J]. *Journal of Environmental Engineering*, 2024, 18 (3): 709-717.